Approche QFT de la dérivation d'équations cinétiques

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Table des matières

1 Introduction **1**
1.1 Introduction 2
1.2 Équation aléatoire 4
1.2.1 Champ aléatoire gaussien 5
1.2.2 Champ aléatoire poissonien 5
1.2.3 Autres aléas 6
1.3 Point de vue de l'espace de Fock 7
1.3.1 Cas gaussien 8
1.3.2 Cas poissonien 8
1.4 Calcul semi-classique 10
1.5 Mesures semi-classiques 11
1.6 Résultats 12
1.6.1 Une dérivation de l'équation de Boltzmann linéaire . . 12
1.6.2 Une formule pour l'évolution associée à un hamiltonien quadratique en dimension infinie 15
1.6.3 Propagation du chaos pour des systèmes constitués d'un grand nombre de bosons en dimension un avec une interaction ponctuelle entre deux bosons. 17
1.7 Quelques aspects du travail présenté 18

2 Dérivation de l'équation de Boltzmann linéaire pour une particule dans un champ aléatoire (rédigé en anglais) **23**
2.1 Model and result 26
2.1.1 Rescaled quantum random field 26
2.1.2 The main result 27
2.2 The linear Boltzmann equation 29
2.2.1 The formal linear Boltzmann equation 29
2.2.2 Properties 30
2.2.3 The linear Boltzmann equation 31
2.2.4 A Trotter-type approximation 32
2.3 From stochastics to the Fock space 34
2.3.1 Classical kinetic regime 35
2.3.2 General Gaussian random fields 36

2.3.3 Wick powers 37
2.3.4 The isomorphism with the Fock space 37
2.3.5 The expression of the dynamic in the Fock space . . . 38
2.3.6 Existence of the dynamic 39
2.4 An approximated equation and its solution 41
2.4.1 The scaling for field operators 41
2.4.2 The second quantization 41
2.4.3 Space translation in the fields and Fourier transform . 42
2.4.4 The approximated equation and its solution 43
2.4.4.1 Results 43
2.4.4.2 A transformation 44
2.4.4.3 The classical movement associated with the approximated equation 44
2.4.4.4 Resolution of the approximated solution and comparison with the exact solution 46
2.5 Measure of an observable for the approximated dynamics 47
2.5.1 Result 47
2.5.2 Expression of the measure of an observable for the approximated equation 49
2.5.3 Two estimates 52
2.5.4 The transport term $m_{\{,\}}$ 53
2.5.5 The collision terms m_- and m_+ 56
2.5.5.1 Computation of the operators $\mathscr{A}_{\pm,P}$ 58
2.5.5.2 Estimate of the error terms $\Delta_{\pm,1}$ 61
2.5.5.3 Estimate of the error terms $\Delta_{\pm,2}$ 63
2.5.5.4 Estimate of the error term $\Delta_{-,3}$ 67
2.5.5.5 Estimate of the error term $\Delta_{+,3}$ 69
2.6 Comparison between approximated and exact dynamics . 70
2.6.1 Step 1: Introduction of cutoffs 71
2.6.2 Step 2: Comparison between truncated solutions . . . 72
2.6.3 Step 3: Release of the truncation on the symbol 76
2.7 The derivation of the Boltzmann equation for the model . . . 77
2.A Stochastics 79
2.B Semiclassical Measures 81
2.C General results on semigroups 82
2.D Lemmas about an approximate identity 83
2.E Formulae 85
2.E.1 Symmetric Fock space 85
2.E.2 Fourier transforms 85
2.E.3 Weyl quantization 85

3 Évolution quadratique d'une observable de Wick (article rédigé en anglais) 93
3.1 Introduction 95
3.2 Wick calculus with polynomial observables 96
3.2.1 Definitions 96
3.2.2 Some examples of Wick quantizations 98
3.2.3 Calculus 98
3.3 Main results and a simple example 99
3.4 Classical evolution of a Wick polynomial under a quadratic evolution 103
3.4.1 Construction of the classical flow without the α term . 103
3.4.2 The strongly continuous dynamical system associated with (α_t) 104
3.4.3 Construction of the classical flow with the α term . . . 104
3.4.4 Composition of a Wick polynomial with the classical evolution 105
3.5 Quantum evolution of a Wick polynomial 105
3.5.1 Without the α term 105
3.5.2 With the α term 108
3.6 Removal of the α part 109
3.7 A Dyson type expansion formula for the Wick symbol of the evolved quantum observable 110
3.8 An exponential type expansion formula for the Wick symbol of the evolved observable 110
3.8.1 Quantum evolution as a Bogoliubov implementation . 110
3.8.2 Action of Bogoliubov transformations on Wick symbols 112
3.8.2.1 Action of Bogoliubov transformations on Weyl quantizations of polynomials in finite dimension 113
3.8.2.2 Action of Bogoliubov transformations on Wick quantization of polynomials in finite dimension 114
3.8.2.3 Extension to infinite dimension on a "cylindrical" class of polynomials 115
3.8.2.4 Extension to general polynomials 116
3.8.3 An evolution formula for the Wick symbol 117
3.8.4 Estimates 118
3.A $\mathbb{R}$-linear symplectic transformations 119
3.B Relations between Weyl and Wick symbols in finite dimension 123
3.C Symplectic Fourier transform 125

4 Propagation du chaos pour un grand nombre de bosons interagissant ponctuellement (article rédigé en anglais) 129
4.1 Introduction 131
4.2 Preliminaries and main results 135

4.3 Many-boson system 140
4.4 The cubic NLS equation 143
4.5 Time-dependent quadratic dynamics 144
4.6 Propagation of coherent states 150
4.7 Propagation of chaos 164
4.A Elementary estimate 167
4.B Commutator theorems 169
4.C Non-autonomous Schrödinger equation 171

Chapitre 1

Introduction

1.1 Introduction

Dans cette thèse nous nous intéressons, dans deux cas particuliers, à l'émergence d'équations cinétiques décrivant l'évolution d'un système macroscopique correspondant à un modèle microscopique donné.

Historiquement, les premières dérivations d'équations cinétiques à partir d'équations microscopiques remontent aux travaux de Ludwig Boltzmann (1844-1906). Dans son livre sur la théorie des gaz [7] il considère des particules se déplaçant en tous sens et s'entrechoquant. Il en déduit l'équation désignée de nos jours comme l'équation de Boltzmann (non-linéaire). Sa démarche est simple sur le principe, il considère un ensemble d'un grand nombre de particules, assimilées à des sphères. Celles-ci se déplacent en ligne droite (cf. figure 1.1.1) sauf lors de chocs au cours desquels elles changent de direction et de vitesse (cf. figure 1.1.2). Dans un premier temps il se cantonne au cas d'un

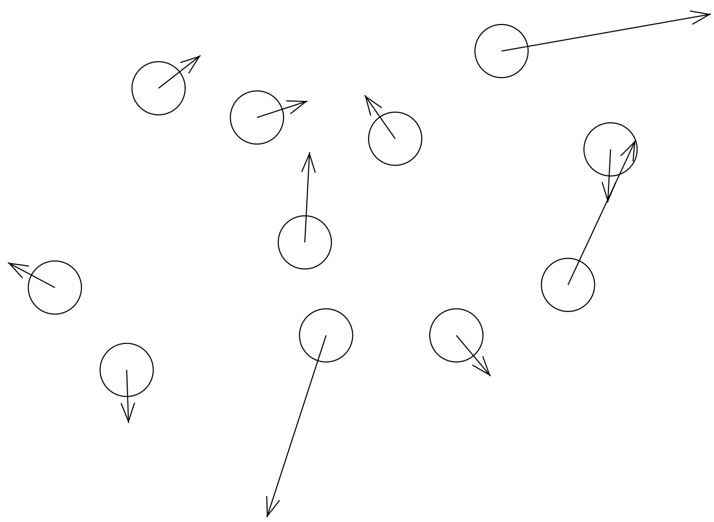

FIG. 1.1.1 – Gaz constitué de particules assimilées à des sphères dures.

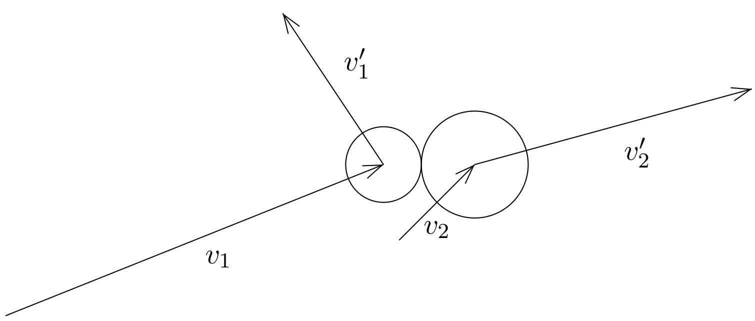

FIG. 1.1.2 – Choc élastique de deux particules assimilées à des sphères dures. Les vitesses avant et après (avec des $'$) le choc sont indiquées.

gaz homogène en espace. Comme un grand nombre de particules est présent par unité de volume (dans l'espace des phases), il peut considérer une densité de particules $f(v)$ dont la vitesse est proche d'une certaine vitesse v. Un bilan sur les différents changements de vitesse lors d'un choc lui permet alors d'en déduire une équation sur la variation de la densité f au cours du temps. Il obtient ainsi un terme dit de collision. Il étend ensuite son raisonnement au cas inhomogène en espace et fait apparaître un terme de transport.

La dérivation de l'équation de Boltzmann (non-linéaire) est d'autant plus intéressante qu'elle présente des difficultés que l'on rencontre dans d'autres cas de dérivation d'équations cinétiques.

1. Une difficulté est de comprendre le passage d'équations réversibles au niveau microscopique à des équations irréversibles au niveau macroscopique. Ce problème était déjà abordé par Boltzmann dans ses travaux et n'est toujours pas complètement résolu.
2. La théorie de l'équation de Boltzmann (non-linéaire), indépendamment de sa dérivation, est déjà complexe. On peut donc s'attendre à des difficultés en ce qui concerne d'éventuels résultats de convergence de solutions du système microscopique vers une solution des équations cinétiques correspondantes.
3. Dans certaines approches mathématiques on se contente de montrer que la limite, par rapport à un certain paramètre, des solutions des équations au niveau microscopique est la solution des équations cinétiques correspondantes. Il faut pour être complet contrôler l'erreur commise pour la valeur donnée par la physique de ce paramètre.

Le comportement individuel des particules considérées est bien évidement classique puisque M. Boltzmann a réalisé ses travaux avant que la théorie atomistique ne soit complètement établie et donc *a fortiori* avant l'avènement de la physique quantique.

On voit donc déjà qu'il peut-être intéressant de dériver les équations cinétiques en partant d'une modélisation des phénomènes microscopiques qui peut-être classique ou quantique.

Nous nous intéressons dans cette thèse à des dérivations de l'équation de *Boltzmann linéaire*

$$\partial_t \mu_t(x,\xi) + 2\xi.\partial_x \mu_t(x,\xi) = \int \sigma(\xi,\xi')\delta(|\xi|^2 - |\xi'|^2)(\mu_t(x,\xi') - \mu_t(x,\xi))\,\mathrm{d}\xi'$$

et de l'équation de *Schrödinger non-linéaire* cubique défocalisante

$$i\partial_t \varphi = -\Delta\varphi + |\varphi|^2 \varphi$$

qui ont une théorie « simple », ce qui évite les difficultés du point 2 ci-dessus.

Plus précisément on s'intéresse à une dérivation de l'équation de Boltzmann linéaire à partir d'une équation de Schrödinger avec un potentiel dépendant d'un paramètre aléatoire

$$ih\partial_t u = -\Delta_x u + \mathcal{V}_\omega^h(x)\, u$$

et à une dérivation de l'équation de Schrödinger non-linéaire cubique dans la limite de champ moyen pour des bosons.

Une autre partie de notre travail a consisté à essayer d'améliorer notre résultat pour la dérivation de l'équation de Boltzmann linéaire. À cette fin nous avons démontré une formule d'évolution des états cohérents comprimés pour un hamiltonien quadratique valable en dimension infinie. Cette formule n'a pas donné les résultats escomptés dans le cas que nous étudiions mais est néanmoins intéressante en elle-même, nous l'avons donc isolée dans un article à part.

Le cas classique On s'intéresse dans cette thèse à des dérivations d'équations cinétiques à partir de systèmes microscopiques décrits par la physique quantique, mais ce sujet a aussi beaucoup été exploré dans le cas classique. On trouve dans l'article [11] une dérivation de l'équation de Boltzmann linéaire pour les fonctions de Green dans le cas d'un gaz de Lorentz. L'article [21] présente une revue de différents modèles microscopiques classiques et d'équations cinétiques obtenues commes limites de ces modèles, mettant en avant le côté markovien approché de l'évolution du système microscopique (quelques modèles quantiques y sont aussi abordés). L'article [6] donne une dérivation de l'équation de Boltzmann linéaire pour la densité de particules dans le cas du modèle de Lorentz.

1.2 Équation aléatoire

On s'intéresse à l'équation de Schrödinger

$$\begin{cases} ih\partial_t u & = -\Delta_x u + \mathcal{V}_\omega^h(x)\, u \\ u_{t=0} & = \psi_0^h \in L^2(\mathbb{R}^d;\mathbb{C}) \end{cases} \tag{1.2.1}$$

où le potentiel $\mathcal{V}_\omega^h(x)$ dépend d'un paramètre aléatoire ω parcourant un espace de probabilité $(\Omega_{\mathbb{P}}, \mathbb{P})$. Le comportement de $\mathcal{V}_\omega^h$ par rapport au paramètre aléatoire ω peut-être choisi de différentes façons. Nous envisageons deux types de champs aléatoires, les champs aléatoires gaussien et poissonien. On peut aussi considérer divers comportements par rapport au petit paramètre h.

Cas du faible couplage Le potentiel prend alors la forme $\mathcal{V}_\omega^h = \sqrt{h}\mathcal{V}_\omega$, $\sqrt{h}$ jouant le rôle d'un paramètre de couplage.

Cas de la faible densité Le potentiel $\mathcal{V}_\omega^h(x)$ est tel que la densité d'obstacles soit de l'ordre de h à l'échelle microscopique, où h représente le rapport entre les échelles microscopique et macroscopique. La forme précise de $\mathcal{V}_\omega^h$ dépend alors du cas considéré, gaussien ou poissonien.

1.2.1 Champ aléatoire gaussien

Un choix possible pour la dépendance du potentiel par rapport à l'aléa est celui d'un champ gaussien centré invariant par translation. Ce champ est particulièrement intéressant de par sa simplicité. Pour qu'un tel champ gaussien soit bien déterminé il est nécessaire et suffisant de fixer sa fonction de covariance

$$\Sigma(x,x') = \mathbb{E}[\mathcal{V}(x)\,\mathcal{V}(x')]\,.$$

On impose de plus la contrainte que le champ aléatoire gaussien centré soit invariant par translation, c'est-à-dire

$$\Sigma(x,x') = G(x-x')\,.$$

Les conditions données par le théorème de Minlos sur les fonctions de type positif, et donc en particulier les fonctions de covariance, suggèrent de prendre G tel que la transformée de Fourier $\hat{G}$ de G soit de la forme

$$\hat{G} = |\hat{V}|^2\,,$$

ce que nous ferons avec de plus V régulière (dans la classe de Schwartz).

Le cas de la limite de faible couplage d'un gaz de Fermi dans un potentiel aléatoire gaussien invariant par translation est traité dans [14] (ainsi que d'autres cas de potentiels aléatoires) et fait intervenir des techniques de combinatoire de graphes dans sa démonstration. On s'intéresse dans cette thèse au cas bosonique. Des résultats d'Erdös et Yau, et plus récemment de Poupaud et Vasseur, existent dans ce contexte, nous les comparerons avec les résultats de cette thèse dans la Section 1.6.1.

Dans le cas des champs aléatoires gaussiens, les hamiltoniens obtenus dans la limite de faible couplage et dans le régime cinétique coïncident.

1.2.2 Champ aléatoire poissonien

La géométrie de l'espace des configurations et les polynômes de Charlier sont abordés dans [1, 15]. Dans le cas d'un champ aléatoire poissonien on considère l'*espace des configurations* $\Gamma_{\mathbb{R}^d}$ défini comme l'ensemble des parties discrètes de $\mathbb{R}^d$,

$$\Gamma_{\mathbb{R}^d} = \left\{\Lambda \subset \mathbb{R}^d,\ \Lambda \text{ localement fini}\right\}\,.$$

L'espace des configurations va nous servir pour décrire l'ensemble des points où des obstacles sont présents. On considérera donc un potentiel de la forme

$$\mathcal{V}_\omega(x) = \sum_{y\in\omega} V(x-y)$$

V étant le potentiel d'interaction avec une particule et ω un point de l'espace des configurations (voir figure 1.2.1).

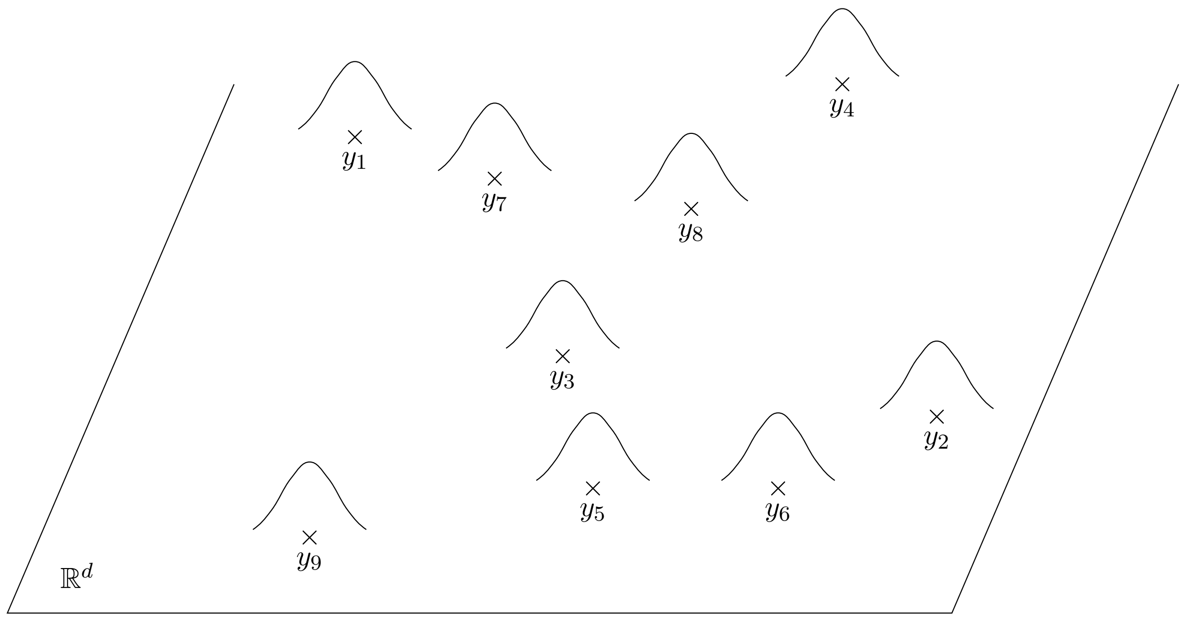

FIG. 1.2.1 – Potentiel poissonien, $\omega = \{y_1, y_2, y_3, \ldots\}$.

On veut considérer le paramètre ω comme un paramètre aléatoire et avoir une densité (uniforme) de particules par unité de volume valant un certaine valeur ρ. Pour cela on construit une mesure de probabilité sur l'espace des configurations. L'espace des configurations étant la limite projective des ensembles $\Gamma_K = \{\Lambda \subset K,\, \Lambda \text{ fini}\}$ pour $K \subset \mathbb{R}^d$ compact. On munit l'espace des configurations d'une mesure $\pi_{\rho\lambda}$ dite de Lebesgue-Poisson de densité $\rho > 0$, construite d'abord sur les Γ_K pour K compact par la formule

$$\pi_{\rho\lambda,K} := e^{-\rho\lambda(K)} \sum_{n=0}^{+\infty} \rho^n \frac{\lambda|_K^{\otimes n}}{n!}$$

où $\lambda^{\otimes n}$ représente la mesure sur $\mathbb{R}^{dn}$ déduite de la mesure de Lebesgue λ sur $\mathbb{R}^d$ et Γ_K est décomposé comme $\sqcup_n \{\omega \in \Gamma_K,\, \#\omega = n\}$ ($\#A$ désigne le cardinal d'un ensemble fini A). On étend ensuite la mesure à l'espace des configurations vu comme limite projective des Γ_K à l'aide du théorème de Kolmogorov.

Erdös et Yau ont aussi obtenu des résultats dans le cas d'un potentiel poissonien [10].

1.2.3 Autres aléas

On pourrait aussi envisager d'autres aléas. On peut notamment se reporter à [17, 16] pour des généralisations de l'aléa poissonien qui peuvent se représenter à l'aide de l'espace de Fock.

1.3 Point de vue de l'espace de Fock

La démarche suivie dans les travaux présentés dans cette thèse est d'exprimer les équations dans l'espace de Fock (bosonique) et d'utiliser les outils géométriques disponibles dans cet espace, à savoir les états cohérents (ou les états cohérents comprimés) associés à un développement en puissances par rapport à un petit paramètre ε. On rappelle donc comment est défini l'espace de Fock et la dépendance par rapport au petit paramètre ε dans la quantification de Wick.

L'*espace de Fock* symétrique $\Gamma\mathcal{Z}$ associé à un espace de Hilbert complexe $\mathcal{Z}$

$$\Gamma\mathcal{Z} = \bigoplus_{n=0}^{+\infty} \bigvee^{n} \mathcal{Z}$$

permet de décrire les états à un nombre quelconque de particules (bosoniques) où $\bigvee$ désigne le produit tensoriel symétrique. Une fonction à variable dans $\mathcal{Z}$ est qualifiée de *monôme* $b \in \mathcal{P}_{p,q}(\mathcal{Z})$ si

$$b(z) = \left\langle z^{\otimes q}, \tilde{b} z^{\otimes p} \right\rangle_{\bigvee^q \mathcal{Z}} \qquad \text{avec} \qquad \tilde{b} \in \mathcal{L}\left(\bigvee^{p} \mathcal{Z}; \bigvee^{q} \mathcal{Z} \right).$$

On adoptera les notations suivantes pour le produit symétrique :

$$f_1 \vee \cdots \vee f_n = \mathcal{S}_n(f_1 \otimes \cdots \otimes f_n) \quad \text{pour} \quad f_j \in \mathcal{Z}\,,$$

$$A_1 \vee \cdots \vee A_n = \mathcal{S}_{q_1+\cdots+q_n}(A_1 \otimes \cdots \otimes A_n)\mathcal{S}_{p_1+\cdots+p_n} \text{ pour } A_j \in \mathcal{L}\left(\bigvee^{p_j} \mathcal{Z}; \bigvee^{q_j} \mathcal{Z} \right),$$

et $\mathcal{S}_m$ est l'opérateur de symétrisation de $\bigotimes^m \mathcal{Z}$ dans $\bigvee^m \mathcal{Z}$ normalisé de sorte que $\mathcal{S}_m$ coïncide avec l'identité sur $\bigvee^m \mathcal{Z}$.

Le quantifié de Wick d'un monôme est défini par ses restrictions aux sous-espaces à n particules

$$b^{Wick}\Big|_{\bigvee^n \mathcal{Z}} = 1_{[p,+\infty[}(n) \frac{\sqrt{n!\,(n-p+q)!}}{(n-p)!} \varepsilon^{\frac{p+q}{2}} \left(\tilde{b} \vee I_{\bigvee^{n-p} \mathcal{Z}} \right)$$

qui sont des éléments de $\mathcal{L}(\bigvee^n \mathcal{Z}; \bigvee^{n-p+q} \mathcal{Z})$. Les *polynômes* sont les combinaisons linéaires finies de monômes, c'est-à-dire les éléments de $\mathcal{P}(\mathcal{Z}) = \bigoplus_{p,q \geq 0} \mathcal{P}_{p,q}(\mathcal{Z})$ et on les quantifie par linéarité à partir des monômes. On note $\mathcal{P}_{\leq m} = \bigoplus_{p+q \leq m} \mathcal{P}_{p,q}$. Pour $f \in \mathcal{Z}$, l'opérateur de champ $\Phi(f)$ est (la fermeture de l'opérateur essentiellement autoadjoint) $\sqrt{2}\Re \langle f, z \rangle^{Wick}$ et l'opérateur de Weyl $W(f)$ est défini par $W(f) = e^{i\Phi(f)}$.

On peut alors définir les *états cohérents*

$$E(f) = e^{-\frac{\|f\|^2}{2\varepsilon}} \sum_{n \geq 0} \varepsilon^{-n/2} \frac{f^{\vee n}}{\sqrt{n!}} = W\left(\frac{\sqrt{2}}{i\varepsilon} f \right) \Omega\,,$$

où $\Omega = (1, 0, 0, \dots) \in \Gamma\mathcal{Z}$. Ces états sont ceux qui se rapprochent le plus d'états classiques car ils sont bien localisés près du point classique f de l'espace des phases $\mathcal{Z}$. On peut les voir en dimension finie comme des gaussiennes, la fonction de covariance étant fixée. Une généralisation de ces états consiste à s'autoriser à changer la covariance de la gaussienne, on aboutit alors à la notion d'état cohérent comprimé.

1.3.1 Cas gaussien

Correspondance entre l'espace gaussien et l'espace de Fock Il existe un isomorphisme entre l'espace gaussien $L^2(\Omega_{\mathbb{P}}, \mathbb{P}; \mathbb{C})$ associé à $L^2(\mathbb{R}^d; \mathbb{R})$ et l'espace de Fock $\Gamma L^2(\mathbb{R}^d)$ symétrique associé à $L^2(\mathbb{R}^d; \mathbb{C})$ (noté $L^2(\mathbb{R}^d)$). On obtient via cet isomorphisme la correspondance

$$\frac{1}{\sqrt{n!}} : \Phi_G(f_1) \cdots \Phi_G(f_n) : \leftrightarrow f_1 \vee \cdots \vee f_n$$

pour des f_j dans $L^2(\mathbb{R}^d; \mathbb{R})$. L'opérateur de champ $\sqrt{2}\Phi(f)$ correspond à la multiplication par $\Phi_G(f)$ via cet isomorphisme et on a $\mathcal{V}_\omega(x) = \Phi_G(V(x - \cdot))$. Plus de détails sur cette correspondance seront donnés dans la section 2.3. On peut aussi consulter [20].

Expression de l'hamiltonien dans l'espace de Fock

Sans petit paramètre L'hamiltonien correspondant dans l'espace de Fock au cas du potentiel $\mathcal{V}_\omega(x) = \Phi_G(V(x - \cdot))$ est donc

$$-\Delta_x + \sqrt{2}\Phi(V(x - \cdot)).$$

Cas de la faible densité (ou du faible couplage) L'hamiltonien initial est envoyé sur

$$-\Delta_x + \sqrt{2h}\Phi(V(x - \cdot)).$$

1.3.2 Cas poissonien

Correspondance entre l'espace poissonien et l'espace de Fock On peut consulter [1, 15] et leurs références au sujet des polynômes de Charlier sur l'espace des configurations. On peut les définir rapidement comme ci-dessous.

Les mesures sur $\mathbb{R}^{dn}$ définies par

$$:\omega^{\otimes n}: = \sum_{\substack{(y_1,\dots,y_n) \\ \{y_1,\dots,y_n\} \subset \omega}} \delta_{(y_1,\dots,y_n)}$$

pour $\omega \in \Gamma_{\mathbb{R}^d}$ avec des y_j distincts et

$$: (\omega - \rho\lambda)^{\otimes n} : \; = \sum_{k=0}^{n} \binom{n}{k} (-1)^k \, (\rho\lambda)^{\vee k} \vee : \omega^{\otimes(n-k)} :$$

permettent de définir les polynômes de Charlier qui sont, pour $f \in \mathcal{C}_0^\infty(\mathbb{R}^d)$, des éléments de $L^2(\Gamma_{\mathbb{R}^d}, \pi_{\rho\lambda})$

$$Q_0(\omega) = 1, \quad Q_n\left(f^{\vee n}\right)(\omega) := \left\langle f^{\vee n}, :(\omega - \rho\lambda)^{\otimes n} : \right\rangle .$$

Ainsi $Q_1(f)(\omega) = \sum_{y \in \omega} f(y) - \int f d(\rho\lambda)$ et le potentiel $\mathcal{V}_\omega(x) = \sum_{y \in \omega} V(x - y)$ peut s'écrire sous la forme

$$\mathcal{V}_\omega(x) = Q_1(V(x - \cdot))(\omega) + \int f \, \mathrm{d}(\rho\lambda) .$$

On dispose de plus d'un isomorphisme entre l'espace de Fock $\Gamma L^2(\mathbb{R}^d)$ et $L^2(\Gamma_{\rho\lambda}, \pi_{\rho\lambda})$ qui donne la correspondance

$$f^{\vee n} \leftrightarrow (\rho^n n!)^{-1/2} Q_n\left(f^{\vee n}\right) .$$

La relation, pour $f,\, g \in \mathcal{C}_0^\infty(\mathbb{R}^d)$,

$$Q_1(f)\, Q_n(g^{\vee n}) = Q_{n+1}(f \vee g^{\vee n}) + Q_n(n(fg) \vee g^{\vee n-1}) + Q_{n-1}(n\langle f, g\rangle_{\rho\lambda} g^{\vee n-1})$$

montre que la multiplication par $Q_1(f)$ dans l'espace de Poisson devient dans l'espace de Fock l'opérateur

$$\sqrt{2\rho}\Phi(f) + \mathrm{d}\Gamma(f \times) .$$

Expression de l'hamiltonien dans l'espace de Fock

Cas du faible couplage On a alors une densité $\rho = 1$ et une constante de couplage $\sqrt{h}$ en facteur du potentiel, d'où le hamiltonien dans l'espace de Fock

$$-\Delta_x + \sqrt{2h}\Phi\left(V(x - \cdot)\right) + \sqrt{h}\, \mathrm{d}\Gamma\left(V(x - \cdot) \times\right) + \sqrt{h} \int V \, \mathrm{d}\lambda .$$

Cas de la faible densité La densité est alors $\rho = h$ (et la constante de couplage vaut 1) d'où le hamiltonien dans l'espace de Fock

$$-\Delta_x + \sqrt{2h}\Phi\left(V(x - \cdot)\right) + \mathrm{d}\Gamma\left(V(x - \cdot) \times\right) + h \int V \, \mathrm{d}\lambda .$$

Les cas de faible densité et de faible couplage sont donc distincts pour un aléa poissonien.

1.4 Calcul semi-classique

Le calcul semi-classique permet de ramener des calculs sur des opérateurs sur des espaces de Hilbert à des calculs sur des fonctions à valeurs scalaires.

Dans cette thèse nous utilisons les quantifications de Weyl et de Wick. Le plus simple pour comprendre ces quantifications est de regarder comment elles se comportent sur des polynômes en dimension 1, c'est-à-dire comment passer d'un polynôme en deux variables b dans $\mathbb{R}[x,\xi]$ à un opérateur sur $L^2(\mathbb{R})$ de sorte à envoyer x sur la multiplication par x et ξ sur $D_x = -i\partial_x$.

Weyl Pour la *quantification de Weyl*, un monôme $x^\alpha\xi^\beta$ est envoyé sur l'opérateur $\frac{1}{2^\alpha}\sum_\gamma \binom{\alpha}{\gamma} x^{\alpha-\gamma} D_x^\beta x^\gamma$, avec $D_x = -i\partial_x$. La quantification des polynômes s'en déduit par linéarité.

On utilisera aussi la quantification de Weyl avec des fonctions dans $\mathcal{C}_0^\infty(\mathbb{R}^{2d};\mathbb{R})$, une formule plus générale pour définir la quantification de Weyl est alors

$$b^{Weyl} = \int e^{i(x-y).\xi} b\left(\frac{x+y}{2},\xi\right) u(y)\frac{\mathrm{d}\xi\,\mathrm{d}y}{(2\pi)^d}\,.$$

Wick On n'utilisera la *quantification de Wick* que sur des polynômes. On peut réécrire un polynôme $P(x,\xi)$ sous la forme $P(\frac{z+\bar z}{2},\frac{z-\bar z}{2i}) = Q(z,\bar z)$ avec $z = x+i\xi$. On peut donc quantifier plutôt des polynômes en z et $\bar z$. On choisit d'envoyer un monôme $\bar z^q z^p$ sur l'opérateur $(x-\partial_x)^q\,(x+\partial_x)^p$.

En dimension d (finie) les monômes sont de la forme $\prod_{j=1}^d \bar z_j^{q_j} z_j^{p_j}$, (notons que ceci est un cas particulier de la forme $\langle z^{\otimes q}, Az^{\otimes p}\rangle$ avec $A\in\mathcal{L}(\mathcal{Z}^{\otimes q};\mathcal{Z}^{\otimes p})$ et $p=\sum_{j=1}^d p_j$, $q=\sum_{j=1}^d q_j$).

Liens entre les différentes quantifications Des formules permettent de faire le lien entre les différentes quantifications et nous exploitons notamment ces formules dans notre travail sur l'évolution d'observables de Wick par un hamiltonien quadratique. Des formules valables pour la quantification de Weyl en dimension finie permettent de déduire des formules valables pour la quantification de Wick en dimension infinie.

On peut faire le lien entre la représentation de Schrödinger et la représentation de Fock dans le cas de la dimension finie à l'aide de la transformation de Bargmann

$$L^2(\mathbb{R}^d) \to \left\{F,\ F \text{ entière et } \int |F(z)|^2 e^{-\frac{2|z|^2}{\varepsilon}}\lambda(\mathrm{d}z) < +\infty\right\}$$
$$f\mapsto B_{2\varepsilon}f\,(z) = \pi^{-\frac{3d}{4}} e^{\frac{z^2}{\varepsilon}} \int_{\mathbb{R}^d} f(y) e^{-\frac{(\sqrt{2}z-y)^2}{\varepsilon}}\,\mathrm{d}y\,.$$

Le développement en série entière de $B_{2\varepsilon}f$ donne alors des coefficients $F_k\in\bigvee^k\mathbb{C}^d$ qui définissent un vecteur de l'espace de Fock $\Gamma\mathbb{C}^d$. On obtient alors un isomorphisme entre $L^2\left(\mathbb{R}^d\right)$ et $\Gamma\mathbb{C}^d$ qui fait se correspondre les deux définitions que nous avons données de la quantification de Wick.

On notera aussi que les états cohérents dans l'espace de Fock sont les images de gaussiennes dans l'espace de Schrödinger via la transformation de Bargmann.

Dimension infinie On parle de quantification en dimension infinie quand, au lieu de quantifier des fonctions définies sur un espace de dimension finie, on quantifie des fonctions définies sur un espace de dimension éventuellement infinie. À cette fin, il sera plus pratique (dans le cas particulier de la dimension finie) de définir des fonctions sur $\mathbb{C}^d$ plutôt que sur $\mathbb{R}^d \times \mathbb{R}^d$.

Un avantage de la quantification de Wick est qu'elle se généralise d'une façon plus agréable en dimension infinie et que la méthode ci-dessus est encore valable, quitte à comprendre dans un premier temps le cas des monômes de la forme $\langle z, f\rangle^q \langle g, z\rangle^p$ et à quantifier $\langle z, f\rangle$ et $\langle g, z\rangle$.

1.5 Mesures semi-classiques

Les mesures semi-classiques sont l'un des outils qui permettent (entre autres applications) de donner un sens rigoureux au passage d'objets quantiques à des objets classiques, et donc de préciser le lien entre les physiques quantique et classique.

Dans le cas qui nous intéresse on considère au niveau quantique des états décrits par des opérateurs positifs de classe trace normalisés et au niveau classique des mesures sur l'espace des phases. Le rapport entre les longueurs pertinentes aux échelles quantique et classique est décrit par un paramètre $h > 0$ sans dimension. Physiquement ce paramètre h a une valeur fixée petite devant 1, mais mathématiquement on considère que le paramètre h parcourt l'intervalle $]0, h_0]$ et on s'intéresse au comportement des états lorsque h tend vers 0.

Soit $(\rho^h)_{h\in]0,h_0]}$ une famille d'états normés sur $L^2\left(\mathbb{R}^2\right)$, c'est-à-dire $\rho \in \mathcal{L}_1^+\left(L_x^2\right)$ et $\operatorname{Tr}\rho = 1$. Une mesure μ_0 est une *mesure semi-classique* associée à (ρ^h) s'il existe une suite h_k de $]0, h_0]$ telle que $h_k \to 0$ et

$$\forall b \in \mathcal{C}_0^\infty\left(\mathbb{R}^{2d}_{x,\xi}\right), \lim_{k\to+\infty} \operatorname{Tr}\left[\rho^h b^W\left(h_k x, D_x\right)\right] = \int_{\mathbb{R}^{2d}_{x,\xi}} b \, \mathrm{d}\mu_0$$

où $b^W\left(hx, D_x\right)$ est la quantification de Weyl du symbole b.

On note $\mathcal{M}((\rho^h)_{h\in]0,h_0]})$ l'ensemble des mesures semi-classiques associées à la famille $(\rho^h)_{h\in]0,h_0]}$.

On pourra considérer qu'une famille d'états quantiques dépendant d'un paramètre h est bien associée à un état classique si l'ensemble des mesures semi-classiques qui lui est associé est réduit à un singleton. On parle alors de famille *pure*.

L'un des points importants concernant les mesures semi-classiques est que l'on peut dans certains cas prouver que l'évolution d'une famille pure par une dynamique donnée conserve le caractère pur de celle-ci. On peut alors considérer que le système classique correspondant a une évolution bien définie et qu'il est décrit par l'unique mesure semi-classique associée à la famille à chaque instant. C'est une approche de ce type que nous utilisons pour dériver l'équation de Boltzmann linéaire.

On peut se réferer à [12, 13, 8, 18, 2, 3] pour plus d'informations sur les mesures semi-classiques ou les mesures de défaut.

1.6 Résultats

1.6.1 Une dérivation de l'équation de Boltzmann linéaire

Soit $d \geq 3$. Soit $G : \mathbb{R}^d \to \mathbb{R}$ de type positif, telle que $\hat{G} = |\hat{V}|^2$ avec $\hat{V} \in \mathcal{S}\left(\mathbb{R}^d;\mathbb{R}\right)$ et $\mathcal{V}_\omega^h(x)$ le champ aléatoire gaussien centré invariant par translation de covariance $hG(x-x')$. On considère la dynamique définie par l'équation de Schrödinger

$$\left\{\begin{array}{rcl} ih\partial_t u &=& -\Delta_x u + \mathcal{V}_\omega(x)\, u \\ u_{t=0} &=& \psi_0 \in L^2\left(\mathbb{R}^d\right) \end{array}\right.$$

avec un renouvellement de l'aléa. Soit $\alpha \in]\frac{3}{4}, 1[$ fixé et $T > 0$. On découpe l'intervalle $[0,T]$ en sous-intervalles de longueur $\Delta t = h^\alpha$ et on pose $N = N^h = T/h^\alpha$. L'aléa est alors renouvelé dès qu'il s'écoule un temps Δt. Plus précisément, étant donné un état ρ normé (c'est-à-dire ρ positif, de classe trace et de trace 1). On définit

$$\rho^h_{N,\Delta t} = \int_{\bar{\Omega}_N} G_{N,\frac{\Delta t}{h},\bar{\omega}_N}\, \rho\, G^{-1}_{N,\frac{\Delta t}{h},\bar{\omega}_N}\, \mathrm{d}\mathbb{P}_N\left(\bar{\omega}_N\right)$$

avec

$$G_{N,\frac{\Delta t}{h},\bar{\omega}_N} = e^{-i\frac{\Delta t}{h}H_{h,\omega_N}}\, e^{-i\frac{\Delta t}{h}H_{h,\omega_{N-1}}} \cdots e^{-i\frac{\Delta t}{h}H_{h,\omega_1}}$$

et $\bar{\omega}_N := (\omega_1, \ldots, \omega_N) \in \bar{\Omega}_N = \Omega_1 \times \cdots \times \Omega_N$, $\bar{\mathbb{P}}_N = \mathbb{P}_1 \times \cdots \times \mathbb{P}_N$.

Théorème 1.6.1. *Supposons la famille $(\rho^h)_{h\in]0,h_0]}$ pure, avec $\mathcal{M}((\rho^h)) = \{\mu_0\}$ et $\mu_0(\mathbb{R}^d_x \times \mathbb{R}^{d*}_\xi) = 1$. Alors la famille $(\rho^h_{N,\Delta t})_{h\in]0,h_0]}$ est pure, avec*

$$\mathcal{M}\left(\left(\rho^h_{N,\Delta t}\right)_{h\in]0,h_0]}\right) = \{\mu_T\}$$

où $\mu_T = \mu_{t=T}$ avec, pour $t \in (0,T)$,

$$\left\{\begin{array}{l} \partial_t\mu_t(x,\xi) + 2\xi.\partial_x\mu_t(x,\xi) = \int \sigma(\xi,\xi')\delta(|\xi|^2 - |\xi'|^2)(\mu_t(x,\xi') - \mu_t(x,\xi))\,\mathrm{d}\xi' \\ \mu_{t=0} = \mu_0 \end{array}\right.,$$

et $\sigma(\xi,\xi') = 2\pi|\hat{V}(\xi-\xi')|^2$.

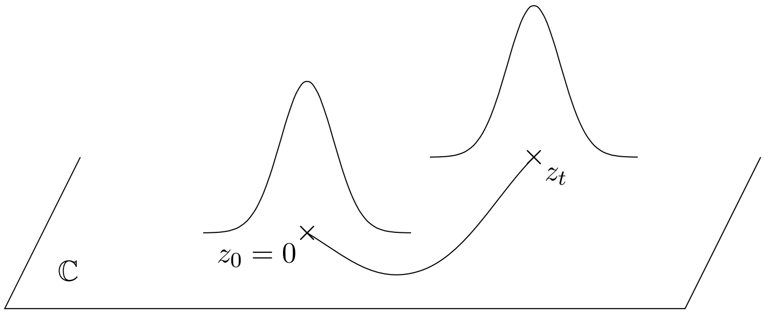

FIG. 1.6.1 – Déplacement d'un état cohérent (représenté pour $\mathcal{Z} = \mathbb{C}$). On mélange deux points de vue dans ce dessin. L'état cohérent est vu comme une gaussienne (représentation de Schrödinger) et son centre est dans $\mathbb{C}$ (représentation de Bargmann).

Traduction du problème dans le formalisme de la théorie quantique des champs

Une approche géométrique Une fois le problème exprimé dans les termes de la théorie quantique des champs on peut approcher l'équation différentielle

$$i\partial_t \boldsymbol{\rho} = [H, \boldsymbol{\rho}] \qquad \text{par} \qquad i\partial_t \boldsymbol{\rho} = [H^{app}, \boldsymbol{\rho}]$$

pour un hamiltonien H^{app} quadratique qui approche convenablement le hamiltonien de départ H pour des données initiales de la forme $\boldsymbol{\rho}_0 = \rho_0 \otimes |\Omega\rangle\langle\Omega|$ et des temps suffisamment courts. On est alors ramené à plusieurs sous-problèmes :

- résoudre explicitement l'équation approchée à l'aide d'états cohérents, (voir la figure 1.6.1) sur l'espace des phases de dimension infinie $\mathcal{Z} = L^2(\mathbb{R}^d; \mathbb{C})$,
- montrer que la solution de l'équation approchée permet de retrouver l'équation duale de l'équation de Boltzmann linéaire, au moins pour des temps courts,
- contrôler la différence entre la solution de l'équation approchée et la solution de l'équation exacte,
- recoller les estimations pour des temps courts en utilisant l'hypothèse de renouvellement de l'aléa,
- on passe de l'équation duale de l'équation de Boltmann linéaire pour des symboles réguliers à l'équation de Boltzmann linéaire pour des mesures.

Sur l'hamiltonien approché L'hamiltonien s'écrit dans le cadre de la théorie quantique des champs

$$D_x^2 + \sqrt{2h}\Phi(V(x - \cdot))\,.$$

Quitte à effectuer une translation on se ramène à l'hamiltonien

$$(D_x - \mathrm{d}\Gamma(D_y))^2 + \sqrt{2h}\Phi(V)$$

que l'on peut approcher par l'hamiltonien

$$D_x^2 - 2D_x.\mathrm{d}\Gamma(D_y) + \mathrm{d}\Gamma(D_y^2) + \sqrt{2h}\Phi(V)$$

quitte à négliger le terme

$$\mathrm{d}\Gamma(D_y)^2 - \mathrm{d}\Gamma(D_y^2)\,.$$

Ce dernier terme est quartique et pour des temps courts doit rester négligeable puisque l'on part d'un état initial vide. La partie restante de l'hamiltonien est la quantification d'un polynôme dans $\mathcal{P}_{\leq 2}(L^2(\mathbb{R}^d))$ et donne une dynamique que l'on peut résoudre explicitement en termes d'états cohérents.

Comparaison avec les résultats de Erdös et Yau Les travaux de Erdös et Yau [9] présentent des résultats, sur le même problème, qui par certains aspect sont meilleurs et par d'autres moins bons que notre travail. Les principales différences sont récapitulées dans le tableau 1.1.

		Erdos, Yau 2000		Breteaux 2011
Hypothèses				
Aléa	+	fixé		renouvelé
État initial		$h^{d/2}f(hx)\exp(\frac{iS(hx)}{h})$ $f,\, S \in \mathcal{S}$	+	famille bornée pure de $\mathcal{L}_1^+(L^2(\mathbb{R}^d))$
Dimension	+	$d \geq 2$		$d \geq 3$
Symétrie de V		Radiale	+	Aucune
Point de vue				
		Combinatoire (graphes)		Géométrique (états cohérents)

Tab. 1.1 – Comparaison avec les résultats de Erdös et Yau [9].

Notons aussi que la régularité demandée pour le profil V est $V \in \mathcal{S}(\mathbb{R}^d)$ dans les deux cas par souci de simplicité, mais cette hypothèse peut être un peu réduite.

Comparaison avec les travaux de Poupaud et Vasseur Dans l'article [19] Poupaud et Vasseur proposent une autre dérivation de l'équation de Boltzmann linéaire.

Leurs hypothèses sur le potentiel aléatoire sont différentes de celles que nous proposons. En effet les potentiels qu'ils considèrent sont notamment bornés presque sûrement ce qui n'est pas le cas des potentiels gaussiens ou poissoniens (qui sont presque sûrement non-bornés pour des potentiels non-nuls). Il n'y a donc pas d'implication entre nos résultats et leurs résultats.

Néanmoins une caractéristique commune avec nos hypothèses est qu'il y a un renouvellement de l'aléa même si ceci est traduit d'une façon différente au niveau des hypothèses.

1.6.2 Une formule pour l'évolution associée à un hamiltonien quadratique en dimension infinie

On essaie de retenir l'information importante en traduisant les équations de départ dans l'espace de Fock et en utilisant la notion d'état cohérent. Dans le cas de la dimension finie, les états cohérents sont des gaussiennes centrées de covariance fixée. Une piste pour améliorer les résultats précédents est donc de considérer des états plus généraux et donc de s'autoriser des covariances variables. On parle alors d'états cohérents comprimés. La connaissance précise de l'évolution d'une observable de Wick par une évolution donnée par un hamiltonien quadratique dépendant du temps peut être intéressante. On a donc développé des formules exactes en vue de les appliquer à la version dans l'espace de Fock de l'équation (1.2.1).

Résultats On considère un espace de Hilbert séparable $\mathcal{Z}$ et les hypothèses suivantes.

H1 Soit $(\alpha_t)_{t\in\mathbb{R}}$ une famille à un paramètre d'opérateurs autoadjoints sur $\mathcal{Z}$ définissant un système dynamique fortement continu $u_\alpha(t,s)$.

H1' On suppose que **H1** est vérifiée et que de plus le système dynamique préserve une partie dense D telle que, pour tout $\psi \in D$, $u_\alpha(\cdot,\cdot)\,\psi$ appartient à $\mathcal{C}^1\left(\mathbb{R}^2;\mathcal{Z}\right)\cap\mathcal{C}^0\left(\mathbb{R}^2;D\right)$.

H2 Soit β dans $\mathcal{C}^0\left(\mathbb{R};\mathcal{Z}^{\vee 2}\right)$, ($\beta_t$ définit un opérateur de Hilbert-Schmidt $\mathbb{C}$-antilinéaire par $z\mapsto (I_{\mathcal{Z}}\vee\langle z|)\,\beta_t$).

Avec **H1'** et **H2**, le *flot classique* associé à une famille $Q_t(z) = \langle z,\alpha_t z\rangle + \Im\left\langle \beta_t, z^{\vee 2}\right\rangle$ de polynômes quadratiques est la solution $\varphi(t,s)$ de l'équation

$$\left\{\begin{array}{rcl} i\partial_t\varphi(t,0)[z] & = & \partial_{\bar z}Q_t(\varphi(t,0)[z]) \\ \varphi(0,0) & = & I_{\mathcal{Z}} \end{array}\right.$$

où $\partial_{\bar z}Q_t(z) = \alpha z + i\,(I_{\mathcal{Z}}\vee\langle z|\,\beta)$, en un sens faible.

L'écriture de l'équation différentielle rend le contexte plus concret mais les hypothèses **H1** et **H2** suffisent à définir un système dynamique $\varphi(t,s)$. La famille $\varphi(t,s)$ est composée de symplectomorphismes de $(\mathcal{Z},\sigma)$ qui se décomposent naturellement en une partie $\mathbb{C}$-linéaire et une partie $\mathbb{C}$-antilinéaire :

$$\varphi = L + A\,,\quad L\in\mathcal{L}(\mathcal{Z})\,,\quad AA^*\in\mathcal{L}_1(\mathcal{Z})\,.$$

De façon similaire le flot quantique associé à Q_t est la solution $U(t,s)$ de

$$\left\{\begin{array}{rcl} i\varepsilon\partial_t U(t,0) & = & Q_t^{Wick} U(t,0) \\ U(0,0) & = & I_{\mathcal{H}} \end{array}\right. .$$

Les deux résultats principaux de ce chapitre traitent de l'évolution d'une observable de Wick b^{Wick}, $b \in \mathcal{P}(\mathcal{Z})$, par le flot quantique, c'est-à-dire

$$U(0,t)\, b^{Wick} U(t,0) \ .$$

(On pose $\langle N\rangle = \sqrt{N^2+1}$, $N = (|z|^2)^{Wick}$)

Théorème 1.6.2. *Supposons **H1** et **H2** verifiées. Soit un polynôme* $b \in \mathcal{P}_{\leq m}(\mathcal{Z})$. *Alors pour tout temps* $t \geq 0$, *la formule*

$$U(0,t)\, b^{Wick} U(t,0) = \left(b^{(0),t}\right)^{Wick} + \sum_{k=1}^{\lfloor m/2\rfloor} \left(\frac{\varepsilon}{2}\right)^k \int_{\Delta_t^k} \left(b^{(k)t,\bar{s}^k}\right)^{Wick} \mathrm{d}\bar{s}^k$$

est vérifiée en tant qu'égalité d'opérateurs continus de $\mathcal{D}(\langle N\rangle^{m/2})$ *dans* $\mathcal{H}$, *où*

- $\bar{s}^k = (s_1,\ldots,s_k) \in \mathbb{R}_+^k$ *et* $\Delta_t^k = \left\{\bar{s}^k \in \mathbb{R}_+^k,\ \sum_{j=1}^k s_j \leq t\right\}$,
- *les polynômes* $b^{(k)t,\bar{s}^k}$ *sont définis récursivement par*

$$\left\{\begin{array}{rcl} b^{(0)t}(z) & = & b(\varphi(t,0)\, z) \\ b^{(k+1)t,\bar{s}^{k+1}} & = & \lambda^{s_{k+1}} b^{(k)t,\bar{s}^k} \end{array}\right. ,$$

avec $\lambda^s c = -i\left\{c\circ\varphi(0,s), Q_s\right\}^{(2)} \circ \varphi(s,0)$ *pour tout polynôme* c.

Théorème 1.6.3. *Supposons **H1** et **H2** verifiées. Soient* $m \geq 2$ *et* $b \in \mathcal{P}_{\leq m}(\mathcal{Z})$ *un polynôme. Alors, en introduisant*

- *le vecteur* $v_t \in \bigotimes^2 \mathcal{Z}$ *tel que pour tous* $z_1,\, z_2 \in \mathcal{Z}$,

$$\langle z_1 \otimes z_2, v_t\rangle = \langle z_1, L^*(t,0)\, A(t,0)\, z_2\rangle \ ,$$

- *l'opérateur sur* $\mathcal{P}(\mathcal{Z})$

$$\Lambda^t c(z) = \mathrm{Tr}\left[-2A^*(t,0)\, A(t,0)\, \partial_{\bar{z}}\partial_z c(z)\right] + \langle v_t|\,.\,\partial_{\bar{z}}^2 c(z) + \partial_z^2 c(z)\,.\,|v_t\rangle \ ,$$

la formule

$$U(0,t)\, b^{Wick} U(t,0) = \left(e^{\frac{\varepsilon}{2}\Lambda^t}\left(b\circ\varphi(t,0)\right)\right)^{Wick}$$

est vérifiée en tant qu'égalité d'opérateurs continus de $\mathcal{D}\left(\langle N\rangle^{m/2}\right)$ *dans* $\mathcal{H}$.

1.6.3 Propagation du chaos pour des systèmes constitués d'un grand nombre de bosons en dimension un avec une interaction ponctuelle entre deux bosons.

On obtient formellement l'équation de Schrödinger cubique défocalisante (avec $\varphi = \varphi(t,x)$, $t \in \mathbb{R}$, $x \in \mathbb{R}^d$)

$$i\partial_t \varphi = -\Delta\varphi + |\varphi|^2 \varphi$$

de façon naturelle à partir de l'équation de Hartree

$$i\partial_t \varphi = -\Delta\varphi + \left(V * |\varphi|^2\right) \varphi$$

en prenant comme potentiel d'interaction la "fonction" de Dirac δ. On présente dans ce travail une dérivation de l'équation de Schrödinger non-linéaire cubique défocalisante en dimension 1 d'espace.

Soit $\varphi_0 \in H^2(\mathbb{R})$ on note φ_t la solution de l'équation de Schrödinger non-linéaire

$$\left\{ \begin{array}{rcl} i\partial_t \varphi & = & -\Delta\varphi + |\varphi|^2 \varphi \\ \varphi|_{t=0} & = & \varphi_0 \end{array} \right. .$$

Soit, pour z dans $\mathcal{S}(\mathbb{R})$, $P(z) = \frac{1}{2}\int_{\mathbb{R}} |z|^4 \, d\lambda$ (où λ est la mesure de Lebesgue) et

$$\begin{aligned} H_\varepsilon &= \mathrm{d}\Gamma_\varepsilon(-\Delta) + P^{Wick} \\ &= \int_{\mathbb{R}} \nabla a_\varepsilon^*(x) \nabla a_\varepsilon(x) \, dx + \frac{1}{2}\int_{\mathbb{R}^2} a_\varepsilon^*(x) a_\varepsilon^*(y) \delta(x-y) a_\varepsilon(x) a_\varepsilon(y) \, \mathrm{d}x \, \mathrm{d}y \,, \end{aligned}$$

où les opérateurs de création et d'annihilation a_ε^* et a_ε sont proportionnels à $\sqrt{\varepsilon}$.

Théorème 1.6.4. *Supposons que $\|\varphi_0\|_{L^2(\mathbb{R})} = 1$. Pour tout polynôme $b \in \mathcal{P}_{p,p}\left(L^2(\mathbb{R})\right)$,*

$$\lim_{n\to+\infty} \left\langle \varphi_0^{\otimes n}, e^{it/\varepsilon_n H_{\varepsilon_n}} b^{Wick} e^{-it/\varepsilon_n H_{\varepsilon_n}} \varphi_0^{\otimes n} \right\rangle = b(\varphi_t) \ ,$$

où $n\varepsilon_n = 1$.

Posons

$$P_2(t)[z] = \frac{D^{(2)}P}{2}(\varphi_t)[z] = \Re \int_{\mathbb{R}} \overline{z(x)}^2 \varphi_t(x)^2 \, dx + 2\int_{\mathbb{R}} |z(x)|^2 |\varphi_t(x)|^2 \, \mathrm{d}x$$

et $\varepsilon A_2(t) = \mathrm{d}\Gamma(-\Delta) + P_2(t)^{Wick}$. On peut alors définir le propagateur unitaire associé à la famille $A_2(t)$,

$$\left\{ \begin{array}{rcl} i\partial_t U_2(t,s) & = & A_2(t) U_2(t,s) \\ U_2(s,s) & = & I_{\Gamma L^2(\mathbb{R})} \end{array} \right. .$$

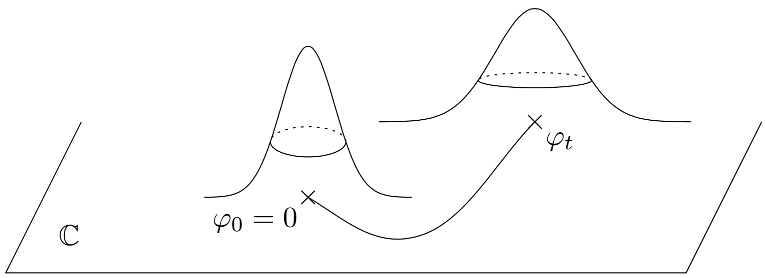

Fig. 1.6.2 – Évolution d'un état cohérent comprimé (représenté pour $\mathcal{Z} = \mathbb{C}$). On mélange deux points de vue dans ce dessin. L'état cohérent est vu comme une gaussienne comprimée (représentation de Schrödinger) et son centre est dans $\mathbb{C}$ (représentation de Bargmann).

Théorème 1.6.5. *Il existe $c > 0$ dépendant seulement de φ_0 tel que l'inégalité*

$$\left\| e^{-it/\varepsilon H_\varepsilon} W\left(\frac{\sqrt{2}}{i\varepsilon}\varphi_0\right)\Omega - e^{i\omega(t)/\varepsilon} W\left(\frac{\sqrt{2}}{i\varepsilon}\varphi_t\right) U_2(t,0)\,\Omega \right\|_{\Gamma L^2(\mathbb{R})} \leq e^{ce^{c|t|}} \varepsilon^{1/8}$$

est vérifiée pour tout $t \in \mathbb{R}$, avec $\omega(t) = \frac{1}{2}\int_0^t \left\|\varphi_s^2\right\|_{L^2(\mathbb{R})}^2 \mathrm{d}s$.

1.7 Quelques aspects du travail présenté

Dimension et dispersion Le résultat sur l'équation de Boltzmann linéaire n'est valable qu'à partir de la dimension trois car les inégalités de dispersion ne permettent de gagner suffisamment dans certaines estimations qu'à partir de la dimension trois pour avoir l'intégrabilité de certains termes. Il est peut-être possible d'atteindre la dimension deux avec un peu de travail supplémentaire.

La restriction à la dimension un dans le cas de l'équation de Schrödinger non-linéaire cubique défocalisante peut être levée quitte à modifier la définition de l'interaction δ.

Positivité et estimations *a priori* Un des ingrédients importants de notre dérivation de l'équation de Boltzmann linéaire est l'utilisation d'estimations *a priori* pour montrer que l'on n'a pas perdu trop de masse dans les mesures lors de notre approximation. On utilise ensuite les propriétés de conservation de la masse et de positivité de l'équation de Boltzmann linéaire pour conclure.

Pas de graphes À la différence des travaux d'Erdös et Yau, on s'est attaché, dans la dérivation de l'équation de Boltzmann linéaire, à éviter la combinatoire des graphes pour essayer de garder un point de vue plus géométrique sur le problème. Néanmoins l'Ansatz que nous utilisons ne permet pas d'atteindre des temps d'ordre 1 comme ceux obtenus par la méthode d'Erdös et Yau.

Théorie quantique des champs et géométrie dans l'espace des phases La théorie quantique des champs est utilisée pour bien voir intervenir la géométrie dans l'espace des phases. On utilise le point de vue de [2], mais en s'intéressant à deux cas qui ne rentrent pas dans le cadre retenu par les auteurs.

D'une part, quand on n'est pas dans un cadre de limite de champ moyen pour la dérivation de l'équation de Boltzmann linéaire, l'introduction d'un paramètre ε est alors artificielle mais permet de garder une trace de l'importance des différents termes.

D'autre part, on considère une interaction plus singulière dans le cas de la dérivation de l'équation de Schrödinger non-linéaire cubique défocalisante, avec un polynôme de Wick qui n'est pas dans la classe $\mathcal{P}(L^2(\mathbb{R}))$ présentée ci-dessus, à cause de l'interaction ponctuelle.

Trotter-Kato On n'obtient pas dans notre résultat le caractère markovien approché de l'évolution de façon satisfaisante. Pour palier ce problème on a introduit un renouvellement de l'aléa de manière artificielle. Les travaux [5, 4] traitent de façon un peu plus sophistiquée de problèmes d'interactions définies « par morceaux ». D'autres Ansätze permettent peut-être d'obtenir une meilleure approximation de la solution du problème de départ et donc d'obtenir le caractère markovien approché de l'évolution.

Perspectives On prévoit d'étudier le cas d'un aléa poissonien, avec le terme supplémentaire $d\Gamma(V(x-\cdot))$ dans l'hamiltonien.

On se propose aussi d'essayer d'autres Ansätze pour tenter d'obtenir de façon plus satisfaisante le caractère markovien de l'évolution limite.

On envisage également d'examiner le cas de la dimension deux pour la dérivation de l'équation de Boltzmann.

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Chapitre 2

Dérivation de l'équation de Boltzmann linéaire pour une particule interagissant avec un champ aléatoire

Rédigé en anglais.

Derivation of the linear Boltzmann equation for a particle interacting with a random field

Sommaire

2.1 Model and result 26

2.1.1 Rescaled quantum random field 26

2.1.2 The main result 27

2.2 The linear Boltzmann equation 29

2.2.1 The formal linear Boltzmann equation 29

2.2.2 Properties 30

2.2.3 The linear Boltzmann equation 31

2.2.4 A Trotter-type approximation 32

2.3 From stochastics to the Fock space 34

2.3.1 Classical kinetic regime 35

2.3.2 General Gaussian random fields 36

2.3.3 Wick powers 37

2.3.4 The isomorphism with the Fock space 37

2.3.5 The expression of the dynamic in the Fock space . 38

2.3.6 Existence of the dynamic 39

2.4 An approximated equation and its solution . . . 41

2.4.1 The scaling for field operators 41

2.4.2 The second quantization 41

2.4.3 Space translation in the fields and Fourier transform 42

2.4.4 The approximated equation and its solution 43

2.5 Measure of an observable for the approximated dynamics 47

2.5.1 Result 47

2.5.2 Expression of the measure of an observable for the approximated equation 49

2.5.3 Two estimates 52

2.5.4 The transport term $m_{\{,\}}$ 53

2.5.5 The collision terms m_- and m_+ 56

2.6 Comparison between approximated and exact dynamics 70

2.6.1 Step 1: Introduction of cutoffs 71

2.6.2 Step 2: Comparison between truncated solutions . 72

2.6.3 Step 3: Release of the truncation on the symbol . 76

2.7 The derivation of the Boltzmann equation for the model 77

2.A Stochastics 79

2.B Semiclassical Measures **81**
2.C General results on semigroups **82**
2.D Lemmas about an approximate identity **83**
2.E Formulae **85**
2.E.1 Symmetric Fock space 85
2.E.2 Fourier transforms 85
2.E.3 Weyl quantization 85

In this text the Hilbert spaces are always separable. The integer $d \geq 1$ denotes the dimension of the space $\mathbb{R}^d_x$. Our result requires $d \geq 3$.

2.1 Model and result

2.1.1 Rescaled quantum random field

Let $G : \mathbb{R}^d \to \mathbb{R}$ positive definite, such that $\hat{G} = |\hat{V}|^2$ with $\hat{V} \in \mathcal{S}\left(\mathbb{R}^d; \mathbb{R}\right)$ and $\mathcal{V}^h_\omega(x)$, $(\omega, x) \in \Omega_\mathbb{P} \times \mathbb{R}^d$, the translation invariant centered Gaussian random field with mean zero and covariance $hG(x - x')$. We consider the Schrödinger equation

$$\begin{cases} ih\partial_t u_{t,\omega}(x) & = H^h_\omega u_{t,\omega}(x) \\ u_{0,\omega}(x) & = \psi_0(x) \in L^2_x \end{cases} \tag{2.1.1}$$

with the Hamiltonian

$$H^h_\omega = -\Delta_x + \mathcal{V}^h_\omega(x) \ . \tag{2.1.2}$$

Let us fix a time T and an integer N. Let $t_k = k\Delta t$ with $\Delta t = \frac{T}{N}$. The dynamics is defined piecewise in the intervals $[t_{k-1}, t_k]$ by the Hamiltonians

$$H_{h,\omega_k} = -\Delta_x + \mathcal{V}_{h,\omega_k}(x)$$

with independent random fields $\mathcal{V}_{h,\omega_k}$, $\omega_k \in \Omega_k$. Thus we get, for an initial data $\psi_0 \in L^2_x$,

$$G_{N,\frac{\Delta t}{h},\bar{\omega}_N} = e^{-i\frac{\Delta t}{h}H_{h,\omega_N}} e^{-i\frac{\Delta t}{h}H_{h,\omega_{N-1}}} \ldots e^{-i\frac{\Delta t}{h}H_{h,\omega_1}} \ , \tag{2.1.3}$$

$$\psi_T(x, \bar{\omega}_N) = G_{N,\frac{\Delta t}{h},\bar{\omega}_N}\psi_0 \ ,$$

with $\bar{\omega}_k := (\omega_1, \ldots, \omega_k) \in \bar{\Omega}_k = \Omega_1 \times \cdots \times \Omega_k$, $\bar{\mathbb{P}}_k = \mathbb{P}_1 \times \cdots \times \mathbb{P}_k$ and $L^2\left(\bar{\Omega}^k, \bar{\mathbb{P}}^k\right) \simeq \bigotimes_{j=1}^k L^2(\Omega_j, \mathbb{P}_j)$.

Definition 2.1.1. Let ρ be a normal state on $\mathcal{L}\left(L^2_x\right)$, *i.e.* $\rho \in \mathcal{L}^+_1\left(L^2_x\right)$ and $\operatorname{Tr}\rho = 1$. We define

$$\rho^h_t = \int_{\Omega_\mathbb{P}} e^{-i\frac{t}{h}H_{h,\omega}}\rho e^{i\frac{t}{h}H_{h,\omega}} \, d\mathbb{P}(\omega) \ , \tag{2.1.4}$$

$$\rho^h_{N,\Delta t}(\bar{\omega}_N) = G_{N,\frac{\Delta t}{h},\bar{\omega}_N} \, \rho \, G^{-1}_{N,\frac{\Delta t}{h},\bar{\omega}_N} \ , \tag{2.1.5}$$

$$\rho^h_{N,\Delta t} = \int_{\bar{\Omega}_N} \rho^h_{N,\Delta t}(\bar{\omega}_N) \, d\mathbb{P}_N(\bar{\omega}_N) \ . \tag{2.1.6}$$

2.1.2 The main result

Let b be a symbol in $\mathcal{C}_0^\infty(\mathbb{R}^{2d}_{x,\xi})$. The measure of the observable $b^W(hx, D_x)$ in a normal state ρ is given by

$$\mathrm{Tr}\left[b^W(hx, D_x)\,\rho\right]$$

where the Weyl quantization is defined by

$$b^W(hx, D_x)u(x) = \frac{1}{(2\pi)^d}\int_{\mathbb{R}^d_\xi}\int_{\mathbb{R}^d_{x'}} e^{i(x-x').\xi} b\left(h\frac{x+x'}{2}, \xi\right) u(x')\,\mathrm{d}x'\,\mathrm{d}\xi\,.$$

One can refer for example to [42] about the properties of the Weyl quantization.

Consider the dynamic given by Equations (2.1.1) and (2.1.2) with renewal as in Equation (2.1.3), $\Delta t = h^\alpha$, $N = N^h = T/h^\alpha$, $\alpha \in]\frac{3}{4}, 1[$.

We say that a family of states (ρ^h), $h \in]0, h_0]$ is pure if there is a measure μ_0 on $\mathbb{R}^{2d}_{x,\xi}$ such that

$$\forall b \in \mathcal{C}_0^\infty\left(\mathbb{R}^{2d}_{x,\xi}\right),\ \lim_{h\to 0^+}\mathrm{Tr}\left[\rho^h b^W(hx, D_x)\right] = \int_{\mathbb{R}^{2d}_{x,\xi}} b\,\mathrm{d}\mu_0\,.$$

We refer the reader to Appendix 2.B and [26, 32, 33, 41] for general information about semiclassical measures.

Theorem 2.1.2. *Assume that $(\rho^h)_{h\in]0,h_0]}$ is pure with $\mu_0(\mathbb{R}^d_x \times \mathbb{R}^{d*}_\xi) = 1$. Then*

$$\forall b \in \mathcal{C}_0^\infty\left(\mathbb{R}^{2d}_{x,\xi}\right),\ \lim_{h\to 0}\mathrm{Tr}\left[\rho^h_{N,\Delta t} b^W(hx, D_x)\right] = \int b\,\mathrm{d}\mu_T$$

where $\mu_T = \mu_{t=T}$ with, for $t \in (0, T)$,

$$\begin{cases} \partial_t\mu_t(x,\xi) + 2\xi.\partial_x\mu_t(x,\xi) = \int \sigma(\xi,\xi')\delta\left(|\xi|^2 - |\xi'|^2\right)\left(\mu_t(x,\xi') - \mu_t(x,\xi)\right)\mathrm{d}\xi'\,, \\ \mu_{t=0} = \mu_0 \end{cases} \tag{2.1.7}$$

and $\sigma(\xi,\xi') = 2\pi|\hat{V}(\xi-\xi')|^2$.

Remark 2.1.3. The meaning of measures solving the linear Boltzmann Equation (2.1.7) is specified in Part 2.2.

The result says that the family $(\rho^h_{N,\Delta t})$ remains pure for every $T\,(= N\Delta t)$ as soon as (ρ^h) is pure.

The justification of the choice of the scaling in the Weyl quantization is the following. Physically the parameter h is the quotient of the microscopic scale over the macroscopic scale, either in time or in position. Thus if we consider an observable $b(X, \Xi)$ varying on a macroscopic scale, the corresponding observable on the microscopic scale will be $b(hx, \xi)$.

The scaling of the random field according to the covariance $hG(x - x')$, is done on a mesoscopic scale imposed by the kinetic regime (see Section 2.3.1).

Sketch of the Proof. Let μ_T in $\mathcal{M}(\rho^h_{N,\Delta t}, h \in]0, h_0[)$ (the set of semiclassical measures defined after extraction of subsequences, see Appendix 2.B). We denote by $\mathcal{B}(t)$ the flow associated with the Boltzmann equation (2.1.7) and $\mathcal{B}^T(t)$ the flow associated with the dual equation, see Section 2.2 for more details about $\mathcal{B}(t)$ and $\mathcal{B}^T(t)$. For any non-negative b in $\mathcal{C}_0^\infty(\mathbb{R}^d_x \times \mathbb{R}^{d*}_\xi)$ we shall prove

1. $\int_{\mathbb{R}^d_x \times \mathbb{R}^{d*}_\xi} b \,\mathrm{d}\mu_T \geq \liminf_{h\to 0} \mathrm{Tr}[\rho^h_{N,\Delta t} b^W(hx, D_x)]$ by the definition of μ_T,
2. $\liminf_{h\to 0} \mathrm{Tr}[\rho^h_{N,\Delta t} b^W(hx, D_x)] \geq \int_{\mathbb{R}^d_x \times \mathbb{R}^{d*}_\xi} (\mathcal{B}^T(T)b) \,\mathrm{d}\mu_0$ (see the remark below),
3. $\int_{\mathbb{R}^d_x \times \mathbb{R}^{d*}_\xi} (\mathcal{B}^T(T)b) \,\mathrm{d}\mu_0 = \int_{\mathbb{R}^d_x \times \mathbb{R}^{d*}_\xi} b \,\mathrm{d}(\mathcal{B}(T)\mu_0)$ by the definition of $\mathcal{B}(T)$.

Taking this for granted, it implies the lower bound

$$\int_{\mathbb{R}^d_x \times \mathbb{R}^{d*}_\xi} b \, d\mu_T \geq \int_{\mathbb{R}^d_x \times \mathbb{R}^{d*}_\xi} b \,\mathrm{d}(\mathcal{B}(T)\,\mu_0)\ .$$

Since this inequality holds for any non-negative b in $\mathcal{C}_0^\infty(\mathbb{R}^d_x \times \mathbb{R}^{d*}_\xi)$ which is dense in $\mathcal{C}^0_\infty(\mathbb{R}^d_x \times \mathbb{R}^{d*}_\xi)$ with dual $\mathcal{M}_b(\mathbb{R}^d_x \times \mathbb{R}^{d*}_\xi)$, we get

$$\mu_T|_{\mathbb{R}^d_x \times \mathbb{R}^{d*}_\xi} \geq \mathcal{B}(T)\,\mu_0|_{\mathbb{R}^d_x \times \mathbb{R}^{d*}_\xi}\ .$$

But we also have $\mathcal{B}(T)\mu_0(\mathbb{R}^d_x \times \mathbb{R}^{d*}_\xi) = 1$ from the properties of the linear Boltzmann equation and $\mu_T(\mathbb{R}^d_x \times \mathbb{R}^d_\xi) \leq 1$ from the properties of semiclassical measures. So, necessarily,

$$\begin{aligned} \mu_T\left(\mathbb{R}^d_x \times \mathbb{R}^{d*}_\xi\right) &= 1 \\ \mu_T\left(\mathbb{R}^d_x \times \{0\}_\xi\right) &= 0 \end{aligned}$$

and $\mu_T = \mathcal{B}(T)\mu_0$. Thus we have the result. □

Remark 2.1.4. The step

$$\liminf_{h\to 0} \mathrm{Tr}\left[\rho^h_{N,\Delta t} b^W(hx, D_x)\right] \geq \int_{\mathbb{R}^d_x \times \mathbb{R}^{d*}_\xi} \left(\mathcal{B}^T(T)\,b\right) \mathrm{d}\mu_0$$

is the technical part which requires various estimates for the quantum dynamics of the whole system particle-random field.

To prove this result we consider first the case without renewal of the stochastics, *i.e.* $N = 1$ for short times in Sections 2.4, 2.5, 2.6 and then glue together the estimates obtained this way N times for N "big" in Section 2.7. To simplify the problem of finding estimates for short times we approximate the equation by a simpler one which is solved and studied in Section 2.4. In

Section 2.5, using the solution to the approximated equation, we carry out explicit computations which give rise to the different terms of the dual linear Boltzmann equation. Then we control the error between the solutions of the approximated equation and the exact equation in Section 2.6. All these computations are done within the framework of quantum field theory. This allows us

- to use conveniently the geometric content of coherent states,
- to keep track of the different orders of importance of the different terms by using the Wick quantization with a parameter ε.

For the reader's convenience, we recall the correspondence between the stochastic and Fock space viewpoints in Section 2.3.

Remark 2.1.5. Our initial data $(\rho^h)_{h\in]0,h_0]}$ are assumed to belong to $\mathcal{L}_1^+L_x^2$ with $\operatorname{Tr}\rho^h = 1$. We will thus make estimates for states ρ in $\mathcal{L}_1^+L_x^2$, with $\operatorname{Tr}\rho = 1$ with constants independent of ρ.

2.2 The linear Boltzmann equation

Information on the linear Boltzmann equation can be found in [28, 29, 44].

In this part suppose that $\sigma \in \mathcal{C}^\infty(\mathbb{R}^d_\xi \times \mathbb{R}^d_{\xi'};\mathbb{R})$ and $\sigma \geq 0$.

2.2.1 The formal linear Boltzmann equation

Since all the objects we use are diagonal in $|\xi|$, the following definitions will be convenient.

Notation: Let $0 < r < r' < +\infty$ we define the Sobolev spaces

$$H^n\left[r,r'\right] = H^n\left(\mathbb{R}^d_x \times A_\xi\left[r,r'\right];\mathbb{R}\right)$$

where $A_\xi[r,r']$ is the annulus $\{\xi,\ |\xi| \in]r,r'[\}$ in the variable ξ. When there is no ambiguity we write A_ξ for $A_\xi[r,r']$. We also define $L^2[r,r'] = H^0[r,r']$.

Definition 2.2.1. The *collision operator* Q is defined for $b \in L^2[r,r']$ by

$$Qb = Q_+b - Q_-b\,, \tag{2.2.1}$$

with

$$Q_+b\,(x,\xi) = \int_{\mathbb{R}^d_{\xi'}} b\,(x,\xi')\,\sigma\,(\xi,\xi')\,\delta\left(|\xi|^2 - \left|\xi'\right|^2\right)\mathrm{d}\xi'$$

and

$$Q_-b\,(x,\xi) = b\,(x,\xi)\int_{\mathbb{R}^d_{\xi'}} \sigma\,(\xi,\xi')\,\delta\left(|\xi|^2 - \left|\xi'\right|^2\right)\mathrm{d}\xi'\,.$$

Remark 2.2.2. For a given ξ these integrals only involve the values of $\sigma(\xi, |\xi|\,\omega)$ and $b(x, |\xi|\,\omega)$ for $\omega \in \mathbb{S}^{d-1}$.

Definition 2.2.3. The *linear Boltzmann equation* is formally the equation

$$\begin{cases} \partial_t f & = \left\{ f, |\xi|^2 \right\} + Qf \\ f_{t=0} & = f_0 \end{cases}$$

and its *dual equation* is

$$\begin{cases} \partial_t b & = -\left\{ b, |\xi|^2 \right\} + Qb = 2\xi.\partial_x b + Qb \\ b_{t=0} & = b_0 \end{cases} .$$

We will see in the next sections that the dual linear Boltzmann equation is solved by a group $(\mathcal{B}^T(t))_{t\in\mathbb{R}}$ of operators on $\mathcal{C}^0_\infty(\mathbb{R}^d_x \times \mathbb{R}^{d*}_\xi; \mathbb{R})$ and this defines by duality a group $(\mathcal{B}(t))_{t\in\mathbb{R}}$ of operators on $\mathcal{M}_b(\mathbb{R}^d_x \times \mathbb{R}^{d*}_\xi; \mathbb{R})$.

2.2.2 Properties

We recall here the main properties of the dual linear Boltzmann equation. (The arguments are the same as for the linear Boltzmann equation.)

Some standard notations and results about semigroups are given in Appendix 2.C. We begin by solving the dual linear Boltzmann equation in $L^2[r, r']$ in the sense of semigroups. We observe that $2\xi.\partial_x$ generates a strongly continuous contraction semigroup on $L^2[r, r']$. Since the operator Q is bounded on $L^2[r, r']$ we get that $2\xi.\partial_x + Q$ generates a semigroup $(\mathcal{B}^T(t))_{t\geq 0}$ bounded by $\exp(t \left\|Q\right\|_{\mathcal{L}(L^2[r,r'])})$ and the associated domain is $D(2\xi.\partial_x)$.

Proposition 2.2.4. *Let $0 < r < r' < +\infty$. The operator Q on $H^n[r, r']$ is well defined and bounded, with*

$$\left\|Q\right\|_{\mathcal{L}(H^n[r,r'])} \leq C_d \sup_{|\alpha|\leq n} \left\|\partial^\alpha \sigma\right\|_{\infty, A^2_\xi[r,r']} .$$

The group of (space-)translation $(e^{2t\xi.\partial_x})_t$ preserves $H^n[r, r']$.

Proposition 2.2.5. *Let $0 < r < r' < +\infty$. The strongly continuous group $(\mathcal{B}^T(t))_{t\geq 0}$ of infinitesimal generator $2\xi.\partial_x + Q$ preserves*

1. *the Sobolev spaces $H^n[r, r']$, for $n \in \mathbb{N}$,*
2. *the set of functions with compact support,*
3. *the set of infinitely differentiable functions with compact support in $\mathbb{R}^d_x \times A_\xi[r, r']$, $\mathcal{C}^\infty_0(\mathbb{R}^d_x \times A_\xi[r, r']; \mathbb{R})$,*
4. *the set of non-negative functions, for $t \geq 0$.*

Proof. For (1) we use Proposition 2.2.4.

For (2) we can use the Trotter approximation

$$\mathcal{B}^T(t) = \lim_{n\to+\infty}\left(e^{2\frac{t}{n}\xi.\partial_x}e^{\frac{t}{n}Q}\right)^n ,$$

the fact that Q is "local" in $(x,|\xi|)$, and that the speed of propagation of the (space-) translations is finite when $\xi \in A_\xi[r,r']$.

For (3) we use (1), (2) and

$$\mathcal{C}_0^\infty\left(\mathbb{R}_x^d \times A_\xi\left[r,r'\right];\mathbb{R}\right) = \bigcap_{n=0}^{\infty} H^n\left[r,r'\right]\bigcap\{f,\,\mathrm{Supp}\,f\text{ compact}\} .$$

For (4) we use both the Trotter approximation

$$\mathcal{B}^T(t) = \lim_{n\to+\infty}\left(e^{2\frac{t}{n}\xi.\partial_x}e^{\frac{t}{n}Q_+}e^{-\frac{t}{n}Q_-}\right)^n$$

and the fact that $e^{2\frac{t}{n}\xi.\partial_x}$ preserves the non-negative functions as a translation, $e^{\frac{t}{n}Q_+}$ preserves the non-negative functions for $t \geq 0$ because Q_+ does, $e^{-\frac{t}{n}Q_-}$ preserves the non-negative functions as a multiplication operator by a positive function. □

Since $\mathcal{C}_0^\infty\left(\mathbb{R}_x^d \times A_\xi;\mathbb{R}\right) \subset D\left(2\xi.\partial_x\right)$ we can give the following result.

Proposition 2.2.6. *For every $b_0 \in \mathcal{C}_0^\infty\left(\mathbb{R}_x^d \times A_\xi;\mathbb{R}\right)$ there exists a unique function $b_t = \mathcal{B}^T(t)\,b_0 \in \mathcal{C}^1\left(\mathbb{R}^+;L^2\left[r,r'\right]\right)\cap\mathcal{C}^0\left(\mathbb{R}^+;D\left(2\xi.\partial_x\right)\right)$ such that for every $t\in\mathbb{R}$,*

$$\begin{cases}\partial_t b_t &= 2\xi.\partial_x b_t + Qb_t\\ b_{t=0} &= b_0\end{cases} .$$

Moreover $\forall t\in\mathbb{R}$, $b_t \in \mathcal{C}_0^\infty\left(\mathbb{R}_x^d \times A_\xi;\mathbb{R}\right)$. If b_0 is non-negative, then $\forall t\geq 0$, b_t is non-negative.

2.2.3 The linear Boltzmann equation

Notation: For X a locally compact, Hausdorff space we denote by $\mathcal{M}_b(X;\mathbb{R})$ the set of Radon measures and by $\mathcal{C}_\infty^0(X;\mathbb{R})$ the set of functions f on X such that for all $\varepsilon>0$ there exists a compact $K_{f,\varepsilon}$ such that $|f(x)|<\varepsilon$ outside of $K_{f,\varepsilon}$ (*i.e.* the set of functions that vanish at infinity).

For a topological space X, locally compact and Hausdorff,

$$\mathcal{M}_b\left(X;\mathbb{R}\right) = \left(\mathcal{C}_\infty^0\left(X;\mathbb{R}\right)\right)' .$$

Proposition 2.2.7. *The semigroup $(\mathcal{B}^T(t))_{t\geq 0}$ defined on $\mathcal{C}_0^0(\mathbb{R}_x^d\times\mathbb{R}_\xi^{d*};\mathbb{R})$ can be extended to a strongly continuous group on $(\mathcal{C}_\infty^0(\mathbb{R}_x^d\times\mathbb{R}_\xi^{d*};\mathbb{R}),\|\cdot\|_\infty)$ and thus defines by duality a (weak* continuous) group $\mathcal{B}(t)$ on $\mathcal{M}_b(\mathbb{R}_x^d\times\mathbb{R}_\xi^{d*};\mathbb{R})$.*

Proof. Using a partition of the unity, we can extend $\mathcal{B}^T(t)$ to $\mathcal{C}^\infty(\mathbb{R}^d_x \times \mathbb{R}^{d*}_\xi;\mathbb{R})$. As $\mathcal{B}^T(t)$ is positive, we have $\mathcal{B}^T(t)(\|b\|_\infty \pm b) \geq 0$ for all b in $\mathcal{C}^\infty_0(\mathbb{R}^d_x \times \mathbb{R}^{d*}_\xi;\mathbb{R})$ and so

$$\left\|\mathcal{B}^T(t)\, b\right\|_\infty \leq \|b\|_\infty \, .$$

We can thus extend continuously $\mathcal{B}^T(t)$ from $\mathcal{C}^\infty_0(\mathbb{R}^d_x \times \mathbb{R}^{d*}_\xi;\mathbb{R})$ to $\mathcal{C}^0_\infty(\mathbb{R}^d_x \times \mathbb{R}^{d*}_\xi;\mathbb{R})$. □

Definition 2.2.8. The *linear Boltzmann group* $(\mathcal{B}(t))$ is defined on $\mathcal{M}_b(\mathbb{R}^d_x \times \mathbb{R}^{d*}_\xi)$ by duality, let $\mu \in \mathcal{M}_b(\mathbb{R}^d_x \times \mathbb{R}^{d*}_\xi)$, then, for any $t \in \mathbb{R}$,

$$\forall b \in \mathcal{C}^0_\infty\left(\mathbb{R}^d_x \times \mathbb{R}^{d*}_\xi\right), \qquad \langle \mathcal{B}(t)\mu, b\rangle = \left\langle \mu, \mathcal{B}^T(t)b\right\rangle \, .$$

2.2.4 A Trotter-type approximation

In this part we will prove a result in the spirit of the approximation of Trotter

$$e^{A+B} = \lim_{N\to\infty}\left(e^{A/N}e^{B/N}\right)^N \, .$$

Notation: For $n \in \mathbb{N}$ and $b \in \mathcal{C}^\infty_0(\mathbb{R}^{2d}_{x,\xi})$, set

$$\mathcal{N}_n(b) := \sup_{|\alpha|\leq n} \|\partial^\alpha b\|_\infty \, . \tag{2.2.2}$$

Proposition 2.2.9. *Let $b \in \mathcal{C}^\infty_0(\mathbb{R}^{2d}_{x,\xi})$, $T > 0$ and $n \in \mathbb{N}$. There are constants $C_{n,Q}$ and $C_{T,b}$ such that for all $N \in \mathbb{N}^*$*

$$\mathcal{N}_n\left(e^{T(2\xi.\partial_x + Q)}b - \left(e^{\frac{T}{N}Q}e^{\frac{T}{N}2\xi.\partial_x}\right)^N b\right) \leq e^{T\left(2n+C_{n,Q}\right)}C_{T,b}\frac{T^2}{N} \, .$$

Definition 2.2.10. Let $Q_t \in \mathcal{L}\left(L^2\left[r,r'\right]\right)$ be the operator defined by $Q_t = e^{t2\xi.\partial_x}Qe^{-t2\xi.\partial_x}$, *i.e.* $Q_t = Q_{+,t} - Q_-$ with

$$Q_{+,t}b\left(x,\xi\right) = \int_{\mathbb{R}^d_{\xi'}} \sigma\left(\xi,\xi'\right)\delta\left(|\xi|^2 - \left|\xi'\right|^2\right) b\left(x - 2t\left(\xi'-\xi\right),\xi'\right)\mathrm{d}\xi'$$

We also define $Q_{-,t} = Q_-$ to have consistent notations in the sequel.

Let $G_Q(t,t_0)$ be the dynamical system associated with the family (Q_t) in $\mathcal{C}(\mathbb{R};\mathcal{L}(L^2[r,r']))$ given by

$$\begin{cases}\partial_t b_t &= Q_t b_t\\ b_{t=t_0} &= b_0 \in L^2_{x,\xi}\end{cases}, \qquad b_t = G_Q\left(t,t_0\right)b_0 \, .$$

Note the relation

$$\mathcal{B}^T(t) = G_Q(t,0)\,e^{2t\xi.\partial_x} = e^{2t\xi.\partial_x}G_Q(0,-t) \, .$$

Lemma 2.2.11. *For any $n \in \mathbb{N}$, $s \geq 0$ and $b \in \mathcal{C}_0^\infty\left(\mathbb{R}_x^d \times A_\xi\left[r, r'\right]\right)$, there exist constants C_1, and C_2 depending on d, r and r' such that*

1. $\mathcal{N}_n\left(Qb\right) \leq C_1 \mathcal{N}_n\left(b\right)$,
2. $\mathcal{N}_n\left(\left(Q - Q_t\right)b\right) \leq C_2 t\left(1 + 2\left|t\right|\right)^n \mathcal{N}_{n+1}\left(b\right)$,
3. $\mathcal{N}_n\left(e^{2t\xi.\partial_x} b\right) \leq \left(1 + 2\left|t\right|\right)^n \mathcal{N}_n\left(b\right)$.

Proof. The first point is clear from the integral expression of Qb.

For the second point derive and estimate the integral formula for $b\left(x - 2t\xi, \xi\right) - b\left(x, \xi\right)$, with $\left|\alpha\right| \leq n$,

$$\begin{aligned}\left|\partial^\alpha\left(b\left(x - 2t\xi, \xi\right) - b\left(x, \xi\right)\right)\right| &\leq \int_0^t \left|\partial^\alpha\left(2\xi.\partial_x b\left(x - 2s\xi, \xi\right)\right)\right| \mathrm{d}s \\ &\leq 2\left|\xi\right| t\left(1 + 2t\right)^n \mathcal{N}_{n+1}\left(b\right)\ .\end{aligned}$$

The last point results from $\left(e^{2t\xi.\partial_x} b\right)\left(x, \xi\right) = b\left(x + 2t\xi, \xi\right)$. □

Definition 2.2.12. For $b \in \mathcal{C}_0^\infty\left(\mathbb{R}_x^d \times A_\xi\left[r, r'\right]\right)$, let

$$\mathcal{N}_n\left(Q\right) = \sup_{b \neq 0} \frac{\mathcal{N}_n\left(Qb\right)}{\mathcal{N}_n b} \text{ and } \mathcal{N}_{n+1,n}\left(s, Q - Q_s\right) = \sup_{b \neq 0} \frac{\mathcal{N}_n\left(\left(Q - Q_s\right)b\right)}{s\left(1 + 2\left|s\right|\right)^n \mathcal{N}_{n+1} b}\,.$$

Lemma 2.2.13. *Let b, $\tilde{b} \in \mathcal{C}_0^\infty\left(\mathbb{R}_x^d \times A_\xi\left[r, r'\right]\right)$, then for all $t \geq 0$,*

$$e^{tQ}\tilde{b} - G_Q\left(t, 0\right)b = e^{tQ}\left(\tilde{b} - b\right) + \int_0^t e^{(t-s)Q}\left(Q - Q_s\right)G_Q\left(s, 0\right)b\,\mathrm{d}s$$

and we have the estimate

$$\begin{aligned}&\mathcal{N}_n\big(e^{tQ}\tilde{b} - G_Q(t,0)b\big) \\ &\leq e^{t\mathcal{N}_n Q}\mathcal{N}_n(\tilde{b} - b) \\ &\quad + t^2(1+2t)^n e^{t\mathcal{N}_n Q} \sup_{s \in [0,t]} \big\{\mathcal{N}_{n+1,n}(s, Q - Q_s)\mathcal{N}_{n+1}\big(G_Q(s,0)\big)\big\}\mathcal{N}_{n+1}(b)\,.\end{aligned}$$

Proof. The equality is clear once we have computed that both sides satisfy the equation

$$\partial_t \Delta_t = Q\Delta_t + \left(Q - Q_t\right)G_Q\left(t, 0\right)b\,.$$

The inequality then follows from Lemma 2.2.11. □

Proof of Proposition 2.2.9 . We fix N and forget the N's in the notations concerning $\tilde{b}$. We set $b_t = \mathcal{B}^T\left(t\right)b$ and define $\tilde{b}_t$ piecewise on $[0, T]$ by setting $t_k = \frac{kT}{N}$, $\tilde{b}_{t_k} = \left(e^{\frac{T}{N}Q}e^{\frac{T}{N}2\xi.\partial_x}\right)^k b_0$ and, for $t \in [t_k, t_{k+1}[$, $\tilde{b}_t = e^{(t-t_k)Q}e^{(t-t_k)2\xi.\partial_x}\tilde{b}_{t_k}$. Let $\delta_k = \mathcal{N}_n\left(b_{t_k} - \tilde{b}_{t_k}\right)$; we get

$$e^{\frac{T}{N}Q}e^{\frac{T}{N}2\xi.\partial_x}\tilde{b}_{t_k} - e^{\frac{T}{N}(2\xi.\partial_x+Q)}b_{t_k} = e^{\frac{T}{N}Q}e^{\frac{T}{N}2\xi.\partial_x}\tilde{b}_{t_k} - G_Q\left(\frac{T}{N}, 0\right)e^{\frac{T}{N}2\xi.\partial_x}b_{t_k}$$

and we can then use Lemma 2.2.13 to obtain

$$\begin{aligned}\delta_{k+1} \leq\ & e^{\frac{T}{N}\mathcal{N}_nQ}\left(1+2\frac{T}{N}\right)^n\delta_k + \left(\frac{T}{N}\right)^2\left(1+2\frac{T}{N}\right)^n e^{\frac{T}{N}\mathcal{N}_nQ} \\ & \sup_{s\in[t_k,t_{k+1}]}\mathcal{N}_{n+1,n}\left(s-t_k, Q-Q_{s-t_k}\right) \\ & \sup_{s\in[t_k,t_{k+1}]}\mathcal{N}_{n+1}\left(G_Q\left(s-t_k,0\right)e^{\frac{T}{N}2\xi.\partial_x}b_{t_k}\right) \\ \leq\ & e^{\frac{T}{N}\mathcal{N}_nQ}e^{2\frac{nT}{N}}\delta_k + \left(\frac{T}{N}\right)^2 e^{\frac{T}{N}\mathcal{N}_nQ}C_{N,T}\end{aligned}$$

where we defined

$$\begin{aligned}C_{N,T,b} = \left(1+2\frac{T}{N}\right)^n & \sup_{s\in[0,T/N]}\mathcal{N}_{n+1,n}\left(s, Q-Q_s\right) \\ & \sup_{k\in\{0,\dots,N-1\}}\sup_{s\in[0,T/N]}\mathcal{N}_{n+1}\left(G_Q\left(s,0\right)e^{-\frac{T}{N}Q}b_{t_{k+1}}\right).\end{aligned}$$

Then we get the recursive formula

$$\delta_{k+1} \leq e^{\frac{T}{N}(2n+\mathcal{N}_nQ)}\delta_k + C_{N,T,b}\left(\frac{T}{N}\right)^2 e^{\frac{T}{N}\mathcal{N}_nQ}$$

so that

$$\delta_N \leq e^{T(2n+\mathcal{N}_nQ)}C_{N,T,b}\frac{T^2}{N}.$$

The only thing remaining is to observe that $C_{N,T,b} \leq C_{T,b}$, with

$$C_{T,b} := (1+2T)^n \sup_{s\in[0,T]}\mathcal{N}_{n+1,n}(s, Q-Q_s)\sup_{s_j\in[0,T]}\mathcal{N}_{n+1}\left(G_Q(s_1,0)e^{-s_2Q}b_{s_3}\right)$$

and for a fixed T this quantity $C_{T,b}$ is finite, so that we get the result. □

2.3 From stochastics to the Fock space

The relation between Gaussian random processes and the Fock space is treated in [45, 38], we recall some facts without proofs which clarify this relation.

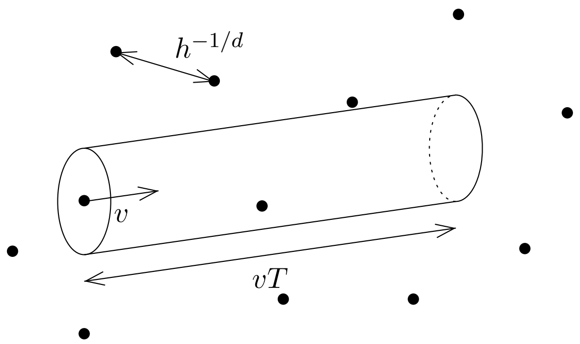

Figure 2.3.1: Kinetic regime.

2.3.1 Classical kinetic regime

In microscopic variable, consider a particle moving among obstacles with a velocity $v \propto 1$ and a distance of interaction $R \propto 1$. During a time T the particle sweeps a volume of order vTR^{d-1}. In the kinetic regime it is assumed that during a long microscopic time $T = t/h$ with $t \propto 1$ the macroscopic time, the average particle encounters a number $\propto 1$ obstacle.

We denote by ρ the density of obstacles and thus obtain $\rho = 1/vTR^{d-1} \propto h$. To get this density of obstacles we need the distance between two nearest obstacles to be of order $h^{-1/d}$.

Thus we consider a Schrödinger equation of the form

$$i\partial_T \psi = -\Delta_x \psi + \mathcal{V}_\omega^h (x) \psi$$

that is

$$ih\partial_t \psi = -\Delta_x \psi + \mathcal{V}_\omega^h (x) \psi .$$

A translation invariant Gaussian random field of covariance $G(x-x')$, $\hat{G} = |\hat{V}|^2$ is $V * W_\omega$ where W_ω is the spatial white noise (see Appendix 2.A) and V describes the interaction potential. In the kinetic regime the obstacles are spread at the mesoscopic scale $h^{1/d}$. Only the white noise W_ω^h is rescaled (and not V) according to

$$\forall \varphi \in \mathcal{S}\left(\mathbb{R}^d;\mathbb{R}\right), \quad \int \varphi\left(h^{1/d}x\right) W_\omega^h (x)\, dx = \int \varphi (x) W_\omega (x)\, \mathrm{d}x ,$$

i.e.

$$W_\omega^h (x) = h W_\omega \left(h^{1/d} x\right) .$$

Thus we get $\mathcal{V}_\omega^h = hV * W_\omega \left(h^{1/d}\cdot\right)$ and $G^h = hG$. See the Appendix 2.A for more details.

2.3.2 General Gaussian random fields

We introduce a different viewpoint on Gaussian random fields.

Definition 2.3.1. Let $(\Omega_{\mathbb{P}}, \mathcal{G}, \mathbb{P})$ be a probability measure space. Let E be a (real) vector space. A *general random field* indexed by E is a map Φ from E to the random variables on $\Omega_{\mathbb{P}}$, so that (almost everywhere)

$$\begin{aligned} \Phi(v+w) &= \Phi(v)+\Phi(w), \quad \forall v, w \in E, \\ \Phi(\alpha v) &= \alpha \Phi(v), \quad \forall \alpha \in \mathbb{R}, \forall v \in E. \end{aligned}$$

Definition 2.3.2. Let $\mathcal{H}_{\mathbb{R}}$ be a real Hilbert space. The *general centered Gaussian random field* indexed by $\mathcal{H}_{\mathbb{R}}$ is a random field Φ_G indexed by $\mathcal{H}_{\mathbb{R}}$ so that

1. $\mathcal{G}$ is the smallest σ-algebra for which al the $\Phi_G(v)$, $v \in \mathcal{H}_{\mathbb{R}}$ are measurable,
2. each $\Phi_G(v)$ is a centered Gaussian random variable,
3. $\mathbb{E}[\Phi_G(v)\Phi_G(w)] = \langle v, w\rangle$ with $\langle \cdot, \cdot \rangle$ the inner product on $\mathcal{H}_{\mathbb{R}}$.

One can refer to [45] for the following two theorems.

Theorem 2.3.3. *Let Φ_G and Φ'_G be two general centered Gaussian random field indexed by $\mathcal{H}_{\mathbb{R}}$ on probability measure spaces $(\Omega_{\mathbb{P}}, \mathcal{G}, \mathbb{P})$ and $(\Omega'_{\mathbb{P}}, \mathcal{G}', \mathbb{P}')$ respectively. Then there exists an isomorphism between the two probability measure spaces so that for every $v \in \mathcal{H}_{\mathbb{R}}$, $\Phi_G(v)$ corresponds to $\Phi'_G(v)$ under the isomorphism.*

Theorem 2.3.4. *Let $\mathcal{H}_{\mathbb{R}}$ be a real Hilbert space. A general centered Gaussian random field indexed by $\mathcal{H}_{\mathbb{R}}$ exists and it is unique (in the sense of the preceding theorem).*

Proposition 2.3.5. *Let $G \in L^1(\mathbb{R}^d;\mathbb{R}) \cap \mathcal{F}L^1(\mathbb{R}^d;\mathbb{C})$ positive definite, we can choose $V \in L^2(\mathbb{R}^d;\mathbb{R})$ such that*

$$\hat{G} = |\hat{V}|^2 .$$

Then the Gaussian random field of mean zero and covariance $\Sigma(x,y) = G(x-y)$ is also the random field obtained as $\Phi_G(\tau_x V)$ where Φ_G is the general Gaussian random field indexed by $L^2(\mathbb{R}^d;\mathbb{R})$.

Proof. From Bochner's theorem we deduce that $\hat{G} \in L^1(\mathbb{R}^d;\mathbb{C})$ has real positive values. Thus we can set $\hat{V} = \sqrt{\hat{G}}$. Then it suffices to prove that the covariance function $\Sigma(x,y)$ of $\Phi_G(\tau_x V)$ is $G(x-y)$.

$$\begin{aligned}\Sigma(x,y) &= \mathbb{E}\left[\Phi_G(\tau_x V)\,\Phi_G(\tau_y V)\right]\\ &= \langle \tau_{x-y}V, V\rangle_{L^2\left(\mathbb{R}^d_x;\mathbb{R}\right)}\\ &= \frac{1}{(2\pi)^d}\left\langle e^{-i(x-y).\xi}\hat{V},\hat{V}\right\rangle_{L^2\left(\mathbb{R}^d_\xi;\mathbb{C}\right)}\\ &= \mathcal{F}^{-1}\left[|\hat{V}|^2\right](y-x)\ .\end{aligned}$$

□

Remark 2.3.6. If we replace G by $G^h = hG$, the field $\sqrt{h}\Phi_G(\tau_x V)$ gives the expected covariance function.

2.3.3 Wick powers

Definition 2.3.7. Let f be a random variable with finite moments, for $n \in \mathbb{N}^*$, $:f^n: \in \mathbb{C}[X]$, the n-th *Wick power* of f is defined recursively by

$$:f^0: = 1\,,\quad \partial_X :f^n: = n:f^{n-1}: \quad \text{and} \quad \tilde{\mathbb{E}}\left[:f^n:\right] = 0\,,$$

where $\tilde{\mathbb{E}} : \mathbb{C}[X] \to \mathbb{C}$ is the linear map defined by $\tilde{\mathbb{E}}[X^n] = \mathbb{E}[f^n]$. We still denote by $:f^n:$ the random variable $:f^n:(f)$.

Remark 2.3.8. For the first terms we have

$$:f^0: = 1\,,\quad :f^1: = f - \mathbb{E}f\,,\quad \text{and} \quad :f^2: = f^2 - 2\mathbb{E}[f]\,f - \mathbb{E}\left[f^2\right] + 2\mathbb{E}[f]^2\ .$$

2.3.4 The isomorphism with the Fock space

Definition 2.3.9. Let $\mathcal{H}_\mathbb{C}$ be a complex Hilbert space, $\vee$ the symmetric tensor product, the *symmetric Fock space* over $\mathcal{H}_\mathbb{C}$ is

$$\Gamma\mathcal{H}_\mathbb{C} = \bigoplus_{n=0}^{+\infty}\Gamma_n\mathcal{H}_\mathbb{C}$$

where $\Gamma_n\mathcal{H}_\mathbb{C} = \mathcal{H}_\mathbb{C}^{\vee n}$ is the Hilbert completion for the norm inherited from the scalar product over $\mathcal{H}_\mathbb{C}$ of the algebraic symmetric n-th power of $\mathcal{H}_\mathbb{C}$, and the sum is also the Hilbert completion of the algebraic sum. We denote by $\Gamma_F\mathcal{H}_\mathbb{C}$ the algebraic sum (but with a completed tensor product) we will eventually refer to this set as the *finite particle vectors.* We define the empty state $\Omega = (1,0,0,\dots) \in \Gamma\mathcal{H}_\mathbb{C}$. The creation $a^*(f)$ and annihilation $a(f)$ operators are defined on $\Gamma_F\mathcal{H}_\mathbb{C}$ by

- $a^*(f)(g^{\vee n}) := (n+1)^{\frac{1}{2}} f \vee g^{\vee n}$,
- $a(f)(g^{\vee n}) := n^{\frac{1}{2}}\langle f, g\rangle\, g^{\vee n-1}$,

for $f,\, g \in \mathcal{H}_{\mathbb{C}}$. The field operator $\Phi(f) = (a^*(f) + a(f))/\sqrt{2}$ is then essentially self-adjoint for $\Gamma_F \mathcal{H}_{\mathbb{C}}$ is a dense set of analytic vectors and we still denote by $\Phi(f)$ its closure.

One can refer to [45] for the following theorem.

Theorem 2.3.10. *Let $\mathcal{H}_{\mathbb{R}}$ be a real Hilbert space and $\mathcal{H}_{\mathbb{C}}$ its complexification. Let Φ_G the general centered Gaussian random field indexed by $\mathcal{H}_{\mathbb{R}}$ over a probability space $(\Omega_{\mathbb{P}}, \mathcal{G}, \mathbb{P})$. The symmetric Fock space $\Gamma\mathcal{H}_{\mathbb{C}}$ is unitarily equivalent to $L^2(\Omega_{\mathbb{P}}, \mathbb{P}; \mathbb{C})$ under a unitary $D : \Gamma\mathcal{H}_{\mathbb{C}} \to L^2(\Omega_{\mathbb{P}}, \mathbb{P}; \mathbb{C})$ such that*

- $D\Omega = 1$,
- $D\Gamma_n\mathcal{H}_{\mathbb{C}} =$ *the closed subspace of* $L^2(\Omega_{\mathbb{P}}, \mathbb{P}; \mathbb{C})$ *generated by*
$$\{ :\Phi_G(f_1)\cdots\Phi_G(f_n): \,,\; f_j \in \mathcal{H}_{\mathbb{R}} \}\ ,$$
- $D\sqrt{2}\Phi(f)\, D^{-1} = \Phi_G(f)$ *for* $f \in \mathcal{H}_{\mathbb{R}}$, *with* $\Phi_G(f)$ *seen as a multiplication operator on* $L^2(\Omega_{\mathbb{P}}, \mathbb{P}; \mathbb{C})$,
- $Df_1 \vee \cdots \vee f_n = \frac{1}{\sqrt{n!}} :\Phi_G(f_1)\cdots\Phi_G(f_n):$ *for* $f_1, \ldots, f_n \in \mathcal{H}_{\mathbb{R}}$.

2.3.5 The expression of the dynamic in the Fock space

We will apply the results of Section 2.3.4 with $\mathcal{H}_{\mathbb{R}} = L^2\left(\mathbb{R}^d_y; \mathbb{R}\right)$ and $\mathcal{H}_{\mathbb{C}} = L^2\left(\mathbb{R}^d_y; \mathbb{C}\right) = L^2_y$ and get an isomorphism

$$D : \Gamma L^2_y \to L^2(\Omega_{\mathbb{P}}, \mathbb{P})\ .$$

We set $\mathrm{Ad}\{A\}[B] = ABA^{-1}$ and for Hilbert spaces $\mathcal{H}$ and $\mathcal{H}'$, $\mathrm{Tr}_{\mathcal{H}'}[A]$ denotes the partial trace of an operator A on $\mathcal{H} \otimes \mathcal{H}'$.

Note that with the stochastic presentation

$$\begin{aligned}
\rho^h_{N,\Delta t} &= \int_{\bar{\Omega}_N} \rho^h_{N,\Delta t}(\bar{\omega}_N)\, \mathrm{d}\mathbb{P}_N(\bar{\omega}_N) \\
&= \int_{\bar{\Omega}_N} \mathrm{Ad}\left[G_{N,\frac{\Delta t}{h},\bar{\omega}_N}\right]\{\rho\}\, \mathrm{d}\mathbb{P}_N(\bar{\omega}_N) \\
&= \int_{\Omega_N} \mathrm{Ad}\left[e^{-i\frac{\Delta t}{h}H_{h,\omega_N}}\right]\left\{ \cdots \int_{\Omega_1} \mathrm{Ad}\left[e^{-i\frac{\Delta t}{h}H_{h,\omega_1}}\right]\{\rho\}\, \mathrm{d}\mathbb{P}(\omega_1)\cdots \right\} \mathrm{d}\mathbb{P}(\omega_N) \\
&= \int_{\Omega_N} \mathrm{Ad}\left[e^{-i\frac{\Delta t}{h}H_{h,\omega_N}}\right]\left\{ \int_{\bar{\Omega}_{N-1}} \rho^h_{N-1,\Delta t}(\bar{\omega}_{N-1})\, \mathrm{d}\mathbb{P}_{N-1}(\bar{\omega}_{N-1}) \right\} \mathrm{d}\mathbb{P}(\omega_N) \\
&= \int_{\Omega_N} \mathrm{Ad}\left[e^{-i\frac{\Delta t}{h}H_{h,\omega_N}}\right]\left\{\rho^h_{N-1,\Delta t}\right\} \mathrm{d}\mathbb{P}(\omega_N)\,.
\end{aligned}$$

The last integral can be expressed using a partial trace as

$$\begin{aligned}
&\int e^{-i\frac{\Delta t}{h}H_{h,\omega}}\rho e^{i\frac{\Delta t}{h}H_{h,\omega}}\,\mathrm{d}\mathbb{P}(\omega) \\
&= \int e^{-i\frac{\Delta t}{h}H_{h,\omega}}\rho 1(\omega)\,1(\omega)\,e^{i\frac{\Delta t}{h}H_{h,\omega}}\,\mathrm{d}\mathbb{P}(\omega) \\
&= \operatorname*{Tr}_{L^2(\Omega_{\mathbb{P}},\mathbb{P})}\left[\int^{\oplus} e^{-i\frac{\Delta t}{h}H_{h,\omega}}\,\mathrm{d}\mathbb{P}(\omega)\,\rho\otimes|1\rangle\langle 1|\int^{\oplus} e^{i\frac{\Delta t}{h}H_{h,\omega'}}\,\mathrm{d}\mathbb{P}(\omega')\right].
\end{aligned}$$

The isomorphism

$$U_{G\leftarrow F} = \mathrm{Id}_{L^2_x}\otimes D : L^2_x\otimes\Gamma L^2_y \to L^2_x\otimes L^2(\Omega_{\mathbb{P}},\mathbb{P})$$

is such that

$$\begin{aligned}
U^{-1}_{G\leftarrow F}\int^{\oplus} e^{-i\frac{\Delta t}{h}H_{h,\omega}}\,\mathrm{d}\mathbb{P}(\omega)\,U_{G\leftarrow F} = e^{-i\frac{\Delta t}{h}H_h}\,, \\
U^{-1}_{G\leftarrow F}\rho\otimes|1\rangle\langle 1|\,U_{G\leftarrow F} = \rho\otimes|\Omega\rangle\langle\Omega|
\end{aligned}$$

with $U^{-1}_{G\leftarrow F}\int^{\oplus} H_{h,\omega}\,\mathrm{d}\mathbb{P}(\omega)\,U_{G\leftarrow F} = H_h$. And thus

$$\begin{aligned}
&\operatorname*{Tr}_{L^2(\Omega_{\mathbb{P}},\mathbb{P})}\left[\int^{\oplus} e^{-i\frac{\Delta t}{h}H_{h,\omega}}\,\mathrm{d}\mathbb{P}(\omega)\,\rho\otimes|1\rangle\langle 1|\int^{\oplus} e^{i\frac{\Delta t}{h}H_{h,\omega'}}\,\mathrm{d}\mathbb{P}(\omega')\right] \\
&\qquad = \operatorname*{Tr}_{\Gamma L^2_y}\left[e^{-i\frac{\Delta t}{h}H_h}\rho\otimes|\Omega\rangle\langle\Omega|\,e^{i\frac{\Delta t}{h}H_h}\right].
\end{aligned}$$

The only thing left is to compute H_h, but $U^{-1}_{G\leftarrow F}\left(\mathcal{V}^h_\omega(x)\times\right)U_{G\leftarrow F} = \Phi_G(\tau_x V)$. We get that in the Fock space formalism

$$\rho^h_{N,\Delta t} = \left(\operatorname*{Tr}_{\Gamma L^2_y}\left[\mathrm{Ad}\left\{e^{-i\frac{\Delta t}{h}H_h}\right\}[\cdot\otimes|\Omega\rangle\langle\Omega|]\right]\right)^N[\rho]$$

with $H_h = U^{-1}_{G\leftarrow F}H_{h,\omega}U_{G\leftarrow F} = -\Delta_x + \sqrt{2h}\,\Phi(\tau_x V)$.

2.3.6 Existence of the dynamic

We will show that the dynamic of the system is well defined and to do so we will show that the Hamiltonian is essentially self-adjoint on a certain domain. We make use of Nelson's commutator theorem which can be found in [43]. Since we work with a fixed $h > 0$ the value of h will be unimportant we take $h = 1$ in this section to clarify our exposition.

Theorem 2.3.11. *Let N' be a self-adjoint operator with $N' \geq 1$. Let H be a symmetric operator with domain D' which is a core for N'. Suppose that:*

1. *For some $C_1 > 0$ and all $u \in D'$,*

$$\|Hu\| \leq C_1\left\|N'u\right\|,$$

2. For some $C_2 > 0$ and all $u \in D'$,

$$\left|\left\langle Hu, N'u\right\rangle - \left\langle N'u, Hu\right\rangle\right| \leq C_2 \left\| N'^{1/2} u \right\|^2 .$$

Then H is essentially self-adjoint on D' and its closure is essentially self-adjoint on any other core for N'.

Let $D' := \mathcal{C}_0^\infty(\mathbb{R}^d) \otimes^{\text{alg}} \Gamma_F L_y^2$ be the domain of both

$$\begin{aligned} N' &= \text{Id} - \Delta_x + N, \\ H &= -\Delta_x + \sqrt{2}\Phi(\tau.V) \end{aligned}$$

where

- $-\Delta_x$ denotes the operator $-\Delta_x \otimes \text{Id}_{\Gamma L_y^2}$,
- N denotes the operator $\text{Id}_{L_x^2} \otimes N$ with N the number operator on ΓL_y^2 and
- $\Phi_F(\tau.V)$ denotes the operator defined on $L^2(\mathbb{R}^d;\Gamma L_y^2) \simeq L^2(\mathbb{R}^d) \otimes \Gamma L_y^2$ by

$$\begin{aligned} L^2(\mathbb{R}^d;\Gamma L_y^2) &\rightarrow L^2(\mathbb{R}^d;\Gamma L_y^2) \\ u &\mapsto \Phi(\tau.V)u \end{aligned}$$

  with $[\Phi(\tau.V)u](x) := [\Phi(\tau_x V)][u(x)]$.

We still denote by N' the closure of the essentially self-adjoint operator N' defined on D'. Then D' is a core for this operator. We remark that $N' \geq I$ on D' and thus also on $D(N')$ as D' is a core for N'.

Proposition 2.3.12. *Suppose that V belongs to $H^2\left(\mathbb{R}^d\right)$. Then the Hamiltonian H satisfies the hypotheses of Theorem 2.3.11.*

Proof. Let $u \in D'$, then

$$\begin{aligned} \|Hu\|_{L_x^2\otimes\Gamma L_y^2} &\leq \|-\Delta_x u\|_{L_x^2\otimes\Gamma L_y^2} + 2\|V\|_{L^2}\left\|\sqrt{N+1}u\right\|_{L_x^2\otimes\Gamma L_y^2}, \\ &\leq (1 + 2\|V\|_{L^2})\left\|N'u\right\|_{L_x^2\otimes\Gamma L_y^2} \end{aligned}$$

which is the first estimate. We also observe that in the sense of quadratic forms

$$\begin{aligned} \left[H, N'\right] &= \sqrt{2}\left[\Phi\left(\tau.V\right), -\Delta_x + N\right], \\ &= \sqrt{2}\Phi\left(\tau.\nabla V\right).\nabla_x + \sqrt{2}\Phi\left(\tau.\Delta V\right) + \left(a^*\left(\tau.V\right) - a\left(\tau.V\right)\right) \end{aligned}$$

so that

$$\begin{aligned} &\left|\left\langle Hu, N'u\right\rangle - \left\langle N'u, Hu\right\rangle\right| \\ &\qquad \leq \left(\sqrt{2}\|\nabla V\|_{L^2} + \sqrt{2}\|\Delta V\|_{L^2} + 2\|V\|_{L^2}\right)\left\|N'^{1/2}u\right\|^2 \end{aligned}$$

which is the second estimate. □

2.4 An approximated equation and its solution

2.4.1 The scaling for field operators

The ε parameter is an intermediate scale which allows to easily identify the graduation in Wick powers. It will in the end be adjusted with respect to h. Let $(D_\varepsilon f)(y) = \varepsilon^{-d/2} f\left(\frac{y}{\varepsilon}\right)$ and

$$H_{h,\varepsilon} = \operatorname{Ad}\left\{\mathrm{Id}_{L^2_x} \otimes \Gamma D_\varepsilon\right\}[H_h] = -\Delta_x \otimes I_{\Gamma_y} + \sqrt{2h}\Phi\left(\varepsilon^{-d/2} V\left(x - \frac{y}{\varepsilon}\right)\right).$$

We now introduce some definitions and notations that will be useful to deal with the Wick quantization and the scaled versions of our objects in the Fock space.

2.4.2 The second quantization

The method of second quantization is exposed in the books [24, 25], an introduction to quantum field theory and second quantization can be found in [31]. The series of articles [34, 35, 36, 37] uses this framework with a small parameter to handle classical or mean field limits by developing the Hepp method [39]. We will use the notation and framework of [22, 23] to handle the second quantization with a small parameter. For the convenience of the reader we expose briefly this framework. We also recall some formulae in Appendix 2.E.1.

Most of our operators on the Fock space will arise as Wick quantizations of polynomials.

Definition 2.4.1. Let $(\mathcal{H}, \langle\cdot,\cdot\rangle)$ be a complex Hilbert space (the scalar product is $\mathbb{C}$-antilinear with respect to the left variable). The symmetric tensor product is denoted by $\vee$. The *polynomials* with variable in $\mathcal{H}$ are the finite linear combinations of monomials $Q : \mathcal{H} \to \mathbb{C}$ of the form

$$Q(z) = \left\langle z^{\vee q}, \tilde{Q} z^{\vee p}\right\rangle$$

where $p, q \in \mathbb{N}$, $\tilde{Q} \in \mathcal{L}(\mathcal{H}^{\vee p}, \mathcal{H}^{\vee q})$ and $\langle\cdot,\cdot\rangle$ denotes the scalar product on $\mathcal{H}^{\vee q}$. The set of such polynomials is denoted by $\mathcal{P}(\mathcal{H})$.

The symmetric *Fock space* associated to $\mathcal{H}$ is

$$\Gamma\mathcal{H} = \bigoplus_{n=0}^{+\infty} \Gamma_n \mathcal{H}$$

with $\Gamma_n\mathcal{H} = \mathcal{H}^{\vee n}$ the completed n-th symmetric power of $\mathcal{H}$ and the sum is completed, the set of *finite particle vectors* $\Gamma_F\mathcal{H}$ is defined as the Fock space but with an algebraic sum.

The *Wick quantization* of a polynomial is defined as the linear combination of the Wick quantizations of its monomials, and for a monomial Q we define $Q^{Wick} : \Gamma_F \mathcal{H} \to \Gamma_F \mathcal{H}$ as the linear operator such that

$$\begin{aligned} Q^{Wick}\Big|_{\mathcal{H}^{\vee n}} &= 1_{[p,+\infty)}(n) \frac{\sqrt{n!\,(n-p+q)!}}{(n-p)!} \varepsilon^{\frac{p+q}{2}} \left(\tilde{Q} \bigvee \mathrm{Id}_{\mathcal{H}^{\vee n-p}}\right) , \\ &\in \mathcal{L}\left(\mathcal{H}^{\vee n}, \mathcal{H}^{\vee n-p+q}\right) . \end{aligned}$$

The field operators $\Phi_\varepsilon(f)$ $(f \in \mathcal{H})$ are defined as the closure of the essentially self-adjoint operators $(\langle z, f\rangle + \langle f, z\rangle)^{Wick} / \sqrt{2}$.

The Weyl operators are then defined by $W(f) = \exp(i\Phi_\varepsilon(f))$. The empty state Ω is $(1, 0, 0, \dots)$ and the coherent states are defined as $E(f) = W\left(\frac{\sqrt{2}}{i\varepsilon} f\right) \Omega$.

Proposition 2.4.2. *For any $Q \in \mathcal{P}(\mathcal{H})$, Q^{Wick} is closable and the domain of its closure contains*

$$\{W(f)\,\phi,\ \phi \in \Gamma_F \mathcal{H},\ f \in \mathcal{H}\} .$$

Definition 2.4.3. For a self-adjoint operator A on $\mathcal{H}$, the self-adjoint operator $d\Gamma_\varepsilon(A)$ is defined by

$$\begin{aligned} \mathrm{d}\Gamma_\varepsilon(A)\big|_{D(A)^{\vee n},\mathrm{alg}} &= \varepsilon n A \vee \mathrm{Id}_{\mathcal{H}}^{\vee n-1} \\ &= \varepsilon\left(A \otimes \mathrm{Id}_{\mathcal{H}} \otimes \cdots \otimes \mathrm{Id}_{\mathcal{H}} + \cdots + \mathrm{Id}_{\mathcal{H}} \otimes \cdots \otimes \mathrm{Id}_{\mathcal{H}} \otimes A\right) \end{aligned}$$

and for a unitary U on $\mathcal{H}$, the unitary operator $\Gamma(U)$ on $\Gamma\mathcal{H}$ is defined by

$$\Gamma(U)|_{\mathcal{H}^{\vee n}} = U^{\vee n} = U \otimes \cdots \otimes U$$

and thus $\Gamma\left(e^{itA}\right) = \exp\left(\frac{it}{\varepsilon} \mathrm{d}\Gamma_\varepsilon(A)\right)$.

2.4.3 Space translation in the fields and Fourier transform

We introduce a notation for an object $X = (X_1, \dots, X_d)$ with d components, like $\xi \in \mathbb{R}^d$, $D_x = (\partial_{x_1}, \dots, \partial_{x_d})$ or $\mathrm{d}\Gamma(D_y)$,

$$X^{.2} := X_1^2 + \cdots + X_d^2 .$$

We would rather have a field operator with no dependence in x. Then we recall that $e^{-ix.D_y} = \tau_x$ and thus

$$\begin{aligned} &\Gamma\left(e^{i\varepsilon x.D_y}\right) H_{h,\varepsilon} \Gamma\left(e^{-i\varepsilon x.D_y}\right) \\ &\quad = D_x^{.2} - 2D_x.\,\mathrm{d}\Gamma_\varepsilon(D_y) + \mathrm{d}\Gamma_\varepsilon(D_y)^{.2} + \sqrt{2}\Phi_\varepsilon\left(\varepsilon^{-d/2}\sqrt{\frac{h}{\varepsilon}} V\left(-\frac{y}{\varepsilon}\right)\right) \end{aligned}$$

where we use an ε-dependent operator $\mathrm{d}\Gamma_\varepsilon$. After a conjugation by the Fourier transform in both the particle and the field variables we get

$$\hat{H}_{h,\varepsilon} = \xi^{\cdot 2} - d\Gamma_\varepsilon\left(2\xi.\eta\right) + d\Gamma_\varepsilon\left(\eta\right)^{\cdot 2} + \sqrt{2}\Phi_\varepsilon\left(f_{h,\varepsilon}\right)$$

with $f_{h,\varepsilon}\left(\eta\right) = \varepsilon^{d/2}\sqrt{\frac{h}{\varepsilon}}\hat{V}\left(-\varepsilon\eta\right)$, *i.e.* $\hat{H}_{h,\varepsilon} = Q_{h,\varepsilon}^{Wick}$ with

$$Q_{h,\varepsilon}\left(z\right) = \xi^{\cdot 2} + \left\langle z, \left(\varepsilon\eta^{\cdot 2} - 2\xi.\eta\right) z\right\rangle + \left\langle z, \eta z\right\rangle^{\cdot 2} + 2\Re\left\langle z, f_{h,\varepsilon}\right\rangle\ .$$

When we neglect the quartic part $\left\langle z, \eta z\right\rangle^{\cdot 2}$ and thus get another polynomial

$$Q_{h,\varepsilon}^{app}\left(z\right) = \xi^{\cdot 2} + \left\langle z, \left(\varepsilon\eta^{\cdot 2} - 2\xi.\eta\right) z\right\rangle + 2\Re\left\langle z, f_{h,\varepsilon}\right\rangle$$

we can solve explicitly the evolution associated with the Hamiltonian

$$\hat{H}_{h,\varepsilon}^{app} = Q_{h,\varepsilon}^{app,Wick} = \xi^{\cdot 2} + \mathrm{d}\Gamma_\varepsilon\left(\varepsilon\eta^{\cdot 2} - 2\xi.\eta\right) + \sqrt{2}\Phi_\varepsilon\left(f_{h,\varepsilon}\right)\ .$$

Definition 2.4.4. Let $\rho \in \mathcal{L}_1\left(L_x^2\right)$, then we define

$$\boldsymbol{\rho}_t = \mathrm{Ad}\left\{e^{-i\frac{t}{\varepsilon}H_{h,\varepsilon}}\right\}\left[\rho \otimes \mathrm{proj}\,\Omega\right]\ , \qquad \boldsymbol{\rho}_t^{app} = \mathrm{Ad}\left\{e^{-i\frac{t}{\varepsilon}H_{h,\varepsilon}^{app}}\right\}\left[\rho \otimes \mathrm{proj}\,\Omega\right]\ ,$$

$$\hat{\boldsymbol{\rho}}_t = \mathrm{Ad}\left\{e^{-i\frac{t}{\varepsilon}\hat{H}_{h,\varepsilon}}\right\}\left[\hat{\rho} \otimes \mathrm{proj}\,\Omega\right]\ , \qquad \hat{\boldsymbol{\rho}}_t^{app} = \mathrm{Ad}\left\{e^{-i\frac{t}{\varepsilon}\hat{H}_{h,\varepsilon}^{app}}\right\}\left[\hat{\rho} \otimes \mathrm{proj}\,\Omega\right]\ ,$$

$$\rho_t^\varepsilon = \underset{\Gamma L_x^2}{\mathrm{Tr}}\,\boldsymbol{\rho}_t\,, \qquad \rho_t^{\varepsilon,app} = \underset{\Gamma L_x^2}{\mathrm{Tr}}\,\boldsymbol{\rho}_t^{app}\,.$$

This definition is consistent with the previous one given for ρ_t^h as $\rho_t^h = \rho_{\frac{\varepsilon}{h}t}^\varepsilon$ and the dilatation acts only in the Fock space part of $L_x^2 \otimes \Gamma L_y^2$.

2.4.4 The approximated equation and its solution

2.4.4.1 Results

Definition 2.4.5. Let $\psi_0 \in L_x^2$. We define

$$\hat{\Psi}_{h,\varepsilon,t} = e^{-i\frac{t}{\varepsilon}\hat{H}_{h,\varepsilon}}\Omega \otimes \hat{\psi}_0 \qquad \text{and} \qquad \hat{\Psi}_{h,\varepsilon,t}^{app} = e^{-i\frac{t}{\varepsilon}\hat{H}_{h,\varepsilon}^{app}}\Omega \otimes \hat{\psi}_0\,.$$

We will show three results in this section.

Proposition 2.4.6. *We have*

$$\hat{\Psi}_{h,\varepsilon,t}^{app} = e^{-i\frac{\omega_{h,\varepsilon,t}}{\varepsilon}}W\left(\frac{\sqrt{2}}{i\varepsilon}z_{h,\varepsilon,t}\right)\Omega \otimes \hat{\psi}_0$$

with $z_{h,\varepsilon,t} = -i\int_0^t e^{-i\frac{s}{\varepsilon}\left(\varepsilon^2\eta^{\cdot 2} - 2\xi.\varepsilon\eta\right)}f_{h,\varepsilon}\,\mathrm{d}s$ *and* $\omega_{h,\varepsilon,t} = t\xi^2 + \int_0^t \Re\left\langle z_s, f_{h,\varepsilon}\right\rangle\mathrm{d}s$.

We have an estimate on the size of z_t.

Proposition 2.4.7. *There exists a constant $C_{G,d}$ depending only on G and the dimension d such that*

$$\left\| |\eta|^{\nu} z_{h,\varepsilon,t} \right\|_{L^2_\eta} \leq C_{G,d} \sqrt{\frac{ht}{\varepsilon}} \varepsilon^{1/2-\nu} .$$

We also have an estimate on the error on $\hat{\Psi}_t$ when considering $\hat{\Psi}_t^{app}$.

Proposition 2.4.8. *Let $T_0 > 0$. There exists a constant $C_{T_0,G,d}$ such that for $\frac{ht}{\varepsilon} \leq T_0$,*

$$\left\| \hat{\Psi}_{h,\varepsilon,t} - \hat{\Psi}^{app}_{h,\varepsilon,t} \right\| \leq C_{T_0,G,d} \left(\frac{ht}{\varepsilon} \right)^2 h^{-1} .$$

2.4.4.2 A transformation

First we get rid of the quadratic part (*i.e.* $\mathrm{d}\Gamma_\varepsilon$).

Definition 2.4.9. Let

$$\tilde{\hat{\Psi}}_{h,\varepsilon,t} = e^{i\frac{t}{\varepsilon}\xi^{.2}} e^{i\frac{t}{\varepsilon} d\Gamma_\varepsilon\left(\varepsilon\eta^{.2} - 2\xi.\eta\right)} \Psi_{h,\varepsilon,t} \text{ and } \tilde{\hat{\Psi}}^{app}_{h,\varepsilon,t} = e^{i\frac{t}{\varepsilon}\xi^{.2}} e^{i\frac{t}{\varepsilon} d\Gamma_\varepsilon\left(\varepsilon\eta^{.2} - 2\xi.\eta\right)} \Psi^{app}_{h,\varepsilon,t} .$$

Proposition 2.4.10. *Then $\tilde{\hat{\Psi}}_t$ (resp. $\tilde{\hat{\Psi}}^{app}_t$) is solution of the equation*

$$i\varepsilon\partial_t \tilde{\Psi}_{h,\varepsilon,t} = \tilde{Q}^{Wick}_{h,\varepsilon} \tilde{\Psi}_{h,\varepsilon,t}$$

(resp. $i\varepsilon\partial_t \tilde{\hat{\Psi}}^{app}_{h,\varepsilon,t} = \tilde{Q}^{app,Wick}_{h,\varepsilon} \tilde{\hat{\Psi}}^{app}_{h,\varepsilon,t}$) with the initial condition $\tilde{\hat{\Psi}}_{h,\varepsilon,t=0} = \Omega$ (resp. $\tilde{\hat{\Psi}}^{app}_{h,\varepsilon,t=0} = \Omega$) and $\tilde{Q}_{h,\varepsilon,t}(z) = 2\Re\langle z, \tilde{f}_{h,\varepsilon,t}\rangle + \langle z, \eta z\rangle^{.2}$ (resp. $\tilde{Q}^{app}_{h,\varepsilon,t}(z) = 2\Re\langle z, \tilde{f}_{h,\varepsilon,t}\rangle$) with $\tilde{f}_{h,\varepsilon,t} = e^{i\frac{t}{\varepsilon}\left(\varepsilon^2\eta^{.2} - 2\xi.\varepsilon\eta\right)} f_{h,\varepsilon}$.

Proof. Indeed

$$\begin{aligned}
i\varepsilon\partial_t \tilde{\hat{\Psi}}_t &= i\varepsilon\partial_t \left[e^{i\frac{t}{\varepsilon}\xi^{.2}} e^{i\frac{t}{\varepsilon}\,\mathrm{d}\Gamma_\varepsilon\left(\varepsilon\eta^{.2} - 2\xi.\eta\right)} \hat{\Psi}_t \right] \\
&= e^{i\frac{t}{\varepsilon}\xi^{.2}} e^{i\frac{t}{\varepsilon}\,\mathrm{d}\Gamma_\varepsilon\left(\varepsilon\eta^{.2} - 2\xi.\eta\right)} \left[2\Re\left\langle z, f\right\rangle + \left\langle z, \eta z\right\rangle^{.2} \right]^{Wick} \hat{\Psi}_t \\
&= \left[2\Re\left\langle z, e^{it\left(\varepsilon\eta^{.2} - 2\xi.\eta\right)} f \right\rangle + \left\langle z, \eta z\right\rangle^{.2} \right]^{Wick} e^{i\frac{t}{\varepsilon}\xi^{.2}} e^{i\frac{t}{\varepsilon} d\Gamma_\varepsilon\left(\varepsilon\eta^{.2} - 2\xi.\eta\right)} \hat{\Psi}_t \\
&= \tilde{Q}^{Wick}_t \tilde{\hat{\Psi}}_t .
\end{aligned}$$

And we can proceed analogously with $\tilde{\Psi}^{app}_t$. □

2.4.4.3 The classical movement associated with the approximated equation

The classical movement is the solution to the equation

$$\begin{cases} i\partial_t \tilde{z}_{h,\varepsilon,t} &= \partial_{\bar{z}} \tilde{Q}_{h,\varepsilon,t}\left(\tilde{z}_{h,\varepsilon,t}\right) = \tilde{f}_{h,\varepsilon,t} \\ \tilde{z}_{h,\varepsilon,t} &= 0 \end{cases} \tag{2.4.1}$$

i.e.

$$\tilde{z}_{h,\varepsilon,t} = -i \int_0^t \tilde{f}_{h,\varepsilon,s}\, \mathrm{d}s = -i \int_0^t e^{i\frac{s}{\varepsilon}\left(\varepsilon^2 \eta^{\cdot 2} - 2\xi.\varepsilon\eta\right)} f_{h,\varepsilon}\, \mathrm{d}s\,.$$

With this simpler dynamics the translation of Proposition 2.4.7 is the following.

Proposition 2.4.11. *There exists a constant $C_{G,d}$ depending only on G and the dimension d such that*

$$\left\| |\eta|^\nu\, \tilde{z}_{h,\varepsilon,t} \right\|_{L^2_\eta} \le C_{G,d} \sqrt{\frac{ht}{\varepsilon}} \varepsilon^{1/2-\nu}\,.$$

Proof. We compute $\left\| |\eta|^\nu\, \tilde{z}_{h,\varepsilon,t} \right\|^2_{L^2_\eta}$

$$\left\| |\eta|^\nu\, \tilde{z}_{h,\varepsilon,t} \right\|^2_{L^2_\eta} = \int_0^t \int_0^t \int_{\mathbb{R}^d_\eta} e^{i\frac{s-s'}{\varepsilon}\left(\varepsilon^2 \eta^{\cdot 2} - 2\xi.\varepsilon\eta\right)} |\eta|^{2\nu} \left|f_{h,\varepsilon}(\eta)\right|^2 \mathrm{d}\eta\, \mathrm{d}s\, \mathrm{d}s'$$

A change of variable $\eta' = \varepsilon\eta - \xi$ gives

$$\int_{\mathbb{R}^d_\eta} e^{i\frac{s-s'}{\varepsilon}\left(\varepsilon^2 \eta^{\cdot 2} - 2\xi.\varepsilon\eta\right)} |\eta|^{2\nu} \left|f_{h,\varepsilon}(\eta)\right|^2 \mathrm{d}\eta$$
$$= \varepsilon^{-2\nu} \frac{h}{\varepsilon} e^{-i\frac{s-s'}{\varepsilon}\xi^{\cdot 2}} \int_{\mathbb{R}^d_\eta} e^{i\frac{s-s'}{\varepsilon}\eta^{\cdot 2}} |\eta+\xi|^{2\nu}\, \hat{G}(\eta+\xi)\, \mathrm{d}\eta$$

as $f_{h,\varepsilon}(\eta) = \varepsilon^{d/2}\sqrt{\frac{h}{\varepsilon}}\hat{V}(-\varepsilon\eta)$ and $\frac{h}{\varepsilon}\hat{G}(\varepsilon\eta)\varepsilon^d = \left|f_{h,\varepsilon}(\eta)\right|^2$.

For $s \ne s'$

$$\left| \int_{\mathbb{R}^d_\eta} e^{i\frac{s-s'}{\varepsilon}\left(\varepsilon^2 \eta^{\cdot 2} - 2\xi.\varepsilon\eta\right)} |\eta|^{2\nu} \left|f_{h,\varepsilon}(\eta)\right|^2 \mathrm{d}\eta \right|$$
$$= \left(\frac{\pi\varepsilon}{s'-s}\right)^{d/2} \varepsilon^{-2\nu} \frac{h}{\varepsilon} \left\| \mathcal{F}\left(\eta \mapsto |\eta+\xi|^{2\nu}\, \hat{G}(\eta+\xi)\right) \right\|_{L^1}$$
$$= \left(\frac{\pi\varepsilon}{s'-s}\right)^{d/2} \varepsilon^{-2\nu} \frac{h}{\varepsilon} \left\| \mathcal{F}\left(\eta \mapsto |\eta|^{2\nu}\, \hat{G}(\eta)\right) \right\|_{L^1}$$

is uniformly bounded by $C_G \varepsilon^{-2\nu}\frac{h}{\varepsilon}$. The squared norm $\left\| |\eta|^\nu\, \tilde{z}^{app}_t \right\|^2_{L^2_\eta}$ is then bounded by

$$\begin{aligned}\left\| |\eta|^\nu\, \tilde{z}_{h,\varepsilon,t} \right\|^2_{L^2_\eta} &\le C_G \frac{h}{\varepsilon}\varepsilon^{-2\nu} \int_0^t \int_0^t \min\left\{ \left(\frac{\pi\varepsilon}{s'-s}\right)^{d/2}, 1 \right\} \mathrm{d}s\, \mathrm{d}s' \\ &\le C_G \frac{h}{\varepsilon}\varepsilon^{-2\nu} \left[\pi^{d/2}\varepsilon^{d/2} \int_{|s-s'|\ge 2\delta, s, s'\in[0,t]} \frac{ds ds'}{(s'-s)^{d/2}} + 2\sqrt{2}t\delta \right] \\ &\le C_G \frac{h}{\varepsilon}\varepsilon^{-2\nu} \left[\pi^{d/2}\varepsilon^{d/2} 2^{d/4} 2\sqrt{2} t \frac{2}{d-2}\delta^{1-d/2} + 2\sqrt{2}t\delta \right]\end{aligned}$$

which is optimal when $\delta = \varepsilon$. This ends the proof. □

Remark 2.4.12. The same estimate holds for z_t with a similar proof.

2.4.4.4 Resolution of the approximated solution and comparison with the exact solution

Proposition 2.4.13. *The solution to the equation*

$$i\varepsilon\partial_t \tilde{\Psi}^{app}_{h,\varepsilon,t} = \tilde{Q}^{app,Wick}_{h,\varepsilon} \tilde{\Psi}^{app}_{h,\varepsilon,t}$$

with initial data $\tilde{\Psi}^{app}_{h,\varepsilon,t=0} = \Omega$ *is*

$$\tilde{\Psi}^{app}_{h,\varepsilon,t} = e^{-i\frac{\tilde{\omega}_{h,\varepsilon,t}}{\varepsilon}} W\left(\frac{\sqrt{2}}{i\varepsilon}\tilde{z}_{h,\varepsilon,t}\right)\Omega$$

with $\tilde{\omega}_{h,\varepsilon,t} = \int_0^t \Re\left\langle \tilde{z}_{h,\varepsilon,s}, \tilde{f}_{h,\varepsilon,s}\right\rangle \mathrm{d}s$.

Proof. Indeed let us apply $i\varepsilon\partial_t$ to the term on the right hand side:

$$\begin{aligned}
& i\varepsilon\partial_t e^{-i\frac{\tilde{\omega}_t}{\varepsilon}} W\left(\frac{\sqrt{2}}{i\varepsilon}\tilde{z}_t\right)\Omega \\
&= \left(\partial_t\tilde{\omega} - i\varepsilon\frac{i\varepsilon}{2}\Im\left\langle \frac{\sqrt{2}}{i\varepsilon}\tilde{z}_t, -\frac{\sqrt{2}}{\varepsilon}\tilde{f}_t\right\rangle + i\varepsilon i\Phi\left(-\frac{\sqrt{2}}{\varepsilon}\tilde{f}_t\right)\right) e^{-i\frac{\omega_t}{\varepsilon}} W\left(\frac{\sqrt{2}}{i\varepsilon}\tilde{z}_t\right)\Omega \\
&= \left(\partial_t\tilde{\omega} - \Im\left\langle \frac{1}{i}\tilde{z}_t, \tilde{f}_t\right\rangle + \sqrt{2}\Phi\left(\tilde{f}_t\right)\right)\tilde{\hat{\Psi}}^{app}_t
\end{aligned}$$

since $\frac{1}{t}\left\langle \varphi, \left[W(z+tu) - W(z)\right]\psi\right\rangle \xrightarrow[t\to 0]{} \left\langle \varphi, \left[-\frac{i\varepsilon}{2}\Im\langle z, u\rangle + i\Phi(u)\right] W(z)\psi\right\rangle$. □

We then compare $\tilde{\Psi}_t$ and $\tilde{\Psi}^{app}_t$.

Proposition 2.4.14. *Let* $\Delta\tilde{\hat{\Psi}}_{h,\varepsilon,t} = \tilde{\hat{\Psi}}_{h,\varepsilon,t} - \tilde{\hat{\Psi}}^{app}_{h,\varepsilon,t}$ *and* $\Delta\tilde{Q}_t(z) = \langle z, \eta z\rangle^{\cdot 2}$, *then*

$$\Delta\tilde{\hat{\Psi}}_{h,\varepsilon,t} = -\frac{i}{\varepsilon}\int_0^t e^{-i\frac{t-s}{\varepsilon}\tilde{Q}^{Wick}_{h,\varepsilon}} \Delta\tilde{Q}^{Wick}\tilde{\hat{\Psi}}^{app}_{h,\varepsilon,s}\,\mathrm{d}s\,.$$

Proof. It suffices to remark that

$$i\varepsilon\partial_t\Delta\tilde{\hat{\Psi}}_t = \tilde{Q}^{Wick}\Delta\tilde{\hat{\Psi}}_t + \Delta\tilde{Q}^{Wick}\tilde{\hat{\Psi}}^{app}_t$$

and that the integral expression satisfies the same differential equation. □

Proposition 2.4.15. *The difference* $\Delta\tilde{\hat{\Psi}}_{h,\varepsilon,t}$ *can be controlled as*

$$\left\|\Delta\tilde{\hat{\Psi}}_{h,\varepsilon,t}\right\| \le \frac{1}{\varepsilon}\int_0^t \left\|\Delta\tilde{Q}^{Wick}\tilde{\hat{\Psi}}^{app}_{h,\varepsilon,s}\right\|\mathrm{d}s = \frac{1}{\varepsilon}\int_0^t \left\|\Delta\tilde{Q}^{Wick}E\left(\tilde{z}_{h,\varepsilon,s}\right)\right\|\mathrm{d}s\,.$$

Proposition 2.4.16. *Let $T_0 > 0$.* There exists a constant $C_{T_0,G,d}$ such that for $\frac{ht}{\varepsilon} \leq T_0$,

$$\left\| \Delta\tilde{Q}^{Wick} E\left(\tilde{z}^{app}_{h,\varepsilon,t}\right)\right\| \leq C_{T_0,G,d}\frac{ht}{\varepsilon}\,.$$

Proof. We make use of the relation valid for coherent states

$$\left\langle E(\tilde{z}_{h,\varepsilon,t}), \left(\Delta\tilde{Q}^{Wick}\right)^{*}\Delta\tilde{Q}^{Wick}E(\tilde{z}_{h,\varepsilon,t})\right\rangle = \overset{Wick}{\mathrm{Symb}}\left(\left(\Delta\tilde{Q}^{Wick}\right)^{*}\Delta\tilde{Q}^{Wick}\right)(\tilde{z}_{h,\varepsilon,t})\,.$$

Since

$$\overset{Wick}{\mathrm{Symb}}\left(\left(\left(\langle z,\eta z\rangle^{.2}\right)^{Wick}\right)^{2}\right)$$
$$= \left(\langle z,\eta z\rangle^{.2}\right)^{2} + 4\varepsilon\left(\langle z,\eta z\rangle\,.\,\langle \eta z|\right)\left(|\eta z\rangle\,.\,\langle z,\eta z\rangle\right) + 2\varepsilon^{2}\left(\langle \eta z|^{.\otimes 2}\right)\left(|\eta z\rangle^{.\otimes 2}\right)\,,$$

using Proposition 2.4.11, we obtain that

$$\left\|\Delta\tilde{Q}^{Wick}E\left(\tilde{z}_{h,\varepsilon,t}\right)\right\|^{2} \leq C_{T_0,G,d}\left(\left(\frac{ht}{\varepsilon}\right)^{4} + 4\varepsilon\left(\frac{ht}{\varepsilon}\right)^{2}\frac{ht}{\varepsilon^{2}} + 2\varepsilon^{2}\left(\frac{ht}{\varepsilon^{2}}\right)^{2}\right)$$

which gives the result for $\frac{ht}{\varepsilon} \leq T_0$. □

Proposition 2.4.17. *Let $T_0 > 0$.* There exists a constant $C_{T_0,G,d}$ such that for $\frac{ht}{\varepsilon} \leq T_0$,

$$\begin{aligned}\left\|\Delta\tilde{\tilde{\Psi}}_{h,\varepsilon,t}\right\| &\leq \frac{1}{\varepsilon}\int_0^t \left\|\Delta\tilde{Q}^{Wick}E\left(\tilde{z}_{h,\varepsilon,t}\right)\right\|\mathrm{d}s\\ &\leq C_{T_0,G,d}h^{-1}\left(\frac{ht}{\varepsilon}\right)^{2}\,.\end{aligned}$$

2.5 Measure of an observable at a mesoscopic scale for the approximated dynamics

2.5.1 Result

In this section we make the connection with the linear Boltzmann equation.

Let b be a symbol in $\mathcal{C}_0^\infty(\mathbb{R}^{2d}_{x,\xi})$ and $\rho \in \mathcal{L}_1^+ L^2_x$, $\mathrm{Tr}\,\rho = 1$. The measure of the observable $b^W(hx, D_x)$ in the state ρ is denoted by

$$m\left(b,\rho\right) \;=\; \mathrm{Tr}\left[b^W\left(hx,D_x\right)\rho\right]\,.$$

Proposition 2.5.1. *Let b be a symbol in $\mathcal{C}_0^\infty(\mathbb{R}^d_x \times \mathbb{R}^{d*}_\xi)$ and $\rho \in \mathcal{L}_1^+ L^2_x$, $\mathrm{Tr}\,\rho \leq 1$ such that the kernel of $\hat{\rho} = \mathrm{Ad}\left\{\mathcal{F}_x\right\}[\rho]$ has a bounded support. Let $\alpha \in [0,1[$. Introduce the symbol $b_t = e^{tQ}e^{2t\xi.\partial_x}b$ where Q is the collision* *operator introduced in Equation 2.2.1 with here* $\sigma(\xi,\xi') = 2\pi\hat{G}(\xi'-\xi) = 2\pi|\hat{V}(\xi-\xi')|^2$. *When* $h^\alpha \leq \frac{ht}{\varepsilon} \leq 1$, *the inequality*

$$m\left(b, \rho_t^{\varepsilon,app}\right) \geq m\left(b_{\frac{ht}{\varepsilon}}, \rho\right) - \mathcal{E}_{2.5}$$

then holds with $\mathcal{E}_{2.5} = C_{b,\mu}\frac{ht}{\varepsilon}\left(\frac{ht}{\varepsilon} + h + \left[h\left(\frac{ht}{\varepsilon}\right)^{-1}\right]^{d/2-1} + h^{\mu(d,\alpha)}\right)$ *for some constant* $C_{b,\mu} > 0$ *and* $\mu(d,\alpha) > 0$.

Remark 2.5.2. This result also holds with b a symbol in $\mathcal{C}_0^\infty(\mathbb{R}_\xi^{d*};\mathbb{C})$. The proof is the same as for Proposition 2.5.1, with the symplectic Fourier transform $\mathcal{F}^\sigma$ replaced by the usual Fourier transform. The special case when $b(\xi) = b_1(|\xi|^2)$ is of particular interest and the symbol b_t in the previous statement does not depend on t.

Proposition 2.5.1 is a by-product of the following stronger result.

Proposition 2.5.3. *Let* $b_s \in \mathcal{C}^1(\mathbb{R};\mathcal{D}(\mathbb{R}^{2d}_{x,\xi}))$ *such that for some* $R > 1$, $\forall s$, $\mathrm{Supp}_\xi\, b_s \subset B_R - B_{R^{-1}}$. *Let* $\rho \in \mathcal{L}_1^+ L_x^2$, $\mathrm{Tr}\,\rho \leq 1$ *such that the kernel of* $\hat{\rho} = \mathrm{Ad}\{\mathcal{F}_x\}[\rho]$ *has a bounded support. Then*

$$\begin{aligned} &m\left(b_{\frac{ht}{\varepsilon}}, \rho_t^{\varepsilon,app}\right) \\ &\geq m(b,\rho) - \frac{i}{\varepsilon}\int_0^t m\left(i\varepsilon\partial_s b_s - ih\left\{b_s, \xi^{.2}\right\} + ihQ_{-\frac{ht}{\varepsilon}} b_s, \rho_s^{\varepsilon,app}\right)\mathrm{d}s - \mathcal{E}_{2.5}\,. \end{aligned}$$

Remark 2.5.4. The conservation of the support in ξ is important and will be provided by the properties of the dual linear Boltzmann equation in the application of this proposition.

Proof that Proposition 2.5.3 implies Proposition 2.5.1. Since one can make mistakes between the notations of those two propositions we use notations with tildes, $\tilde{b}$ for Proposition 2.5.1 and without tildes for Proposition 2.5.3. Thus we want

$$\tilde{b} = b_{\frac{ht}{\varepsilon}}\,, \qquad \tilde{b}_{\frac{ht}{\varepsilon}} = b\,.$$

Denote by $\tilde{G}(t,t_0)$ the dynamical system associated with $(-2\xi.\partial_x - Q_{-t})_t$ given by

$$\begin{cases} \partial_t b_t &= (-2\xi.\partial_x - Q_{-t})\, b_t \\ b_{t=t_0} &= b_0 \end{cases}, \qquad b_t = \tilde{G}(t,t_0)\, b_0\,.$$

To have a vanishing term for b in the integral we require $b_{ht/\varepsilon} = \tilde{G}(\frac{ht}{\varepsilon},0)b$, so that with $\tilde{b}_{ht/\varepsilon} = \tilde{G}(0,-\frac{ht}{\varepsilon})\tilde{b}$, we will get the expected result. The only thing remaining to prove is $\tilde{G}(0,-t) = e^{tQ}e^{2t\xi.\partial_x}$. It is equivalent to show that

$$e^{2t\xi.\partial_x}\tilde{G}(t,0) = e^{-tQ}\,,$$

which is clear by derivation and using that $Q_t = e^{t2\xi.\partial_x}Qe^{-t2\xi.\partial_x}$. □

2.5.2 Expression of the measure of an observable for the approximated equation

We carry out an explicit computation using only the approximated equation. We recall (see Proposition 2.4.13) that the solution of the approximated equation with initial data $\Psi^{app}_{t=0} = \psi_0 \otimes \Omega$ is (after translation and Fourier transform)

$$\hat{\Psi}^{app}_{h,\varepsilon,t} = \hat{\psi}_0(\xi)\, e^{-i\frac{\omega^{\xi}_{h,\varepsilon,t}}{\varepsilon}} W\left(\frac{\sqrt{2}}{i\varepsilon} z^{\xi}_{h,\varepsilon,t}\right)\Omega$$

with $z_{h,\varepsilon,t} = -i\int_0^t e^{-i\frac{s}{\varepsilon}\left(\varepsilon^2\eta^{\cdot 2} - 2\xi.\varepsilon\eta\right)} f_{h,\varepsilon}\,\mathrm{d}s$ and $\omega_t = t\xi^2 + \int_0^t \Re\langle z_{h,\varepsilon,s}, f_{h,\varepsilon}\rangle\,\mathrm{d}s$ and $f_{h,\varepsilon}(\eta) = \varepsilon^{d/2}\sqrt{\frac{h}{\varepsilon}}\hat{V}(-\varepsilon\eta)$.

Definition 2.5.5. Let $\sigma(X_1, X_2) = \xi_1.x_2 - x_1.\xi_2$ ($X_j = (x_j, \xi_j) \in \mathbb{R}^{2d}_{x,\xi}$) be the standard symplectic form on $\mathbb{R}^{2d}_{x,\xi}$.

Let $X' = (x', \xi') \in \mathbb{R}^{2d}_{x,\xi}$, the Weyl operators on L^2_x are defined by

$$\tau^h_{X'} = \left(e^{-i\sigma(\cdot,X')}\right)^W (hx, D_x) = e^{-i\sigma(\cdot,X')^W(hx,D_x)} = e^{i(\xi'\cdot hx - x'\cdot D_x)},$$

their Fourier transform is denoted by $\hat{\tau}^h_P := \mathrm{Ad}\{\mathcal{F}_x\}\left[\tau^h_P\right]$.

The symplectic Fourier transform $\mathcal{F}^\sigma$ is defined on $L^2\left(\mathbb{R}^{2d}_{x,\xi};\mathbb{C}\right)$ by

$$\mathcal{F}^\sigma b(X) = \int_{\mathbb{R}^{2d}} e^{-i\sigma(X,X')} b(X')\,\text{đ}X'$$

with $\text{đ}X = \mathrm{d}X/(2\pi)^d$.

Proposition 2.5.6. *Let b be a symbol in $\mathcal{C}^\infty_0\left(\mathbb{R}^{2d}_{x,\xi}\right)$ and $\rho \in \mathcal{L}^+_1 L^2_x$, $\mathrm{Tr}\,\rho \le 1$, then*

$$m\left(b, \rho^{\varepsilon,app}_t\right) = \iiint \mathcal{F}^\sigma b(P)\, e^{-\frac{i[\omega]+[\varphi]_1-[\varphi,p_x]_2}{\varepsilon}}\, \hat{\tau}^h_P(\xi_2,\xi_1)\,\hat{\rho}(\xi_1,\xi_2)\,\mathrm{d}\xi_1\,\mathrm{d}\xi_2\,\text{đ}P$$

with

$$\begin{aligned}
[\omega] &= \omega^{\xi_1}_t - \omega^{\xi_2}_t && (2.5.1)\\
[\varphi]_1 &= [\varphi]_{1,1} + [\varphi]_{1,2} && (2.5.2)\\
[\varphi]_{1,j} &= \frac{1}{2}|z^{\xi_j}_t|^2,\ j = 1,2 && (2.5.3)\\
[\varphi, p_x]_2 &= \left\langle z^{\xi_2}_t, e^{ip_x\cdot\varepsilon\eta} z^{\xi_1}_t\right\rangle. && (2.5.4)
\end{aligned}$$

Remark 2.5.7. From $e^{i\varepsilon x.\lambda}\tau_P^h e^{-i\varepsilon x.\lambda} = e^{i\varepsilon\lambda.p_x}\tau_P^h$ and taking λ as the spectral parameter of $\mathrm{d}\Gamma_\varepsilon(D_y)$,

$$\Gamma\left(e^{i\varepsilon x.D_y}\right)\tau_P^h\Gamma\left(e^{-i\varepsilon x.D_y}\right) = \Gamma\left(e^{ip_x\cdot\varepsilon D_y}\right)\tau_P^h$$

and after conjugating with the Fourier transforms, we obtain

$$\mathrm{Ad}\left\{(\mathcal{F}_x\otimes\Gamma\mathcal{F}_y)\Gamma\left(e^{i\varepsilon x D_y}\right)\right\}\left[\tau_P^h\right] = \Gamma\left(e^{ip_x\cdot\varepsilon\eta}\right)\hat{\tau}_P^h\,.$$

Proof. As $b^W(hx, D_x) = \int\mathcal{F}^\sigma b(P)\,\tau_P^h\,đP$, we have for $\rho\in\mathcal{L}_1^+$

$$m(b,\rho) = \int\mathcal{F}^\sigma b(P)\,\mathrm{Tr}\left[\tau_P^h\rho\right]đP\,.$$

By translating and Fourier transforming we get the expression

$$m(b,\rho_t^{\varepsilon,app}) = \int\mathcal{F}^\sigma b(P)\,\mathrm{Tr}\left[\hat{\boldsymbol{\rho}}_t^{app}\Gamma\left(e^{ip_x\cdot\varepsilon\eta}\right)\hat{\tau}_P^h\right]đP\,.$$

We conclude with the Lemma 2.5.8 below. □

Lemma 2.5.8. *The kernel K_P of the operator $\mathrm{Tr}_{\Gamma L^2_\eta}[\hat{\boldsymbol{\rho}}_t^{app}\Gamma(e^{ip_x\cdot\varepsilon\eta})]$ on L^2_ξ is*

$$K_P(\xi_1,\xi_2) = e^{-i\frac{\omega_{h,\varepsilon,t}^{\xi_1}-\omega_{h,\varepsilon,t}^{\xi_2}}{\varepsilon}}\hat{\rho}(\xi_1,\xi_2)e^{-|z_{h,\varepsilon,t}^{\xi_1}|^2/2\varepsilon-|z_{h,\varepsilon,t}^{\xi_2}|^2/2\varepsilon+\frac{1}{\varepsilon}\langle z_{h,\varepsilon,t}^{\xi_2},e^{ip_x\cdot\varepsilon\eta}z_{h,\varepsilon,t}^{\xi_1}\rangle}\,.$$

Proof. Using $\hat{\rho}\otimes|\Omega\rangle\langle\Omega| = \int_{\xi_1}^\oplus\int_{\xi_2}^\oplus\hat{\rho}(\xi_1,\xi_2)|\Omega\rangle\langle\Omega|\,\mathrm{d}\xi_1\,\mathrm{d}\xi_2$ we get

$$\begin{aligned}&\mathop{\mathrm{Tr}}_{\Gamma L^2_\eta}\left[\hat{\boldsymbol{\rho}}_t^{app}\Gamma(e^{ip_x\cdot\varepsilon\eta})\right]\\ &= \mathop{\mathrm{Tr}}_{\Gamma L^2_\eta}\left[\int_{\mathbb{R}^d_{\xi_1}}^\oplus\int_{\mathbb{R}^d_{\xi_2}}^\oplus\left|E(z_t^{\xi_1})\right\rangle\left\langle E(z_t^{\xi_2})\right|e^{-i\frac{\omega_t^{\xi_1}}{\varepsilon}}e^{i\frac{\omega_t^{\xi_2}}{\varepsilon}}\hat{\rho}(\xi_1,\xi_2)\,\mathrm{d}\xi_1\,\mathrm{d}\xi_2\Gamma(e^{ip_x\cdot\varepsilon\eta})\right]\end{aligned}$$

and by the rules of calculus on coherent states we obtain

$$\begin{aligned}K_P(\xi_1,\xi_2) &= e^{-i\frac{\omega_t^{\xi_1}-\omega_t^{\xi_2}}{\varepsilon}}\hat{\rho}(\xi_1,\xi_2)\left\langle E\left(z_t^{\xi_2}\right)\right|\Gamma\left(e^{ip_x\cdot\varepsilon\eta}\right)\left|E\left(z_t^{\xi_1}\right)\right\rangle\\ &= e^{-i\frac{\omega_t^{\xi_1}-\omega_t^{\xi_2}}{\varepsilon}}\hat{\rho}(\xi_1,\xi_2)\,e^{-\left|z_t^{\xi_1}\right|^2/2\varepsilon-\left|z_t^{\xi_2}\right|^2/2\varepsilon+\frac{1}{\varepsilon}\left\langle z_t^{\xi_2},e^{ip_x\cdot\varepsilon\eta}z_t^{\xi_1}\right\rangle}\end{aligned}$$

which is the result of the Lemma. □

Definition 2.5.9. For $j = \{,\},-,+$ we define

$$m_j = \int_{\mathbb{R}^{2d}_P}\mathcal{F}^\sigma b(P)\,\mathrm{Tr}\left[\hat{\boldsymbol{\rho}}_t^{app}\Gamma\left(e^{ip_x\cdot\varepsilon\eta}\right)\mathscr{A}_{j,P}\right]đP$$

where the operators $\mathscr{A}_{j,P}$ are defined by their kernels, according to the notations of Equations (2.5.1), (2.5.2), (2.5.3) and (2.5.4),

$$ih\mathscr{A}_{\{,\},P}(\xi_1,\xi_2) = \hat{\tau}_P^h(\xi_2,\xi_1)\,\partial_t[\omega]\ , \tag{2.5.5}$$

$$ih\mathscr{A}_{\{,\},j,P}(\xi_j) = \hat{\tau}_P^h(\xi_2,\xi_1)\,\partial_t\omega_t^{\xi_j}\ ,\ j=1,2\,, \tag{2.5.6}$$

$$ih\mathscr{A}_{-,P}(\xi_1,\xi_2) = i\partial_t[\varphi]_1\,\hat{\tau}_P^h(\xi_2,\xi_1)\ , \tag{2.5.7}$$

$$ih\mathscr{A}_{-,j,P}(\xi_j) = i\partial_t[\varphi]_{1,j}\,\hat{\tau}_P^h(\xi_2,\xi_1)\ ,\ j=1,2\,, \tag{2.5.8}$$

$$ih\mathscr{A}_{+,P}(\xi_1,\xi_2) = i\partial_t[\varphi,p_x]_2\,\hat{\tau}_P^h(\xi_2,\xi_1) \tag{2.5.9}$$

and $\mathscr{A}_{\{,\}} = \mathscr{A}_{\{,\},1} - \mathscr{A}_{\{,\},2}$, $\mathscr{A}_{-} = \mathscr{A}_{-,1} + \mathscr{A}_{-,2}$.

The indexes $\{,\}$, $-$ and $+$ were chosen to recall the terms of the linear Boltzmann equation, $\{,\}$ corresponding to $\left\{\xi^2,\cdot\right\}$, $+$ to Q_+ and $-$ to Q_-.

Proposition 2.5.10. *Let $b_t \in \mathcal{C}^1(\mathbb{R};\mathcal{C}_0^\infty(\mathbb{R}^{2d}_{x,\xi}))$, then the equality*

$$i\varepsilon\partial_t m\left(b_t,\rho_t^{\varepsilon,app}\right) = m\left(i\varepsilon\partial_t b_t,\rho_t^{\varepsilon,app}\right) + ih\left(m_{\{,\}} - m_- + m_+\right)$$

holds.

Remark 2.5.11. Later we will put each of those terms m_j in the form

$$m_j = m\left(c_j,\rho_t^{\varepsilon,app}\right) + \Delta_j$$

where Δ_j denotes a small error term.

Proof of Proposition 2.5.10. Indeed

$$\begin{aligned}
&i\varepsilon\partial_t m\left(b,\rho_t^{\varepsilon,app}\right)\\
&\quad= \iiint_{P,\xi_1,\xi_2}\left[\mathcal{F}^\sigma i\varepsilon\partial_t b(P) + \mathcal{F}^\sigma b(P)\left\{\partial_t[\omega] - i\partial_t[\varphi]_1 + i\partial_t[\varphi,p_x]_2\right\}\right]\\
&\qquad\qquad e^{-\frac{i[\omega]+[\varphi]_1-[\varphi,p_x]_2}{\varepsilon}}\,\hat{\tau}_P^h(\xi_2,\xi_1)\,\hat{\rho}(\xi_1,\xi_2)\,\mathrm{d}\xi_1\,\mathrm{d}\xi_2\,\text{đ}P
\end{aligned}$$

and so it suffices to prove the following lemma. □

Lemma 2.5.12. *For $j = \{,\}$, $-$, $+$, the formula*

$$\operatorname{Tr}\left[\hat{\boldsymbol{\rho}}_t^{app}\Gamma\left(e^{ip_x\cdot\varepsilon\eta}\right)\mathscr{A}_{j,P}\right] = \iint \mathscr{A}_j(P,\xi_1,\xi_2)\,e^{-\frac{i[\omega]+[\varphi]_1-[\varphi,p_x]_2}{\varepsilon}}\,\hat{\rho}(\xi_1,\xi_2)\,\mathrm{d}\xi_1\,\mathrm{d}\xi_2$$

holds.

Proof. Indeed

$$\begin{aligned}
&\operatorname{Tr}\left[\hat{\boldsymbol{\rho}}_t^{app}\Gamma\left(e^{ip_x\cdot\varepsilon\eta}\right)\mathscr{A}_{j,P}\right]\\
&= \iint \hat{\rho}(\xi_1,\xi_2)\left\langle E\left(z_t^{\xi_2}\right)\middle|\,\Gamma\left(e^{ip_x\cdot\varepsilon\eta}\right)\middle|E\left(z_t^{\xi_1}\right)\right\rangle e^{-i\frac{\omega_t^{\xi_1}-\omega_t^{\xi_2}}{\varepsilon}}\,\mathscr{A}_j(P,\xi_1,\xi_2)\,\mathrm{d}\xi_1\,\mathrm{d}\xi_2\\
&= \iint \hat{\rho}(\xi_1,\xi_2)\,e^{-\frac{i[\omega]+[\varphi]_1+[\varphi,p_x]_2}{\varepsilon}}\,\mathscr{A}_j(P,\xi_1,\xi_2)\,\mathrm{d}\xi_1\,\mathrm{d}\xi_2\,.
\end{aligned}$$

□

2.5.3 Two estimates

We will need several times these estimates to get rid of the term $\Gamma(e^{ip_x\cdot\varepsilon\eta})$ and then control small errors on the operators $\mathcal{A}_P$.

Proposition 2.5.13. *Let $\mathscr{A}_P$ be a P-dependent family of operators in $\mathcal{L}(L^2_\xi)$. Then*

$$\langle P\rangle^{-k}\left|\mathrm{Tr}\left[\hat{\boldsymbol{\rho}}_t^{app}\left(\Gamma\left(e^{ip_x\cdot\varepsilon\eta}\right)-\mathrm{Id}\right)\mathscr{A}_P\right]\right|\leq\frac{ht}{\varepsilon}\sup_{P\in\mathbb{R}^{2d}}\langle P\rangle^{-k}\left\|\mathscr{A}_P\right\|_{\mathcal{L}\left(L^2_\xi\right)}$$

and

$$\left|\int_{\mathbb{R}^{2d}_P}\mathcal{F}^\sigma b\left(P\right)\mathrm{Tr}\left[\hat{\boldsymbol{\rho}}_t^{app}\left(\Gamma\left(e^{ip_x\cdot\varepsilon\eta}\right)-\mathrm{Id}\right)\mathscr{A}_P\right]đP\right|$$
$$\leq\frac{ht}{\varepsilon}\left\|\langle\cdot\rangle^k\mathcal{F}^\sigma b\right\|_{L^1_P}\sup_P\langle P\rangle^{-k}\left\|\mathscr{A}_P\right\|_{\mathcal{L}\left(L^2_\xi\right)}.$$

This can be proved in two steps.

Remark 2.5.14. It suffices to prove this property with $\rho=|\psi\rangle\langle\psi|$ with a $\hat{\psi}$ with bounded support as any $\rho\in\mathcal{L}_1^+L^2_x$, $\mathrm{Tr}\,\rho=1$ can be decomposed as

$$\rho=\sum_{j\geq 0}\lambda_j\left|\psi_j\right\rangle\left\langle\psi_j\right|$$

with positive λ_j's and $\sum_j\lambda_j=1$, and

$$\mathrm{Supp}\,\hat{\rho}\left(\xi,\xi'\right)\subset B_M^2\Leftrightarrow\forall j,\ \mathrm{Supp}\,\hat{\psi}_j\subset B_M\,.$$

Lemma 2.5.15. *Let $\mathscr{A}_P$ be a P-dependent family of operators in $\mathcal{L}(L^2_\eta)$ and $\hat{\Psi}$ be a normed vector in $L^2_\xi\otimes\Gamma L^2_\eta$. Then*

$$\left|\mathrm{Tr}\left[\mathrm{proj}\,\hat{\Psi}\left(\Gamma\left(e^{ip_x\cdot\varepsilon\eta}\right)-\mathrm{Id}\right)\mathscr{A}_P\right]\right|\leq\left\|\left(\Gamma\left(e^{ip_x\cdot\varepsilon\eta}\right)-\mathrm{Id}\right)\hat{\Psi}\right\|\left\|\mathscr{A}_P\right\|_{\mathcal{L}\left(L^2_\xi\right)}.$$

Lemma 2.5.16. *There exists a constant $C_{G,d}$ which depends only on G and d such that*

$$\left\|\left(\Gamma\left(e^{ip_x\cdot\varepsilon\eta}\right)-\mathrm{Id}\right)\hat{\Psi}^{app}_{h,\varepsilon,t}\right\|\leq C_{G,d}\frac{ht}{\varepsilon}\,.$$

Proof. The calculus rules on coherent states give

$$\begin{aligned}\left\|\left(\Gamma\left(e^{ip_x\cdot\varepsilon\eta}\right)-\mathrm{Id}\right)\hat{\Psi}^{app}_{h,\varepsilon,t}\right\|^2&=\sup_\xi\left\|E\left(e^{ip_x\cdot\varepsilon\eta}z^\xi_{h,\varepsilon,t}\right)-E\left(z^\xi_{h,\varepsilon,t}\right)\right\|^2\\&=\sup_\xi 2\left(1-\cos\left(\frac{1}{\varepsilon}\Im\left\langle e^{ip_x.\varepsilon\eta}z^\xi_{h,\varepsilon,t},z^\xi_{h,\varepsilon,t}\right\rangle\right)\right)\\&\leq C_{G,d}\left(\frac{ht}{\varepsilon}\right)^2,\end{aligned}$$

where the last inequality is obtained using $|1-\cos t|\leq t^2/2$ and the estimates on $\|z_t\|$. □

Proposition 2.5.17. *Let $\mathscr{E}_P$ be a P-dependent family of operators in $\mathcal{L}(L^2_\xi)$ and $\hat{\boldsymbol{\rho}}$ be a state on $L^2_\xi \otimes \Gamma L^2_\eta$. Then for any integer k (with possibly infinite quantities)*

$$\left| \int_{\mathbb{R}^{2d}_P} \mathcal{F}^\sigma b\,(P)\,|\mathrm{Tr}\,[\hat{\boldsymbol{\rho}}\mathscr{E}_P]|\,\text{đ}P \right| \leq \left\| \langle \cdot \rangle^k \mathcal{F}^\sigma b \right\|_{L^1_P} \sup_P \left\| \langle P \rangle^{-k} \mathscr{E}_P \right\|_{\mathcal{L}(L^2_\xi)} .$$

2.5.4 The transport term $m_{\{,\}}$

The result of this section is the following.

Proposition 2.5.18. *Let $\rho \in \mathcal{L}^+_1 L^2_x$, $\mathrm{Tr}\,\rho \leq 1$ and $b \in \mathcal{C}^\infty_0(\mathbb{R}^{2d}_{x,\xi})$ such that $\mathrm{Supp}\,\hat{\rho}(\xi,\xi') \subset B^2_R$, and $\mathrm{Supp}_\xi\, b \subset B_R$ for some $R > 0$ then*

$$m_{\{,\}} = m\left(-\left\{b, \xi^{\cdot 2}\right\}, t\right) + \Delta_{\{,\}}$$

with $|\Delta_{\{,\}}| \leq C_{G,R,b}(\frac{ht}{\varepsilon} + h + (\frac{\varepsilon}{t})^{d/2})$.

It is a consequence of the following more accurate result.

Proposition 2.5.19. *Suppose the hypotheses of Proposition 2.5.18 are satisfied and keep the same notations. The term Δ_1 can be decomposed as*

$$\Delta_{\{,\}} = \sum_{j=1}^{3} \Delta_{\{,\},j}$$

with, for some integer k,

1. $\left|\Delta_{\{,\},1}\right| \leq 2\frac{ht}{\varepsilon} \| \langle \cdot \rangle^k \mathcal{F}^\sigma b \|_{L^1_P} \mathcal{O}\left(1 + h + [h(\frac{ht}{\varepsilon})^{-1}]^{d/2-1}\right)$,
2. $\left|\Delta_{\{,\},2}\right| \leq \left(\|\mathcal{F}^\sigma b\|_{L^1_P} + \| \langle \cdot \rangle^k \mathcal{F}^\sigma b \|_{L^1_P} \right) \mathcal{O}\left(h + (\frac{\varepsilon}{t})^{\frac{d}{2}-1}\right)$,
3. $\left|\Delta_{\{,\},3}\right| \leq \frac{ht}{\varepsilon} \|\mathcal{F}^\sigma \{b, \xi^{\cdot 2}\}\|_{L^1_P}$.

Remark 2.5.20. The operator $\mathscr{A}_{\{,\},P}$ is actually

$$\mathscr{A}_{\{,\},P} = \frac{1}{ih}\left[\hat{\tau}^h_P, \partial_t \omega \times\right] .$$

Remark 2.5.21. We can introduce a cutoff function $\chi_R \in \mathcal{C}^\infty_0(\mathbb{R}^d_\xi)$ such that $\chi_R(B_R) = \{1\}$, $\chi_R(\mathbb{R}^d_\xi - B_{R+1}) = \{0\}$ and $\chi_R(\mathbb{R}^d_\xi) \subset [0,1]$.

This result will be proved by considering successively every error term. These error terms $\Delta_{\{,\},j}$, $j = 1, 2, 3$ are given by the following approximation process (where we write shortly B^W for $B^W(-hD_\xi, \xi)$).

$$\begin{aligned}
m_{\{,\}} &= \int_P \mathcal{F}^\sigma b\,(P)\,\mathrm{Tr}\left[\hat{\boldsymbol{\rho}}_t^{app}\Gamma\left(e^{ip_x\cdot\varepsilon\eta}\right)\frac{1}{ih}\left[\hat{\tau}_P^h,\partial_t\omega\times\right]\right]\mathrm{d}P\\
&= \int_P \mathcal{F}^\sigma b\,(P)\,\mathrm{Tr}\left[\hat{\boldsymbol{\rho}}_t^{app}\Gamma\left(e^{ip_x\cdot\varepsilon\eta}\right)\frac{1}{ih}\left[\hat{\tau}_P^h,\chi_R\partial_t\omega\times\right]\right]\mathrm{d}P\\
&= \int_P \mathcal{F}^\sigma b\,(P)\,\mathrm{Tr}\left[\hat{\boldsymbol{\rho}}_t^{app}\frac{1}{ih}\left[\hat{\tau}_P^h,\chi_R\partial_t\omega\times\right]\right]\mathrm{d}P+\Delta_{\{,\},1}\\
&= \mathrm{Tr}\left[\hat{\boldsymbol{\rho}}_t^{app}\frac{1}{ih}\left[b^W,\chi_R\partial_t\omega\times\right]\right]\mathrm{d}P+\Delta_{\{,\},1}\\
&= -\,\mathrm{Tr}\left[\hat{\boldsymbol{\rho}}_t^{app}\left\{b,\chi_R\xi^{\cdot 2}\right\}^W\right]\mathrm{d}P+\sum_{j=1}^{2}\Delta_{\{,\},j}\\
&= \int_P \mathcal{F}^\sigma\left(-\left\{b,\xi^{\cdot 2}\right\}\right)(P)\,\mathrm{Tr}\left[\hat{\boldsymbol{\rho}}_t^{app}\hat{\tau}_P^h\right]\mathrm{d}P+\sum_{j=1}^{2}\Delta_{\{,\},j}\\
&= \int_P \mathcal{F}^\sigma\left(-\left\{b,\xi^{\cdot 2}\right\}\right)(P)\,\mathrm{Tr}\left[\hat{\boldsymbol{\rho}}_t^{app}\Gamma\left(e^{ip_x\cdot\varepsilon\eta}\right)\hat{\tau}_P^h\right]\mathrm{d}P+\sum_{j=1}^{3}\Delta_{\{,\},j}\\
&= m\left(-\left\{b,\xi^{\cdot 2}\right\},t\right)+\sum_{j=1}^{3}\Delta_{\{,\},j}\,.
\end{aligned}$$

The quantities $\Delta_{\{,\},j}$ are defined by

$$\begin{aligned}
\Delta_{\{,\},1} &= \int_P \mathcal{F}^\sigma b\,(P)\,\mathrm{Tr}\left[\hat{\boldsymbol{\rho}}_t^{app}\left(\Gamma\left(e^{ip_x\cdot\varepsilon\eta}\right)-\mathrm{Id}\right)\frac{1}{ih}\left[\hat{\tau}_P^h,\chi_R\partial_t\omega\times\right]\right]\mathrm{d}P\,,\\
\Delta_{\{,\},2} &= \mathrm{Tr}\left[\hat{\boldsymbol{\rho}}_t^{app}\frac{1}{ih}\left(\left[b,\chi_R\partial_t\omega\times\right]-\frac{h}{i}\left\{b,\chi_R\xi^{\cdot 2}\right\}^W\right)\right]\mathrm{d}P\,,\\
\Delta_{\{,\},3} &= \int_P \mathcal{F}^\sigma\left(-\left\{b,\xi^{\cdot 2}\right\}\right)(P)\,\mathrm{Tr}\left[\hat{\boldsymbol{\rho}}_t^{app}\left(\mathrm{Id}-\Gamma\left(e^{ip_x\cdot\varepsilon\eta}\right)\right)\hat{\tau}_P^h\right]\mathrm{d}P\,.
\end{aligned}$$

We will use the structure of $\partial_t\omega$:

Proposition 2.5.22. *The time derivative of ω is given by*

$$\partial_t\omega_{h,\varepsilon,t}=\xi^{\cdot 2}-h\Im\int_0^{t/\varepsilon}\int_{\mathbb{R}^d_\eta}e^{is\left(\eta^{\cdot 2}-2\xi.\eta\right)}\hat{G}\,(\eta)\,\mathrm{d}\eta\,\mathrm{d}s\,.$$

Proof. Differentiating ω with respect to t,

$$\begin{aligned}
\partial_t\omega_{h,\varepsilon,t} &= \xi^{\cdot 2}+\Re\left\langle z^\xi_{h,\varepsilon,t},f_{h,\varepsilon}\right\rangle\\
&= \xi^{\cdot 2}+\Re\int_{\mathbb{R}^d_\eta}i\int_0^t e^{-i\frac{s}{\varepsilon}\left(\varepsilon^2\eta^{\cdot 2}-2\xi.\varepsilon\eta\right)}\left|f_{h,\varepsilon}\left(\eta\right)\right|^2\mathrm{d}s e^{i\frac{t}{\varepsilon}\left(\varepsilon^2\eta^{\cdot 2}-2\xi.\varepsilon\eta\right)}\,\mathrm{d}\eta
\end{aligned}$$

which is the result once we replace $f_{h,\varepsilon}$ by its expression in terms of $\hat{V}$, use $\hat{G}=|\hat{V}|^2$ and make a change of variable. □

Lemma 2.5.23. *We have, for some integer k,*

$$\left[\hat{\tau}_P^h, \chi_R \partial_t \omega_{h,\varepsilon,t} \times\right] = \frac{h}{i}\left\{e^{i\sigma(P,X)}, \chi_R \xi^2\right\}^W (-hD_\xi, \xi) + h\mathcal{O}\Big(\langle P\rangle^k h + \Big(\frac{\varepsilon}{t}\Big)^{\frac{d}{2}-1}\Big).$$

and in particular $\left\|\left[\hat{\tau}_P^h, \chi_R \partial_t \omega \times\right]\right\|_{\mathcal{L}(L_\xi^2)} \leq \langle P\rangle^k \mathcal{O}(h)$.

Remark 2.5.24. We use in this proposition that $G \in L_x^1$.

Proof of Lemma 2.5.23. We split the commutator in three parts

$$\left[\hat{\tau}_P^h, \chi_R \partial_t \omega \times\right] = \left[\hat{\tau}_P^h, \chi_R(\xi)\,\xi^{\cdot 2} - h g_1(\xi) + h R_1\left(\frac{t}{\varepsilon}, \xi\right) \times\right]$$

with

$$g_1(\xi) := \chi_R(\xi)\,\Im \lim_{M \to +\infty} \int_0^M \int_{\mathbb{R}_\eta^d} e^{is\left(\eta^{\cdot 2} - 2\xi.\eta\right)} \hat{G}(\eta)\, \mathrm{d}\eta\, \mathrm{d}s\,,$$

$$R_1(u, \xi) := \chi_R(\xi)\,\Im \lim_{M \to +\infty} \int_u^M \int_{\mathbb{R}_\eta^d} e^{is\left(\eta^{\cdot 2} - 2\xi.\eta\right)} \hat{G}(\eta)\, \mathrm{d}\eta\, \mathrm{d}s\,.$$

The biggest part, in $\xi^{\cdot 2}$, gives the only relevant contribution

$$\left[\hat{\tau}_P^h, \chi_R \xi^{\cdot 2} \times\right] = \frac{h}{i}\left\{e^{i\sigma(P,X)}, \chi_R \xi^{\cdot 2} \times\right\}^{Weyl} + \langle P\rangle^k \mathcal{O}_{h\to 0}\left(h^2\right)\,.$$

One of the other parts can be estimated without using the commutator structure

$$\left\|\left[\hat{\tau}_P^h, R_1\left(\frac{t}{\varepsilon}, \xi\right) \times\right]\right\|_{\mathcal{L}(L_\xi^2)} \leq 2\left\|\hat{\tau}_P^h\right\|_{\mathcal{L}(L_\xi^2)} \left\|R_1\left(\frac{t}{\varepsilon}, \xi\right) \times\right\|_{L_\xi^\infty} \leq C\left(\frac{\varepsilon}{t}\right)^{\frac{d}{2}-1}$$

since

$$\int_{\mathbb{R}_\eta^d} e^{is\left(\eta^{\cdot 2} - 2\xi.\eta\right)} \hat{G}(\eta)\, \mathrm{d}\eta = e^{-is\xi^{\cdot 2}} \int_{\mathbb{R}_x^d} G(x)\, e^{-ix.\xi} \left(\frac{2\pi}{|s|}\right)^{d/2} e^{id\,\mathrm{sign}\, s\frac{\pi}{4}} e^{\frac{x^2}{2is}}\, \mathrm{d}x$$

and thus

$$\left|\int_{\mathbb{R}_\eta^d} e^{is\left(\eta^{\cdot 2} - 2\xi.\eta\right)} \hat{G}(\eta)\, \mathrm{d}\eta\right| \leq \left(\frac{2\pi}{|s|}\right)^{d/2} \|G\|_{L^1}\,.$$

Since g_1 is in $\mathcal{C}_0^\infty(\mathbb{R}_\xi^d)$ we can apply the symbolic calculus

$$\left[\hat{\tau}_P^h, h g_1(\xi) \times\right] = \frac{h^2}{i}\left\{e^{i\sigma(P,X)}, g_1(\xi)\right\}^W (-hD_\xi, \xi) + \mathcal{O}\left(h^2 \langle P\rangle^k\right)$$

where for some integer k,

$$\left\|\left\{e^{i\sigma(P,X)}, g_1(\xi) \times\right\}^W (-hD_\xi, \xi)\right\|_{\mathcal{L}(L_\xi^2)} = \langle P\rangle^k \mathcal{O}_{h\to 0}(1)\,,$$

which concludes the proof of the lemma. □

We can then estimate the three error terms $\Delta_{\{,\},j}$.

Proof of 1 in Proposition 2.5.19. It is a result of Proposition 2.5.13 and the estimate of

$$\left\| \left[\hat{\tau}_P^h, \chi_R \partial_t \omega_{h,\varepsilon,t} \times \right] \right\|_{\mathcal{L}\left(L^2_\xi\right)}$$

of the lemma. □

Proof of 2 in Proposition 2.5.19. The second error term can be expressed as

$$\Delta_{\{,\},2} = \int_{\mathbb{R}^{2d}_P} \mathcal{F}^\sigma b(P) \operatorname{Tr}\left[\hat{\boldsymbol{\rho}}_t^{app} \frac{1}{ih} \left(\left[\hat{\tau}_P^h, \chi_R \partial_t \omega_{h,\varepsilon,t} \times \right] - \frac{h}{i} \left\{ \hat{\tau}_P^h, \chi_R \xi^{\cdot 2} \right\}^W \right) \right] \text{đ}P$$

so that the lemma and Proposition 2.5.17 give the estimation. □

Proof of 3 in Proposition 2.5.19. It is an application of Proposition 2.5.13. □

2.5.5 The collision terms m_- and m_+

Proposition 2.5.25. *Let $b \in \mathcal{C}_0^\infty(\mathbb{R}^d_x \times \mathbb{R}^{d*}_\xi)$ and $\rho \in \mathcal{L}_1^+ L^2_x$, $\operatorname{Tr} \rho \leq 1$ such that for some $R > 0$, $\operatorname{Supp}_\xi b \subset B_R - B_{1/R}$ and $\operatorname{Supp} \hat{\rho}\left(\xi, \xi'\right) \subset B_R^2$. Then*

$$m_\pm = m\left(Q_{\pm,t}\left(b\right), t\right) + \Delta_\pm$$

and for any $\alpha \in [0,1[$, there are constants $\mu = \mu\left(d,\alpha\right) > 0$ and $C_{R,b,G,d,\alpha,\mu} > 0$, such that for $h^\alpha \leq \frac{th}{\varepsilon} \leq 1$,

$$\left|\Delta_\pm\right| \leq C_{R,b,G,\mu} \left(\frac{ht}{\varepsilon} + h^\mu \right) .$$

Definition 2.5.26. For $\zeta > 0$, $r \in \mathbb{R}$ and $P \in \mathbb{R}^{2d}_{p_x,p_\xi}$, set

$$\begin{aligned}
\kappa^\zeta\left(r\right) &= \frac{1}{\pi} \frac{\zeta}{r^2 + \zeta^2} , \\
\mathfrak{c}\left(\xi\right) &= 2\pi \int_{\mathbb{R}^d_\eta} \hat{G}\left(\eta + \xi\right) \delta\left(\eta^{\cdot 2} - \xi^{\cdot 2}\right) \mathrm{d}\eta , \\
\mathfrak{c}^\zeta\left(\xi\right) &= 2\pi \int_{\mathbb{R}^d_\eta} \hat{G}\left(\eta\right) \kappa^\zeta\left(\eta^{\cdot 2} - 2\xi.\eta\right) \mathrm{d}\eta , \\
\mathfrak{c}^\zeta_{P,t}\left(x,\xi\right) &= 2\pi \int_{\mathbb{R}^d_\eta} \hat{G}\left(\eta\right) e^{i\sigma(P,(-2t\eta,-\eta))} \kappa^\zeta\left(\eta^{\cdot 2} - 2\xi.\eta\right) \mathrm{d}\eta .
\end{aligned}$$

Associate with these functions the operators $Q_{\pm}$, $Q^{\zeta}_{\pm,t}$ defined by

$$\begin{aligned} Q_{-}(b) &= \mathfrak{c} b\,, \\ Q^{\zeta}_{-}(b) &= \mathfrak{c}^{\zeta} b\,, \\ Q^{\zeta}_{+,t} b(x,\xi) &= \int_{\mathbb{R}^{2d}_P} \mathcal{F}^{\sigma} b(P)\, e^{i\sigma(P,X)} \mathfrak{c}^{\zeta}_{P,t}(x,\xi)\, \text{đ}P\,, \end{aligned}$$

for $b \in \mathcal{C}^{\infty}_0(\mathbb{R}^d_x \times \mathbb{R}^{d*}_{\xi})$.

Proposition 2.5.27. *For $d \geq 3$, and $h^{\alpha} \leq \frac{ht}{\varepsilon} \leq 1$,*

$$\begin{aligned} m_{\pm} &= \int_P \mathcal{F}^{\sigma} b(P) \operatorname{Tr}\left[\hat{\boldsymbol{\rho}}^{app}_t \Gamma\left(e^{ip_x\cdot\varepsilon\eta}\right) \mathscr{A}_{\pm,P}\right] \text{đ}P \\ &= m\left(Q_{\pm,t}(b), t\right) + \sum_{k=1}^{4} \Delta_{\pm,k} \end{aligned}$$

with

- $|\Delta_{\pm,1}| \leq \frac{ht}{\varepsilon} C_d \max\left\{\|\hat{G}\|_{L^1}, \|G\|_{L^1}\right\} \|\mathcal{F}^{\sigma} b\|_{L^1_P}$,
- $|\Delta_{\pm,2}| \leq C_{\alpha,\beta,\nu,G,d} h^{\nu}$,
- $|\Delta_{\pm,3}| \leq \zeta^{\gamma} \mathcal{N}_{k(d)}(b)\, C_{d,G,C,\gamma}$ *for* $\gamma \in]0,1[$,
- $|\Delta_{\pm,4}| \leq \frac{ht}{\varepsilon} \left\|\mathcal{F}^{\sigma}\left(Q_{\pm,\frac{ht}{\varepsilon}}(b)\right)\right\|_{L^1_P}$

for some ν, $\beta > 0$ with $\zeta = h^{\beta}$.

This result will be proved in the next paragraphs by considering successively all the error terms. These error terms $\Delta_{\pm,j}$, $j = 1, \ldots, 4$ are given by the following approximation process (where we write shortly B^W for $B^W(-hD_{\xi}, \xi)$)

$$\begin{aligned} m_{\pm} &= \int \mathcal{F}^{\sigma} b(P) \operatorname{Tr}\left[\hat{\boldsymbol{\rho}}^{app}_t \Gamma\left(e^{ip_x\cdot\varepsilon\eta}\right) \mathscr{A}_{\pm,P}\right] \text{đ}P \\ &= \int \mathcal{F}^{\sigma} b(P) \operatorname{Tr}\left[\hat{\boldsymbol{\rho}}^{app}_t \mathscr{A}_{\pm,P}\right] \text{đ}P + \Delta_{\pm,1} \\ &= \int \mathcal{F}^{\sigma} b(P) \operatorname{Tr}\left[\hat{\boldsymbol{\rho}}^{app}_t \left(\mathfrak{c}^{\zeta}_{\pm,P} e^{i\sigma(P,\cdot)}\right)^W\right] \text{đ}P + \sum_{j=1}^{2} \Delta_{\pm,j} \\ &= \operatorname{Tr}\left[\hat{\boldsymbol{\rho}}^{app}_t \left(Q^{\zeta}_{\pm,\frac{ht}{\varepsilon}} b\right)^W\right] + \sum_{j=1}^{2} \Delta_{\pm,j} \\ &= \operatorname{Tr}\left[\hat{\boldsymbol{\rho}}^{app}_t \left(Q_{\pm,\frac{ht}{\varepsilon}} b\right)^W\right] + \sum_{j=1}^{3} \Delta_{\pm,j} \end{aligned}$$

$$
\begin{aligned}
&= \int \mathcal{F}^{\sigma}\left(Q_{\pm,\frac{ht}{\varepsilon}} b\right)(P) \operatorname{Tr}\left[\hat{\boldsymbol{\rho}}_t^{app} \hat{\tau}_P^h\right] \text{đ}P + \sum_{j=1}^{3} \Delta_{\pm,j} \\
&= \int \mathcal{F}^{\sigma}\left(Q_{\pm,\frac{ht}{\varepsilon}} b\right)(P) \operatorname{Tr}\left[\hat{\boldsymbol{\rho}}_t^{app} \Gamma\left(e^{ip_x\cdot\varepsilon\eta}\right) \hat{\tau}_P^h\right] \text{đ}P + \sum_{j=1}^{4} \Delta_{\pm,j} \\
&= m\left(Q_{\pm,\frac{ht}{\varepsilon}} b, t\right) + \sum_{j=1}^{4} \Delta_{\pm,j} .
\end{aligned}
$$

The error terms $\Delta_{\pm,j}$ are thus given by

$$
\Delta_{\pm,1} = \int \mathcal{F}^{\sigma} b(P) \operatorname{Tr}\left[\hat{\boldsymbol{\rho}}_t^{app} \left(\Gamma\left(e^{ip_x\cdot\varepsilon\eta}\right) - \mathrm{Id}\right) \mathscr{A}_{\pm,P}\right] \text{đ}P , \tag{2.5.10}
$$

$$
\Delta_{\pm,2} = \int \mathcal{F}^{\sigma} b(P) \operatorname{Tr}\left[\hat{\boldsymbol{\rho}}_t^{app} \left(\mathscr{A}_{\pm,P} - \left(\mathfrak{c}^{\zeta}_{\pm,P} e^{i\sigma(P,\cdot)}\right)^W\right)\right] \text{đ}P , \tag{2.5.11}
$$

$$
\Delta_{\pm,3} = \operatorname{Tr}\left[\hat{\boldsymbol{\rho}}_t^{app} \left(Q^{\zeta}_{\pm,\frac{ht}{\varepsilon}} b - Q_{\pm,\frac{ht}{\varepsilon}} b\right)^W\right] , \tag{2.5.12}
$$

$$
\Delta_{\pm,4} = \int \mathcal{F}^{\sigma}\left(Q_{\pm,\frac{ht}{\varepsilon}} b\right)(P) \operatorname{Tr}\left[\hat{\boldsymbol{\rho}}_t^{app} \left(\mathrm{Id} - \Gamma\left(e^{ip_x\cdot\varepsilon\eta}\right)\right) \hat{\tau}_P^h\right] \text{đ}P , \tag{2.5.13}
$$

since $\hat{\tau}_P^h = \left(e^{i\sigma(P,\cdot)}\right)^W$,

$$
\left(Q^{\zeta}_{\pm,\frac{ht}{\varepsilon}} b\right)^W = \int_{\mathbb{R}^{2d}_P} \mathcal{F}^{\sigma} b(P) \left(\mathfrak{c}^{\zeta}_{\pm,P} e^{i\sigma(P,\cdot)}\right)^W \text{đ}P ,
$$

and the same relation holds without ζ and

$$
\int_P \mathcal{F}^{\sigma}\left(Q_{\pm,\frac{ht}{\varepsilon}} b\right)(P) \operatorname{Tr}\left[\hat{\boldsymbol{\rho}}_t^{app} \Gamma\left(e^{ip_x\cdot\varepsilon\eta}\right) \hat{\tau}_P^h\right] \text{đ}P = m\left(Q_{\pm,\frac{ht}{\varepsilon}} b, t\right) .
$$

The term $\Delta_{\pm,4}$ can be estimated right away using Proposition 2.5.13.

2.5.5.1 Computation of the operators $\mathscr{A}_{\pm,P}$

We recall that the operators $\mathscr{A}_{\pm,P}$ and $\mathscr{A}_{-,j,P}\mathscr{A}_{-} = \mathscr{A}_{-,1} + \mathscr{A}_{-,2}$ are defined in Equations (2.5.5), (2.5.6), (2.5.7), (2.5.8), (2.5.9) by their kernels

$$
\begin{aligned}
\mathscr{A}_{-,P}(\xi_1,\xi_2) &= \mathscr{A}_{-,1,P}(\xi_1) + \mathscr{A}_{-,2,P}(\xi_2) , \\
ih\mathscr{A}_{-,j,P}(\xi_j) &= i\partial_t\left(\frac{1}{2}\left|z^{\xi_j}_{h,\varepsilon,t}\right|^2\right) \hat{\tau}_P^h(\xi_2,\xi_1) , \; j = 1,2 , \\
ih\mathscr{A}_{+,P}(\xi_1,\xi_2) &= i\partial_t\left[\varphi, p_x\right]_2 \hat{\tau}_P^h(\xi_2,\xi_1) .
\end{aligned}
$$

Thus we need to compute $\partial_t(\frac{1}{2}|z^{\xi_j}_{h,\varepsilon,t}|^2)$ and $\partial_t\left[\varphi, p_x\right]_2$.

Lemma 2.5.28. *The time derivative of* $\frac{1}{2}|z_{h,\varepsilon,t}|^2$ *is given by*

$$\partial_t \left(\frac{1}{2} |z_{h,\varepsilon,t}|^2 \right) = h \Re \int_{\mathbb{R}^d_\eta} \int_0^{t/\varepsilon} e^{is\left(\eta^{\cdot 2} - 2\xi_j . \eta\right)} \hat{G}(\eta) \, \mathrm{d}s \, \mathrm{d}\eta \, .$$

Proof. For $z_t = -i \int_0^t e^{-i\frac{s}{\varepsilon}\left(\varepsilon^2 \eta^{\cdot 2} - 2\xi . \varepsilon\eta\right)} f_{h,\varepsilon} \, \mathrm{d}s$ with $f_{h,\varepsilon}(\eta) = \varepsilon^{d/2} \sqrt{\frac{h}{\varepsilon}} \hat{V}(-\varepsilon\eta)$,

$$\partial_t \left(\frac{1}{2} |z_t|^2 \right) = \Re \int_{\mathbb{R}^d_\eta} \bar{z}_t \partial_t z_t$$

and $\partial_t z_t = -ie^{-i\frac{t}{\varepsilon}\left(\varepsilon^2 \eta^{\cdot 2} - 2\xi . \varepsilon\eta\right)} f_{h,\varepsilon}$. A simple computation gives

$$\begin{aligned} \partial_t \left(\frac{1}{2} |z_t|^2 \right) &= \Re \int_{\mathbb{R}^d_\eta} \int_0^t e^{i\frac{t-s}{\varepsilon}\left(\varepsilon^2 \eta^{\cdot 2} - 2\xi . \varepsilon\eta\right)} |f_{h,\varepsilon}(\eta)|^2 \, \mathrm{d}s \, \mathrm{d}\eta \\ &= h \Re \int_{\mathbb{R}^d_\eta} \int_0^{t/\varepsilon} e^{is\left(\eta^{\cdot 2} - 2\xi . \eta\right)} \hat{G}(\eta) \, \mathrm{d}s \, \mathrm{d}\eta \end{aligned}$$

which is the expected result. □

Lemma 2.5.29. *The time derivative of* $[\varphi, p_x]_2$ *is given by*

$$\begin{aligned} \partial_t [\varphi, p_x]_2 = \quad & h \int_{\mathbb{R}^d_\eta} \int_0^{t/\varepsilon} e^{ip_x \cdot \eta} e^{is\left(\eta^{\cdot 2} - 2\xi_1 . \eta\right)} e^{-i\frac{t}{\varepsilon}\left(\eta^{\cdot 2} - 2\xi_2 . \eta\right)} \, \mathrm{d}s \hat{G}(\eta) \, \mathrm{d}\eta \\ & + h \int_{\mathbb{R}^d_\eta} \int_0^{t/\varepsilon} e^{ip_x \cdot \eta} e^{i\frac{t}{\varepsilon}\left(\eta^{\cdot 2} - 2\xi_1 . \eta\right)} e^{-is\left(\eta^{\cdot 2} - 2\xi_2 . \eta\right)} \, \mathrm{d}s \hat{G}(\eta) \, \mathrm{d}\eta \, . \end{aligned}$$

Proof. Two analogous terms appear in this computation

$$\begin{aligned} \partial_t [\varphi, p_x]_2 &= \partial_t \left\langle z_t^{\xi_2}, e^{ip_x \cdot \varepsilon\eta} z_t^{\xi_1} \right\rangle_{L^2_\eta} \\ &= \left\langle z_t^{\xi_2}, e^{ip_x \cdot \varepsilon\eta} \partial_t z_t^{\xi_1} \right\rangle_{L^2_\eta} + \left\langle \partial_t z_t^{\xi_2}, e^{ip_x \cdot \varepsilon\eta} z_t^{\xi_1} \right\rangle_{L^2_\eta} . \end{aligned}$$

Consider the first one:

$$\begin{aligned} & \left\langle \partial_t z_t^{\xi_2}, e^{ip_x \cdot \varepsilon\eta} z_t^{\xi_1} \right\rangle_{L^2_\eta} \\ &= \left\langle e^{i\frac{t}{\varepsilon}\left(\varepsilon^2 \eta^{\cdot 2} - 2\xi_2 . \varepsilon\eta\right)} f_{h,\varepsilon}, e^{ip_x \cdot \varepsilon\eta} \int_0^t e^{i\frac{s}{\varepsilon}\left(\varepsilon^2 \eta^{\cdot 2} - 2\xi_1 . \varepsilon\eta\right)} f_{h,\varepsilon} \, \mathrm{d}s \right\rangle \\ &= \int_{\mathbb{R}^d_\eta} \int_0^t e^{ip_x \cdot \varepsilon\eta} e^{i\frac{s}{\varepsilon}\left(\varepsilon^2 \eta^{\cdot 2} - 2\xi_1 . \varepsilon\eta\right)} e^{-i\frac{t}{\varepsilon}\left(\varepsilon^2 \eta^{\cdot 2} - 2\xi_2 . \varepsilon\eta\right)} \, \mathrm{d}s \, |f_{h,\varepsilon}(\eta)|^2 \, \mathrm{d}\eta \\ &= h \int_{\mathbb{R}^d_\eta} \int_0^{t/\varepsilon} e^{ip_x \cdot \eta} e^{is\left(\eta^{\cdot 2} - 2\xi_1 . \eta\right)} e^{-i\frac{t}{\varepsilon}\left(\eta^{\cdot 2} - 2\xi_2 . \eta\right)} \, \mathrm{d}s \hat{G}(\eta) \, \mathrm{d}\eta \, . \end{aligned}$$

With analogous computations we get the result for the second one. □

Proposition 2.5.30. *The operators $\mathscr{A}_{-,j}$ can be expressed as*

$$\mathscr{A}_{-,1,P} = \int_{\mathbb{R}^d_\eta} \int_0^{t/\varepsilon} \hat{\tau}^h_P \circ \Re\left(e^{is\left(\eta^{\cdot 2} - 2\xi.\eta\right)}\right) \times \hat{G}(\eta)\, \mathrm{d}s\, \mathrm{d}\eta\,,$$
$$\mathscr{A}_{-,2,P} = \int_{\mathbb{R}^d_\eta} \int_0^{t/\varepsilon} \Re\left(e^{is\left(\eta^{\cdot 2} - 2\xi.\eta\right)}\right) \times \circ\hat{\tau}^h_P \hat{G}(\eta)\, \mathrm{d}s\, \mathrm{d}\eta\,.$$

Proof. From the definition of $\mathscr{A}_{-,j,P}$ in terms of their kernel, we get

$$ih\mathscr{A}_{-,1,P} = i\hat{\tau}^h_P \circ \left[\partial_t \left(\frac{1}{2}\left|z^\xi_t\right|^2\right) \times\right],$$
$$ih\mathscr{A}_{-,2,P} = i\left[\partial_t \left(\frac{1}{2}\left|z^\xi_t\right|^2\right) \times\right] \circ \hat{\tau}^h_P\,.$$

Lemma 2.5.28 yields the result. □

Consider now the term $\mathscr{A}_+$.

Proposition 2.5.31. *The operators $\mathscr{A}_{+,j}$ can be expressed as*

$$\mathscr{A}_{+,1,P} = \int_0^{t/\varepsilon} \int_{\mathbb{R}^d_\eta} e^{-i\sigma\left(P,\left(2\frac{t}{\varepsilon}\eta,\eta\right)\right)} \hat{\tau}^h_P \circ e^{-is\left(\eta^{\cdot 2} - 2\xi.\eta\right)} \hat{G}(\eta)\, \mathrm{d}\eta\, \mathrm{d}s\,,$$
$$\mathscr{A}_{+,2,P} = \int_0^{t/\varepsilon} \int_{\mathbb{R}^d_\eta} e^{-i\sigma\left(P,\left(2\frac{t}{\varepsilon}\eta,\eta\right)\right)} e^{is\left(\eta^{\cdot 2} - 2\xi.\eta\right)} \circ \hat{\tau}^h_P \hat{G}(\eta)\, \mathrm{d}\eta\, \mathrm{d}s\,.$$

Proof. Lemma 2.5.29 allows us to write

$$\mathscr{A}_{+,1,P} = \int_0^{t/\varepsilon} \int_{\mathbb{R}^d_\eta} e^{ip_x\cdot\eta} e^{-i\frac{t}{\varepsilon}\left(\eta^{\cdot 2} - 2\xi.\eta\right)} \circ \hat{\tau}^h_P \circ e^{is\left(\eta^{\cdot 2} - 2\xi.\eta\right)} \hat{G}(\eta)\, \mathrm{d}\eta\, \mathrm{d}s\,,$$
$$\mathscr{A}_{+,2,P} = \int_0^{t/\varepsilon} \int_{\mathbb{R}^d_\eta} e^{ip_x\cdot\eta} e^{-is\left(\eta^{\cdot 2} - 2\xi.\eta\right)} \circ \hat{\tau}^h_P \circ e^{i\frac{t}{\varepsilon}\left(\eta^{\cdot 2} - 2\xi.\eta\right)} \hat{G}(\eta)\, \mathrm{d}\eta\, \mathrm{d}s\,.$$

Since

$$e^{2i\frac{t}{\varepsilon}\xi.\eta} \circ \hat{\tau}^h_P = e^{-2i\frac{t}{\varepsilon}p_\xi\eta} \hat{\tau}^h_P \circ e^{2i\frac{t}{\varepsilon}\xi.\eta}\,,$$
$$\hat{\tau}^h_P \circ e^{-2i\frac{t}{\varepsilon}2\xi.\eta} = e^{-2i\frac{t}{\varepsilon}p_\xi\eta} e^{-2i\frac{t}{\varepsilon}2\xi.\eta} \circ \hat{\tau}^h_P\,,$$

we get

$$\mathscr{A}_{+,1,P} = \int_0^{t/\varepsilon} \int_{\mathbb{R}^d_\eta} e^{-i\sigma\left(P,\left(2\frac{t}{\varepsilon}\eta,\eta\right)\right)} \hat{\tau}^h_P \circ e^{-i\left(\frac{t}{\varepsilon}-s\right)\left(\eta^{\cdot 2} - 2\xi.\eta\right)} \hat{G}(\eta)\, \mathrm{d}\eta\, \mathrm{d}s\,,$$
$$\mathscr{A}_{+,2,P} = \int_0^{t/\varepsilon} \int_{\mathbb{R}^d_\eta} e^{-i\sigma\left(P,\left(2\frac{t}{\varepsilon}\eta,\eta\right)\right)} e^{i\left(\frac{t}{\varepsilon}-s\right)\left(\eta^{\cdot 2} - 2\xi.\eta\right)} \circ \hat{\tau}^h_P \hat{G}(\eta)\, \mathrm{d}\eta\, \mathrm{d}s$$

and with a change of variable we obtain the expected result. □

Thus we get six different terms (four for the $\mathscr{A}_-$ terms due to the real parts and two for the $\mathscr{A}_+$ terms) with a very similar structure. In order to avoid repeating analogous calculations several times we introduce the following notations.

Notation: Set (by writing shortly B^W for $B^W(-hD_\xi, \xi)$)

$$\mathscr{A}^1_{\vec{\mu}}(s) = \int_{\mathbb{R}^d_\eta} \hat{G}(\eta)\, e^{\mu_1 i\tilde{\sigma}} \hat{\tau}^h_P \circ e^{-\mu_2 is\left(\eta^{\cdot 2} - 2\xi.\eta\right)}\, \mathrm{d}\eta\,, \tag{2.5.14}$$

$$\mathscr{B}^1_{\vec{\mu}}(s) = \int_{\mathbb{R}^d_\eta} \hat{G}(\eta)\, e^{\mu_1 i\tilde{\sigma}} \hat{\tau}^h_{\left(p_x - \mu_2 2s\eta, p_\xi\right)} e^{-\mu_2 is\eta^{\cdot 2}}\, \mathrm{d}\eta\,, \tag{2.5.15}$$

$$\mathscr{C}^{1,\zeta}_{\vec{\mu}} = \int_{\mathbb{R}^d_\eta} \hat{G}(\eta) \left(e^{\mu_1 i\tilde{\sigma}} e^{i\sigma(P,\cdot)}\right)^W \frac{\mathrm{d}\eta}{\zeta + \mu_2 i\left(\eta^{\cdot 2} - 2\xi.\eta\right)}\,, \tag{2.5.16}$$

$$\mathscr{A}^2_{\vec{\mu}}(s) = \int_{\mathbb{R}^d_\eta} \hat{G}(\eta)\, e^{\mu_1 i\tilde{\sigma}} e^{\mu_2 is\left(\eta^{\cdot 2} - 2\xi.\eta\right)} \circ \hat{\tau}^h_P\, \mathrm{d}\eta\,, \tag{2.5.17}$$

$$\mathscr{B}^2_{\vec{\mu}}(s) = \int_{\mathbb{R}^d_\eta} \hat{G}(\eta)\, e^{\mu_1 i\tilde{\sigma}} \hat{\tau}^h_{\left(p_x + \mu_2 2s\eta, p_\xi\right)} e^{\mu_2 is\eta^{\cdot 2}}\, \mathrm{d}\eta\,, \tag{2.5.18}$$

$$\mathscr{C}^{2,\zeta}_{\vec{\mu}} = \int_{\mathbb{R}^d_\eta} \hat{G}(\eta) \left(e^{\mu_1 i\tilde{\sigma}} e^{i\sigma(P,\cdot)}\right)^W \frac{\mathrm{d}\eta}{\zeta - \mu_2 i\left(\eta^{\cdot 2} - 2\xi.\eta\right)}\,, \tag{2.5.19}$$

with $\tilde{\sigma} = \sigma\left(P, \left(-2h\frac{t}{\varepsilon}\eta, -\eta\right)\right)$. The terms μ_1, μ_2 are chosen to adapt to the cases of the terms $m_\pm$.

More precisely, for $j = 1, 2$, the previous quantities become

$$\mathscr{A}_{-,j} = \frac{1}{2}\int_0^{t/\varepsilon} \left(\mathscr{A}^j_{0,1}(s) + \mathscr{A}^j_{0,-1}(s)\right) \mathrm{d}s\,,$$

$$\mathscr{A}_{+,j} = \int_0^{t/\varepsilon} \mathscr{A}^j_{1,1}(s)\, ds\,.$$

We will first show that the operators $\mathscr{C}^\zeta_{\vec{\mu}}$ are good approximations of the operators $\mathscr{A}_{\vec{\mu}} = \int_0^{t/\varepsilon} \mathscr{A}_{\vec{\mu}}(s)\, \mathrm{d}s$ if the parameter ζ is well chosen. We use the operators $\int_0^{t/\varepsilon} \mathscr{B}_{\vec{\mu}}(s)\, \mathrm{d}s$ as an intermediate step.

Then we study the limit of the operators $\mathscr{C}^\zeta_{\vec{\mu}}$, with a distinction between the cases m_- and m_+.

2.5.5.2 Estimate of the error terms $\Delta_{\pm,1}$

Proposition 2.5.32. *For $d \geq 3$, the inequality*

$$|\Delta_{\pm,1}| \leq \frac{ht}{\varepsilon} C_d \max\left\{\|\hat{G}\|_{L^1}, \|G\|_{L^1}\right\} \|\mathcal{F}^\sigma b\|_{L^1_P}$$

holds.

Proof. The term $\Delta_{\pm,1}$ was defined in Equation (2.5.10). This inequality follows from Propositions 2.5.13 and 2.5.33 below since $s \mapsto \min\{1, s^{-d/2}\}$ is integrable on $\mathbb{R}^+$ for $d \geq 3$. □

Proposition 2.5.33. *The families of operators $\mathscr{A}(s) = \mathscr{A}^j_{\vec{\mu}}(s)$ satisfy*

$$\|\mathscr{A}(s)\|_{\mathcal{L}(L^2_\xi)} \leq C_d \max\{\|\hat{G}\|_{L^1}, \|G\|_{L^1}\} \min\{1, s^{-d/2}\}.$$

Proof. By a uniform estimate of Equations (2.5.14), (2.5.17) we get

$$\left\|\mathscr{A}^j_{\vec{\mu}}(s)\right\|_{\mathcal{L}(L^2_\xi)} \leq C_d \|\hat{G}\|_{L^1}.$$

In order to obtain the part of the estimate with the dependence in s, we use the formula

$$\left\|\mathscr{A}^j_{\vec{\mu}}(s)\right\|_{\mathcal{L}(L^2_\xi)} = \sup_{\|\psi\|_{L^2_\xi} = \|\varphi\|_{L^2_\xi} = 1} \left|\left\langle \psi, \mathscr{A}^j_{\vec{\mu}}(s)\varphi \right\rangle\right|.$$

We can then compute, for ψ, $\varphi \in L^2_\xi$,

$$\begin{aligned}
&\left\langle \psi, \mathscr{A}^j_{\vec{\mu}}(s)\varphi \right\rangle \\
&= \int_{\mathbb{R}^d_\eta} \left\langle \psi, \hat{G}(\eta) e^{i\mu_1 \tilde{\sigma}} \hat{\tau}^h_P \circ e^{-\mu_2 is\left(\eta^{\cdot 2} - 2\xi.\eta\right)} \varphi \right\rangle_\xi \mathrm{d}\eta \\
&= \int_{\mathbb{R}^d_\xi} \left\langle \hat{G}(\eta) \hat{\tau}^h_{-P} \psi(\xi), e^{\mu_1 i \tilde{\sigma}} e^{-\mu_2 is\left(\eta^{\cdot 2} - 2\xi.\eta\right)} \varphi(\xi) \right\rangle_\eta \mathrm{d}\xi \\
&= \int_{\mathbb{R}^d_\theta} \left\langle \psi_\theta, \varphi_{\vec{\mu},\theta} \right\rangle_\xi \frac{1}{(2\pi)^d} \mathrm{d}\theta,
\end{aligned}$$

where we defined, for $\theta \in \mathbb{R}^d_\theta$,

$$\begin{aligned}
\varphi_{\vec{\mu},\theta} &= \int e^{i\theta\eta} e^{\mu_1 i \tilde{\sigma}} e^{-\mu_2 is\left(\eta^{\cdot 2} - 2\xi.\eta\right)} \varphi(\xi) \,\mathrm{d}\eta, \\
\psi_\theta &= \int e^{i\theta\eta} \hat{G}(\eta) \hat{\tau}^h_{-P} \psi(\xi) \,\mathrm{d}\eta.
\end{aligned}$$

We first compute

$$\varphi_{\vec{\mu},\theta}(\xi) = \left(\frac{\pi}{s}\right)^{d/2} e^{i\frac{\left(\theta + \mu_2 2s\xi + \mu_1\left(2hsp_\xi - p_x\right)\right)^2}{4\mu_2 s}} e^{i\frac{\pi}{4}d} \varphi(\xi)$$

where we used the formula

$$\int e^{-ix\eta} e^{-a\eta^2} d\eta = \left(\frac{\pi}{a}\right)^{d/2} e^{-x^2/4a}$$

with $a = \mu_2 is$ and $x = -(\theta + \mu_2 2s\xi + \mu_1 (2hsp_\xi - p_x))$ and so for a fixed θ

$$\left\|\varphi_{\vec{\mu},\theta}\right\|_{L^2_\xi} \leq \left(\frac{\pi}{s}\right)^{d/2} \|\varphi\|_{L^2_\xi}\,.$$

We now observe that in $L^1(\mathbb{R}^d_\theta;\mathcal{L}(L^2_\xi))$

$$\left\|\int e^{i\theta\eta}\hat{G}(\eta)\,\hat{\tau}^h_{-P} d\eta\right\|_{L^1\left(\mathbb{R}^d_\theta;\mathcal{L}\left(L^2_\xi\right)\right)} \leq (2\pi)^d \|G\|_{L^1}$$

so that $\|\psi_\theta\|_{L^1\left(\mathbb{R}^d_\theta;L^2_\xi\right)} \leq C_d \|G\|_{L^1} \|\psi\|_{L^2_\xi}$. And finally

$$\begin{aligned}\left|\left\langle\psi, \mathscr{A}_{\vec{\mu}}(s)\,\varphi\right\rangle\right| &\leq \frac{1}{(2\pi)^d} \|\psi_\theta\|_{L^1\left(\mathbb{R}^d_\theta;L^2_\xi\right)} \left\|\varphi_{\vec{\mu},\theta}\right\|_{L^\infty\left(\mathbb{R}^d_\theta;L^2_\xi\right)} \\ &\leq C_d \|G\|_{L^1} \left(\frac{\pi}{s}\right)^{d/2} \|\varphi\|_{L^2_\xi} \|\psi\|_{L^2_\xi}\end{aligned}$$

and we obtain the desired result $\|\mathscr{A}_{\vec{\mu}}(s)\|_{\mathcal{L}\left(L^2_\xi\right)} \leq C_d \|G\|_{L^1} s^{-d/2}$. □

2.5.5.3 Estimate of the error terms $\Delta_{\pm,2}$

Proposition 2.5.34. *Let $\alpha \in \,]0,1]$. There are constants $\beta = \beta(d,\alpha) \in \,]0,1[$, $\nu = \nu(d,\alpha) \in \,]0,1[$ and $C = C(\alpha,\beta,\nu,d,G) > 0$ such that, for $h^\alpha \leq \frac{th}{\varepsilon} \leq 1$, and $\zeta = h^\beta$,*

$$|\Delta_{\pm,2}| \leq \|\langle\cdot\rangle^k \mathcal{F}^\sigma b\|_{L^1} C h^\nu\,.$$

In order to prove this result we use Proposition 2.5.17 and thus control

$$\left\|\int_0^{t/\varepsilon} \mathscr{A}(s)\,\mathrm{d}s - \mathscr{C}^\zeta\right\|_{\mathcal{L}\left(L^2_\xi\right)}\,.$$

We first give an abstract result and then show that our cases fit within this framework.

Proposition 2.5.35. *For M, t, ε such that $1 \leq M \leq \frac{t}{\varepsilon}$. Suppose given $(\mathscr{A}(s))_{s\geq 0}$, $(\mathscr{B}(s))_{s\geq 0}$ and $(\mathscr{C}^\zeta)_{0<\zeta<1}$ three families of operators in $\mathcal{L}(L^2_\xi)$ (also dependent on h and $P = (p_x,p_\xi)$) such that for some constants $C_\mathscr{A}$, $C_{\mathscr{A},\mathscr{B}}$, $C_{\mathscr{B},\mathscr{C}}$, independent of $h,\varepsilon,t,P,M,\zeta$,*

1. $\|\mathscr{A}(s)\|_{\mathcal{L}\left(L^2_\xi\right)} \leq C_\mathscr{A} \min\left\{1, s^{-d/2}\right\}$,
2. $\|\mathscr{A}(s) - \mathscr{B}(s)\|_{\mathcal{L}\left(L^2_\xi\right)} \leq C_{\mathscr{A},\mathscr{B}} hs\,|p_\xi|$,

3. $r_{\zeta,M}(x,\xi) := \mathrm{Symb}^{Weyl}(\int_0^M \mathscr{B}(s)\, e^{-\zeta s}\, \mathrm{d}s - \mathscr{C}^\zeta)$ *satisfies for some* $k = k(d) \in \mathbb{N}$,

$$\sup_{|\alpha|\leq k} \left\| \partial^\alpha_{x,\xi} r_{\zeta,M} \right\|_{L^\infty_{x,\xi}} \leq C_{\mathscr{B},\mathscr{C}} \langle P \rangle^k \left(\frac{M}{\zeta} \right)^k e^{-\zeta M} .$$

Then, for $\zeta M \geq 1$,

1. $\| \int_0^{t/\varepsilon} \mathscr{A}(s)\, \mathrm{d}s \|_{\mathcal{L}(L^2_\xi)} \leq \frac{d}{d-2} C_{\mathscr{A}}$,

2. $\| \int_0^{t/\varepsilon} \mathscr{A}(s)\, \mathrm{d}s - \int_0^M \mathscr{A}(s)\, \mathrm{d}s \|_{\mathcal{L}(L^2_\xi)} \leq \frac{2}{d-2} C_{\mathscr{A}} M^{1-\frac{d}{2}}$,

3. depending on d,

$$\begin{aligned} \| \int_0^M \mathscr{A}(s) \left(1 - e^{-\zeta s} \right) \mathrm{d}s \|_{\mathcal{L}(L^2_\xi)} &\leq \frac{9}{2} C_{\mathscr{A}} \zeta^{1/2} \quad \mathit{if} d = 3 \\ &\leq \frac{3}{2} C_{\mathscr{A}} \zeta \left| \log \zeta \right| \quad \mathit{if} d = 4 \\ &\leq C_{\mathscr{A}} \zeta \frac{d+2}{2d-4} \quad \mathit{if} d \geq 5 \\ &(\leq 5 C_{\mathscr{A}} \zeta^{1/2} \quad \mathit{if} d \geq 3), \end{aligned}$$

4. $\| \int_0^M (\mathscr{A}(s) - \mathscr{B}(s))\, e^{-\zeta s}\, \mathrm{d}s \|_{\mathcal{L}(L^2_\xi)} \leq \frac{1}{2} C_{\mathscr{A},\mathscr{B}} h \zeta^{-2} |p_\xi|$,

5. for some integer $k = k(d)$,

$$\left\| \int_0^M \mathscr{B}(s)\, e^{-\zeta s}\, \mathrm{d}s - \mathscr{C}^\zeta \right\|_{\mathcal{L}(L^2_\xi)} \leq C_{d,k'} C_{\mathscr{B},\mathscr{C}} \langle P \rangle^k \left(\frac{M}{\zeta} \right)^k e^{-\zeta M} .$$

6. Let $\frac{ht}{\varepsilon} \geq h^\alpha$, $\zeta = h^\beta$ *with* $\beta \in \left]0, \frac{1}{2}\right[$ *and* $\beta + \alpha < 1$, *and* $\nu = \nu(d,\alpha,\beta) < \min\{(1-\alpha)\left(\frac{d}{2} - 1\right), \tilde\beta(d), 1 - 2\beta\}$ *with* $\tilde\beta(3,\beta) = \beta/2$, $\tilde\beta(4,\beta) = \beta$ *and* $\tilde\beta(d \geq 5, \beta) = \beta$ *we have*

$$\left\| \int_0^{\frac{t}{\varepsilon}} \mathscr{A}(s)\, \mathrm{d}s - \mathscr{C}^\zeta \right\|_{\mathcal{L}(L^2_\xi)} \leq C h^\nu$$

with $C = C(\nu, \alpha, \beta, C_{\mathscr{A}}, C_{\mathscr{A}\mathscr{B}}, C_{\mathscr{B}\mathscr{C}})$.

Proofs of 1 and 2. By integration of the first assumed estimate and using $1 \leq M \leq \frac{t}{\varepsilon}$ for *2.* □

Proof of 3. By integration of the first assumed estimate, using $1-e^{-\zeta s} \leq \zeta s$ for $\zeta s \leq 1$ and $1-e^{-\zeta s} \leq 1$ for $\zeta s \geq 1$,

$$\begin{aligned}
&\int_0^M \left(1-e^{-\zeta s}\right) \min\left\{1, s^{-d/2}\right\} \mathrm{d}s \\
&\quad \leq \zeta \int_0^1 s \, \mathrm{d}s + \zeta \int_1^{1/\zeta} s^{1-\frac{d}{2}} \, \mathrm{d}s + \int_{1/\zeta}^{+\infty} s^{-d/2} \, \mathrm{d}s \,, \qquad \text{if } d = 3, 4, \\
&\quad \leq \zeta \int_0^1 s \, \mathrm{d}s + \zeta \int_1^{+\infty} s^{1-\frac{d}{2}} \, \mathrm{d}s \,, \qquad \text{if } d \geq 5 \,,
\end{aligned}$$

which brings the result. □

Proof of 4. We control $\|\mathscr{A}(s) - \mathscr{B}(s)\|_{\mathcal{L}\left(L^2_\xi\right)}$ using the second assumption and use

$$\int_0^M s e^{-\zeta s} \, \mathrm{d}s \leq \zeta^{-2} \int_0^{+\infty} u e^{-u} \, \mathrm{d}u \,.$$

□

Proof of 5. The known estimates for pseudodifferential operators give

$$\begin{aligned}
\left\| r^W(-hD_\xi, \xi) \right\| &\leq C_{1,k} \sum_{|\alpha| \leq N_k} \left\| \partial^\alpha_{x,\xi} r \right\|_{L^\infty\left(\mathbb{R}^{2d}\right)} \\
&\leq C_{2,k} \sup_{|\alpha| \leq N_k} \left\| \partial^\alpha_{x,\xi} r \right\|_{L^\infty\left(\mathbb{R}^{2d}\right)} \,.
\end{aligned}$$

This and the third hypothesis imply the result. □

Proof of 6. We would like to choose the (h-dependent) parameters M and ζ such that the quantity

$$M^{1-\frac{d}{2}} + \tilde{\zeta}(d, \zeta) + h\zeta^{-2} + \left(\frac{M}{\zeta}\right)^k e^{-\zeta M} \,,$$

with ($\tilde{\zeta}(3,\zeta) = \sqrt{\zeta}$, $\tilde{\zeta}(4,\zeta) = \zeta\,|\log\zeta|$, $\tilde{\zeta}(d \geq 5, \zeta) = \zeta$), is small when h tends to 0 and M not too big. We choose $hM = h^\alpha$ and $\zeta = h^\beta$ with $\beta + \alpha < 1$, $\alpha, \beta > 0$ so that the previous quantity is smaller than

$$h^{(1-\alpha)\left(\frac{d}{2}-1\right)} + h^{\tilde{\beta}(d,\beta)} + h^{1-2\beta} + h^{-k(1-\alpha+\beta)} \exp\left(-\left(h^{\beta+\alpha-1}\right)\right)$$

(with $\tilde{\beta}(3,\beta) = \beta/2$, $\tilde{\beta}(4,\beta) = \beta^-$ and $\tilde{\beta}(d \geq 5, \beta) = \beta$). In order to get a small quantity it suffices to require $\beta < \frac{1}{2}$. Then we get an error term whose size is controlled by $h^{\nu(d,\alpha,\beta)}$. □

Proposition 2.5.36. *The families of operators* $\mathscr{A}(s) = \mathscr{A}^j_{\vec{\mu}}(s)$, $\mathscr{B}(s) = \mathscr{B}^j_{\vec{\mu}}(s)$ *and* $\mathscr{C}^\zeta = \mathscr{C}^{j,\zeta}_{\vec{\mu}}$ *satisfy the hypotheses of Proposition 2.5.35 with*

$$C_{\mathscr{A}} = C_d \max\left\{\|\hat{G}\|_{L^1}, \|G\|_{L^1}\right\}, \; C_{\mathscr{A},\mathscr{B}} = \left\||\cdot|\,\hat{G}\right\|_{L^1}, \; C_{\mathscr{B},\mathscr{C}} = \left\|\langle\cdot\rangle^k\,\hat{G}\right\|_{L^1},$$

for some integer k.

Proof of 1. See Proposition 2.5.33. □

Proof of 2. We show the result for $\mathscr{A}^1_{\vec{\mu}}$ and $\mathscr{B}^1_{\vec{\mu}}$, the proof can be adapted to the case of $\mathscr{A}^2_{\vec{\mu}}$ and $\mathscr{B}^2_{\vec{\mu}}$. We observe that

$$\hat{\tau}^h_P \circ \left(e^{\mu_2 is2\xi.\eta}\times\right) = e^{-\mu_2 is\eta hp_\xi}\hat{\tau}^h_{P-(\mu_2 2s\eta,0)}$$

and

$$\left(e^{i\sigma(P,X)}e^{\mu_2 is2\xi.\eta}\right)^W(-hD_\xi,\xi) = \hat{\tau}^h_{\left(p_x-\mu_2 2s\eta,p_\xi\right)}.$$

Thus we obtain the estimation

$$\left\|\hat{\tau}^h_P \circ \left(e^{\mu_2 is2\xi.\eta}\times\right) - \left(e^{i\sigma(P,X)}e^{\mu_2 is2\xi.\eta}\right)^W(-hD_\xi,\xi)\right\|_{\mathcal{L}\left(L^2_\xi\right)} \leq hs\,|\eta|\,|p_\xi|$$

Since the Weyl symbol of $\mathscr{B}^1_{\vec{\mu}}(s)$ is

$$\frac{1}{2}\int_{\mathbb{R}^d_\eta}\hat{G}(\eta)\,e^{i\mu_1\tilde{\sigma}}e^{i\sigma(P,X)}e^{-\mu_2 is\left(\eta^{.2}-2\xi.\eta\right)}\,\mathrm{d}\eta$$

we finally get

$$\left\|\mathscr{A}^1_{\vec{\mu}}(s) - \mathscr{B}^1_{\vec{\mu}}(s)\right\|_{\mathcal{L}\left(L^2_\xi\right)} \leq hs\,|p_\xi|\int_{\mathbb{R}^d_\eta}\hat{G}(\eta)\,|\eta|\,\mathrm{d}\eta$$

and this concludes the proof. □

Proof of 3. The Weyl symbol of $\int_0^M \mathscr{B}^1_{\vec{\mu}}(s)\,e^{-\zeta s}\,\mathrm{d}s$ is

$$\begin{aligned}
&\overset{Weyl}{\mathrm{Symb}}\int_0^M \mathscr{B}^1_{\vec{\mu}}(s)\,e^{-\zeta s}\,\mathrm{d}s\\
&= \int_{\mathbb{R}^d_\eta}\hat{G}(\eta)\,e^{\mu_1 i\tilde{\sigma}}e^{i\sigma(P,X)}\left[\frac{e^{-\mu_2 is\left(\eta^{.2}-2\xi.\eta\right)-\zeta s}}{-\mu_2 i\left(\eta^{.2}-2\xi.\eta\right)-\zeta}\right]_0^M\mathrm{d}\eta\\
&= \overset{Weyl}{\mathrm{Symb}}\,\mathscr{C}^{1,\zeta}_{\vec{\mu}} + r_{\zeta,M}
\end{aligned}$$

with

$$r_{\zeta,M}(x,\xi) = -\int_{\mathbb{R}^d_\eta} \hat{G}(\eta)\, e^{\mu_1 i\tilde{\sigma}} e^{i\sigma(P,X)} \frac{e^{-\mu_2 iM\left(\eta^{\cdot 2}-2\xi.\eta\right)-\zeta M}}{\mu_2 i\left(\eta^{\cdot 2}-2\xi.\eta\right)+\zeta}\, \mathrm{d}\eta\,.$$

The remainder term $r_{\zeta,M}$ is in the symbol class $\mathcal{S}(1)$, and for $k = k(d)$, the operator norm $\left\|r^W_{\zeta,M}(-hD_\xi,\xi)\right\|_{\mathcal{L}\left(L^2_\xi\right)}$ can be controlled by

$$\sup_{|\alpha|\le k} \left\|\partial^\alpha_{x,\xi} r_{\zeta,M}\right\|_{L^\infty_{x,\xi}}\,.$$

Thus we consider

$$\begin{aligned}\left|\partial^\alpha_{x,\xi} r_{\zeta,M}(x,\xi)\right| &\le \int_{\mathbb{R}^d_\eta} \hat{G}(\eta)\,\langle P\rangle^k \left(M\langle\eta\rangle\right)^k \frac{1}{\zeta^{k+1}} e^{-\zeta M}\,\mathrm{d}\eta\\ &\le \langle P\rangle^k \left(\frac{M}{\zeta}\right)^{k+1} e^{-\zeta M} \int_{\mathbb{R}^d_\eta} \hat{G}(\eta)\,\langle\eta\rangle^k\,\mathrm{d}\eta\,.\end{aligned}$$

This yields the result

$$\left\|\int_0^M \mathscr{B}^1_{\vec{\mu}}(s)\, e^{-\zeta s} ds - \mathscr{C}^{1,\zeta}_{\vec{\mu}}\right\|_{\mathcal{L}\left(L^2_\xi\right)} \le \langle P\rangle^k \left(\frac{M}{\zeta}\right)^k e^{-\zeta M} \int_{\mathbb{R}^d_\eta} \hat{G}(\eta)\,\langle\eta\rangle^k\,\mathrm{d}\eta\,,$$

for some $k = k(d)$. The same proof holds for $\mathscr{B}^2_{\vec{\mu}}(s)$ and $\mathscr{C}^{2,\zeta}_{\vec{\mu}}$. □

2.5.5.4 Estimate of the error term $\Delta_{-,3}$

Proposition 2.5.37. *Let $b \in \mathcal{C}^\infty_0(\mathbb{R}^{2d}_{x,\xi})$ with $\mathrm{Supp}_\xi\, b \subset B_R - B_{1/R}$ for some $R > 1$. Let $\gamma \in]0,1[$. There exists a constant $C_{G,b,\gamma} > 0$ such that, for all $\zeta > 0$,*

$$|\Delta_{-,3}| \le \zeta^\gamma \mathcal{N}_k(b)\, C_{G,b,\gamma}$$

for some integer $k = k(d)$ big enough.

Proof. We recall that

$$\Delta_{-,3} = \mathrm{Tr}\left[\hat{\boldsymbol{\rho}}^{app}_t \left(Q^\zeta_- b - Qb\right)^W \left(-hD_\xi, \xi - \mathrm{d}\Gamma_\varepsilon(\eta)\right)\right]$$

so that

$$\begin{aligned}|\Delta_{-,3}| &\le \left\|\left(Q^\zeta_- b - Q_- b\right)^W \left(-hD_\xi, \xi - \mathrm{d}\Gamma_\varepsilon(\eta)\right)\right\|_{\mathcal{L}\left(L^2_\xi\otimes\Gamma L^2_\eta\right)}\\ &\le C_{k,d}\mathcal{N}_k\left(Q^\zeta_- b - Q_- b\right)\end{aligned}$$

for some integer k big enough. By recalling $Q_-^\zeta(b) = \mathfrak{c}^\zeta b$ and $Q_-(b) = \mathfrak{c} b$ it is then sufficient to prove that

$$\sup_{|\alpha|\leq k}\sup_{\xi\in[R^{-1},R]}\left|\partial_\xi^\alpha\left(\mathfrak{c}^\zeta-\mathfrak{c}\right)(\xi)\right|\leq C_{k,\gamma,G,R}\zeta^\gamma\,.$$

This is a consequence of the Lemma 2.5.38 below. □

Lemma 2.5.38. *For any integer k and γ in $[0,1[$, there exists a positive constant $C_{k,\gamma,G,C}$ such that for $\zeta\in\,]0,\zeta_0[$*

$$\sup_{|\alpha|\leq k}\sup_{|\xi|\in[R^{-1},R]}\left|\partial_\xi^\alpha\left(\mathfrak{c}^\zeta-\mathfrak{c}\right)(\xi)\right|\leq C_{k,\gamma,G,R}\zeta^\gamma\,.$$

Proof. With κ^ζ, $\mathfrak{c}$, $\mathfrak{c}^\zeta$ introduced in Definition 2.5.26, $\mathfrak{c}^\zeta-\mathfrak{c}$ can be expressed as

$$\left(\mathfrak{c}^\zeta-\mathfrak{c}\right)(\xi)=\int_{\mathbb{R}^d_\eta}\hat{G}(\eta)\,\kappa^\zeta\left(\eta^{\cdot 2}-2\xi.\eta\right)\mathrm{d}\eta-\int_{\mathbb{R}^d_\eta}\hat{G}(\xi+\eta)\,\delta\left(|\eta|^2-|\xi|^2\right)\mathrm{d}\eta\,.$$

We express the first integral as

$$\begin{aligned}\int_{\mathbb{R}^d_\eta}\hat{G}(\eta)\,\kappa^\zeta\left((\eta-\xi)^{\cdot 2}-\xi^{\cdot 2}\right)\mathrm{d}\eta&=\int_{S^{d-1}}\int_{\mathbb{R}_\rho}f_{\xi,\omega}(r)\,\kappa^\zeta\left(\xi^{\cdot 2}-r\right)\mathrm{d}r\,\mathrm{d}\omega\\&=\int_{S^{d-1}}f_{\xi,\omega}*\kappa^\zeta\left(\xi^{\cdot 2}\right)\mathrm{d}\omega\end{aligned}$$

and $f_{\xi,\omega}(r):=\frac{1}{2}r^{\frac{d-2}{2}}g(\xi+\sqrt{r}\omega)\,1_{[0,+\infty[}(r)$. The partial derivative

$$\partial_{\xi_j}f_{\xi,\omega}(r)=\frac{1}{2}r^{\frac{d-2}{2}}\partial_{\xi_j}g\left(\xi+\sqrt{r}\omega\right)1_{[0,+\infty[}(r)$$

has the same form as the function f_ξ. Then we observe that

$$\begin{aligned}&\partial_{\xi_j}\left(f_{\xi,\omega}*\kappa^\zeta-f_{\xi,\omega}\right)\left(|\xi|^2\right)\\&\quad=\left[\left(\partial_{\xi_j}f_{\xi,\omega}\right)*\kappa^\zeta-\partial_{\xi_j}f_{\xi,\omega}\right]\left(|\xi|^2\right)+\left[\partial_r\left(f_{\xi,\omega}*\kappa^\zeta-f_{\xi,\omega}\right)\right]\left(|\xi|^2\right)2\xi_j\end{aligned}$$

so that by doing successive derivations it suffices to deal only with quantities of the form

$$\partial_r^k\left(\partial_\xi^\beta f_{\xi,\omega}*\kappa^\zeta-\partial_\xi^\beta f_{\xi,\omega}\right)$$

which are in fact of the form $\partial_r^k\left(f*\kappa^\zeta-f\right)$ with f satisfying the hypotheses of Proposition 2.D.2 uniformly in ω so that we get the expected control, by integration over ω. □

2.5.5.5 Estimate of the error term $\Delta_{+,3}$

Remark 2.5.39. Throughout this section we will make definitions that are dependent on the value of $\frac{th}{\varepsilon}$. This will not be a problem as long as $\frac{th}{\varepsilon} \leq 1$ which will be satisfied with our choice of $\varepsilon = \varepsilon(h) \gg h$.

Proposition 2.5.40. *Let $b \in \mathcal{C}_0^\infty(\mathbb{R}^{2d}_{x,\xi})$ with $\mathrm{Supp}_\xi\, b \subset B_R - B_{1/R}$ for some $R > 1$. Let $\gamma \in]0,1[$. There exists a constant $C_{G,R,\gamma} > 0$ such that, for all $\zeta > 0$,*

$$|\Delta_{+,3}| \leq \zeta^\gamma \mathcal{N}_k(b)\, C_{G,R,\gamma}$$

for some integer $k = k(d)$ big enough.

Proof. We recall that

$$\Delta_{+,3} = \mathrm{Tr}\left[\hat{\boldsymbol{\rho}}_t^{app}\left(Q^\zeta_{+,\frac{ht}{\varepsilon}}b - Q_{+,\frac{ht}{\varepsilon}}b\right)^W(-hD_\xi, \xi - \mathrm{d}\Gamma_\varepsilon(\eta))\right]$$

so that

$$\begin{aligned}|\Delta_{+,3}| &\leq \left\|\left(Q^\zeta_{+,\frac{ht}{\varepsilon}}b - Q_{+,\frac{ht}{\varepsilon}}b\right)^W(-hD_\xi, \xi - \mathrm{d}\Gamma_\varepsilon(\eta))\right\|_{\mathcal{L}\left(L^2_\xi \otimes \Gamma L^2_\eta\right)}\\ &\leq C_{k,d}\mathcal{N}_k\left(Q^\zeta_{+,\frac{ht}{\varepsilon}}b - Q_{+,\frac{ht}{\varepsilon}}b\right)\end{aligned}$$

for some integer $k = k(d)$ big enough.

Thus we boil down to prove that for any integer $k \geq 0$ there is a constant $C_{k,b,G,\gamma} > 0$ such that for any $\zeta > 0$

$$\mathcal{N}_k\left(Q^\zeta_{+,\frac{ht}{\varepsilon}}b - Q_{+,\frac{ht}{\varepsilon}}b\right) \leq C_{k,G,\gamma}\mathcal{N}_k(b)\,\zeta^\gamma.$$

But we have a convenient expression for $Q^\zeta_{+,\frac{ht}{\varepsilon}}$

$$\begin{aligned}Q^\zeta_{+,\frac{ht}{\varepsilon}}b(x,\xi) &= 2\pi\int_{\mathbb{R}^d_\eta}\hat{G}(\eta)\, b\left(x - 2\frac{t}{\varepsilon}h\eta, \xi - \eta\right)\kappa^\zeta\left(\eta^{\cdot 2} - 2\xi.\eta\right)\mathrm{d}\eta\\ &= 2\pi\int_{\mathbb{R}^d_\eta}\hat{G}(\xi - \eta)\, b\left(x - 2\frac{t}{\varepsilon}h\xi + 2\frac{t}{\varepsilon}h\eta, \eta\right)\kappa^\zeta\left(\eta^{\cdot 2} - 2\xi.\eta\right)\mathrm{d}\eta\\ &= \pi\int_{\mathbb{S}^{d-1}_\omega}\int_{\mathbb{R}^+_r}\varphi_\omega(x,\xi,r)\, K^\zeta\left(r - \xi^{\cdot 2}\right)\mathrm{d}r\,\mathrm{d}\omega\,,\end{aligned}$$

with $\varphi_\omega(x,\xi,r) = 0$ for $r \leq 0$, and for $r \geq 0$,

$$\varphi_\omega(x,\xi,r) = \hat{G}\left(\xi - \sqrt{r}\omega\right) b\left(x - 2\frac{ht}{\varepsilon}\xi + 2\frac{ht}{\varepsilon}\sqrt{r}\omega, \sqrt{r}\omega\right) r^{d/2-1} \quad (2.5.20)$$

defined for $\omega \in \mathbb{S}^{d-1}$ and $x, \xi \in \mathbb{R}^d$. We also have a convenient expression for $Q_{+,\frac{ht}{\varepsilon}} b$ in terms of φ_ω,

$$Q_{+,\frac{ht}{\varepsilon}} b\,(x,\xi) = \pi \int_{\mathbb{S}_\omega^{d-1}} \varphi_\omega\left(x,\xi,\xi^{\cdot 2}\right) \mathrm{d}\omega\,.$$

The conclusion is then given by Lemma 2.5.41. □

Lemma 2.5.41. *For any $\gamma \in \,]0,1[$, uniformly in $\omega \in \mathbb{S}_\omega^{d-1}$,*

$$\mathcal{N}_k\left(\int_{\mathbb{R}_r^+} \varphi_\omega\,(x,\xi,r)\,\kappa^\zeta\left(r-\xi^{\cdot 2}\right) dr - \varphi_\omega\left(x,\xi,\xi^{\cdot 2}\right)\right) \leq C_{k,G,\gamma}\zeta^\gamma\,.$$

Proof. The integral can be expressed as a convolution product

$$\int_{\mathbb{R}_r} \varphi_\omega\,(x,\xi,r)\,\kappa^\zeta\left(r-\xi^{\cdot 2}\right) dr = \left(\varphi\,(x,\xi,\cdot) * \kappa^\zeta\right)\left(\xi^{\cdot 2}\right)\,.$$

Since the derivation behaves well with the difference, *i.e.*

$$\partial_x^\alpha \partial_\xi^\beta \left(\left(\varphi_\omega\,(x,\xi,\cdot) * \kappa^\zeta\right)\left(\xi^{\cdot 2}\right) - \varphi_\omega\left(x,\xi,\xi^{\cdot 2}\right)\right) = \sum_{\alpha',\beta',\gamma'} c_{\alpha',\beta',\gamma'} 2^{|\gamma'|} \xi^{\gamma'} \times$$
$$\left[\left(\left(\partial_x^{\alpha'}\partial_\xi^{\beta'}\partial_r^{\gamma'}\varphi_\omega\right)(x,\xi,\cdot) * \kappa^\zeta\right)\left(\xi^{\cdot 2}\right) - \left(\partial_x^{\alpha'}\partial_\xi^{\beta'}\partial_r^{\gamma'}\varphi_\omega\right)\left(x,\xi,\xi^{\cdot 2}\right)\right],$$

it suffices to apply Proposition 2.D.1. □

2.6 Comparisons of the measures of an observable at a mesoscopic scale for the original and approximated dynamics

Proposition 2.6.1. *Let $b \in \mathcal{C}_0^\infty(\mathbb{R}_{x,\xi}^{2d})$, $\rho \in \mathcal{L}_1 L_x^2$ and $t \geq 0$,*

$$m\left(b,\rho_t^\varepsilon\right) = \mathrm{Tr}\left[b^W\left(-hD_\xi, \xi - \mathrm{d}\Gamma_\varepsilon\,(\eta)\right)\hat{\boldsymbol{\rho}}_t\right],$$
$$m\left(b,\rho_t^{\varepsilon,app}\right) = \mathrm{Tr}\left[b^W\left(-hD_\xi, \xi - \mathrm{d}\Gamma_\varepsilon\,(\eta)\right)\hat{\boldsymbol{\rho}}_t^{app}\right].$$

Definition 2.6.2. Let $b \in \mathcal{C}_0^\infty(\mathbb{R}_{x,\xi}^{2d})$, $\rho \in \mathcal{L}_1 L_x^2$ a state, $t \geq 0$ and $\chi \in \mathcal{C}_0^\infty(\mathbb{R}_{x,\xi}^{2d})$ we define

$$m\,(b,\rho,t,\chi) = \mathrm{Tr}\left[\chi\left(\mathrm{d}\Gamma_\varepsilon\,(\eta)\right) b^W\left(-hD_\xi, \xi - \mathrm{d}\Gamma_\varepsilon\,(\eta)\right)\chi\left(\mathrm{d}\Gamma_\varepsilon\,(\eta)\right)\hat{\boldsymbol{\rho}}_t\right]$$
$$m^{app}\,(b,\rho,t,\chi) = \mathrm{Tr}\left[\chi\left(\mathrm{d}\Gamma_\varepsilon\,(\eta)\right) b^W\left(-hD_\xi, \xi - \mathrm{d}\Gamma_\varepsilon\,(\eta)\right)\chi\left(\mathrm{d}\Gamma_\varepsilon\,(\eta)\right)\hat{\boldsymbol{\rho}}_t^{app}\right].$$

Proposition 2.6.3. *Let b be a symbol in $\mathcal{C}_0^\infty(\mathbb{R}^{2d}_{x,\xi})$ with positive values such that $\mathrm{Supp}_\xi\, b \subset B_R - B_{1/R}$ for some $R > 0$, $\rho \in \mathcal{L}_1^+ L_x^2$ with $\mathrm{Tr}\,\rho \leq 1$ and for $j = 1, 2$, $\chi_j \in \mathcal{C}_0^\infty(\mathbb{R}^d_\lambda)$ with values in $[0,1]$, $\chi_j(B_{M_j}) = \{1\}$ for $M_1 = 3R$ and with $\chi_2(\mathbb{R}^d - B_{R+1}) = \{0\}$. There is a constant C_{R,b,χ_1,χ_2} (which does not depend on ρ) such that*

$$m\left(b, \rho_t\right) - m^{app}\left(b, (\rho_{\chi_2})_t^{app}\right) \geq -\mathcal{E}_{2.6}$$

with $\mathcal{E}_{2.6} = \mathcal{E}_{2.6.1} + \mathcal{E}_{2.6.2} + \mathcal{E}_{2.6.3}$ and $\rho_{\chi_2} = \chi_2(D_x)\rho\chi_2(D_x)$.

$$\mathcal{E}_{2.6} = C_{R,b,\chi_1,\chi_2}\left(h + \left(\frac{ht}{\varepsilon}\right)^3 h^{-3/2} + \left(\frac{ht}{\varepsilon}\right)^4 h^{-2} + \mathcal{E}_{2.5}\right).$$

We shall prove it in three steps:

1. $m\left(b, \rho_t\right) - m\left(b, \rho_{\chi_2}, t, \chi_1\right) \geq -\mathcal{E}_{2.6.1}$,
$$\mathcal{E}_{2.6.1} = Ch\,,$$
2. $m\left(b, \rho_{\chi_2}, t, \chi_1\right) - m^{app}\left(b, \rho_{\chi_2}, t, \chi_1\right) \geq -\mathcal{E}_{2.6.2}$,
$$\mathcal{E}_{2.6.2} = C_{b,R,\chi_1}\left(\left(\frac{ht}{\varepsilon}\right)^3 h^{-3/2} + \left(\frac{ht}{\varepsilon}\right)^4 h^{-2}\right),$$
3. $m^{app}\left(b, \rho_{\chi_2}, t, \chi_1\right) - m\left(b, (\rho_{\chi_2})_t^{app}\right) \geq -\mathcal{E}_{2.6.3}$,
$$\mathcal{E}_{2.6.3} = \mathcal{E}_{2.5} + Ch\,.$$

2.6.1 Step 1: Introduction of cutoffs

We will introduce cutoff functions both on the state ρ and the observable $b^W(-hD_\xi, \xi - d\Gamma_\varepsilon(\eta))$.

Proposition 2.6.4. *Let $b \in \mathcal{C}_0^\infty(\mathbb{R}^{2d}_{x,\xi})$ non-negative such that $\mathrm{Supp}_\xi\, b \subset B_R$ for some $R > 0$, $\rho \in \mathcal{L}_1^+ L_x^2$, $\mathrm{Tr}\,\rho \leq 1$, and, for $j = 1, 2$, $\chi_j \in \mathcal{C}_0^\infty(\mathbb{R}^d_\lambda)$ with values in $[0,1]$ and $\chi_j(B_{M_j}) = \{1\}$ for some $M_j > 0$. Then there is a constant C_{b,χ_1,χ_2} such that*

$$m\left(b, \rho_t\right) \geq m\left(b, \rho_{\chi_2}, t, \chi_1\right) - \mathcal{E}_{2.6.1}$$

with $\mathcal{E}_{2.6.1} = C_{b,\chi_1,\chi_2} h$ and $\rho_{\chi_2} = \chi_2(D_x) \circ \rho \circ \chi_2(D_x)$.

Proof. Using the functional calculus for the self-adjoint operator $d\Gamma_\varepsilon\left(\eta\right)$ and since

$$\begin{aligned} b\left(x, \xi - \lambda\right) &\geq \chi_2\left(\xi\right) b\left(x, \xi - \lambda\right) \chi_1\left(\lambda\right) \chi_2\left(\xi\right) \\ &\geq \chi_2\left(\xi\right) \sharp^h b\left(x, \xi - \lambda\right) \chi_1\left(\lambda\right) \sharp^h \chi_2\left(\xi\right) - C_{b,\chi_1,\chi_2} h \end{aligned}$$

holds uniformly in λ, we can write

$$\begin{aligned} &b^W\left(-hD_\xi,\xi-\mathrm{d}\Gamma_\varepsilon(\eta)\right)\\ &\qquad\geq \chi_2(\xi)\circ b^W\left(-hD_\xi,\xi-\mathrm{d}\Gamma_\varepsilon(\eta)\right)\chi_1\left(\mathrm{d}\Gamma_\varepsilon(\eta)\right)\circ\chi_2(\xi)-C_{b,\chi_1,\chi_2}h\,. \end{aligned}$$

And thus

$$\begin{aligned} m(b,\rho_t)&=\mathrm{Tr}\left[b^W\left(-hD_\xi,\xi-\mathrm{d}\Gamma_\varepsilon(\eta)\right)\hat{\boldsymbol{\rho}}_t\right]\\ &\geq \mathrm{Tr}\left[b^W\left(-hD_\xi,\xi-\mathrm{d}\Gamma_\varepsilon(\eta)\right)\chi_1\left(d\Gamma(\eta)\right)\widehat{\boldsymbol{\rho_{\chi_2}}_t}\right]-C_{b,\chi_1,\chi_2}h \end{aligned}$$

since $[H_\varepsilon,\chi_2]=0$. □

2.6.2 Step 2: Comparison between truncated solutions

Proposition 2.6.5. *Let b be a symbol in $\mathcal{C}_0^\infty(\mathbb{R}^{2d}_{x,\xi})$ with positive values, $\rho\in\mathcal{L}_1^+L_x^2$, $\mathrm{Tr}\,\rho\leq 1$ and $\chi\in\mathcal{C}_0^\infty(\mathbb{R}^d_\lambda)$ with values in $[0,1]$, and $\chi(B_M)=\{1\}$ for some $M>0$, then there is a constant $C_{G,b,\chi}$ such that*

$$\left|m(b,\rho,t,\chi)-m^{app}(b,\rho,t,\chi)\right|\leq\mathcal{E}_{2.6.2}$$

with $\mathcal{E}_{2.6.2}=C_{G,b,\chi}\left(\left(\frac{ht}{\varepsilon}\right)^3h^{-3/2}+\left(\frac{ht}{\varepsilon}\right)^4h^{-2}\right)$.

We will need the following number estimate.

Lemma 2.6.6. *Let $\hat{\psi}_0\in L^2_\xi$ be a normed vector. We have, for $\hat{\Psi}^\sharp_{h,\varepsilon,t}=\hat{\Psi}_{h,\varepsilon,t}=e^{-i\frac{t}{\varepsilon}\hat{H}}\hat{\psi}_0\otimes\Omega$ or $\hat{\Psi}^\sharp_{h,\varepsilon,t}=\hat{\Psi}^{app}_{h,\varepsilon,t}=e^{-i\frac{t}{\varepsilon}\hat{H}^{app}_{h,\varepsilon}}\hat{\psi}_0\otimes\Omega$,*

$$\left\|(\varepsilon+N_\varepsilon)^{1/2}\hat{\Psi}^\sharp_{h,\varepsilon,t}\right\|\leq C_d\left(\sqrt{\varepsilon}+\sqrt{\frac{t}{2}\frac{ht}{\varepsilon}\|\hat{G}\|_{L^1}}\right)\,.$$

Proof of the Lemma. Indeed let us define $\gamma_t=\|(\varepsilon+N_\varepsilon)^{1/2}\hat{\Psi}^\sharp_t\|$. Then

$$i\varepsilon\partial_t\left(\gamma_t^2\right)=\left\langle\hat{\Psi}^\sharp_t,\left[\Phi_\varepsilon\left(f_{h,\varepsilon}\right),N_\varepsilon\right]\hat{\Psi}^\sharp_t\right\rangle$$

with $f_{h,\varepsilon}=\sqrt{\frac{h}{\varepsilon}}\varepsilon^{d/2}\overline{\hat{V}(\varepsilon\eta)}$ since ξ and $d\Gamma_\varepsilon(\eta)$ commute with N_ε. Using $N_\varepsilon=d\Gamma_\varepsilon(1)$, we get

$$\begin{aligned} \left[a_\varepsilon\left(f_{h,\varepsilon}\right),d\Gamma_\varepsilon(1)\right]&=i\partial_s\left[\Gamma\left(e^{i\varepsilon s}\right)a_\varepsilon\left(f_{h,\varepsilon}\right)\Gamma\left(e^{-i\varepsilon s}\right)\right]\Big|_{s=0}\\ &=a_\varepsilon\left(\varepsilon f_{h,\varepsilon}\right)\,. \end{aligned}$$

The other term of the commutator can be computed analogously (but $a_\varepsilon(\cdot)$ is $\mathbb{C}$-antilinear whereas $a^*_\varepsilon(\cdot)$ is $\mathbb{C}$-linear). Introducing this relation into the differential equation and taking the modulus, we get

$$\left|i\varepsilon\partial_t\left(\gamma_t^2\right)\right|\leq\frac{1}{\sqrt{2}}\left\|\hat{\Psi}^\sharp_t\right\|\left(\left\|a_\varepsilon\left(\varepsilon f_{h,\varepsilon}\right)\hat{\Psi}^\sharp_t\right\|+\left\|a^*_\varepsilon\left(\varepsilon f_{h,\varepsilon}\right)\hat{\Psi}^\sharp_t\right\|\right)\,.$$

But

$$\left\| a_\varepsilon\left(\varepsilon f_{h,\varepsilon}\right)\hat{\Psi}_t^\sharp \right\|^2 \leq \|\varepsilon f_{h,\varepsilon}\|_{L^2_\xi}^2 \left\langle \hat{\Psi}_t^\sharp, N_\varepsilon \hat{\Psi}_t^\sharp \right\rangle ,$$
$$\left\| a_\varepsilon^*\left(\varepsilon f_{h,\varepsilon}\right)\hat{\Psi}_t^\sharp \right\|^2 \leq \|\varepsilon f_{h,\varepsilon}\|_{L^2_\xi}^2 \left\langle \hat{\Psi}_t^\sharp, \left(\varepsilon + N_\varepsilon\right) \hat{\Psi}_t^\sharp \right\rangle .$$

Using $\|\hat{G}\|_{L^1} = \frac{h}{\varepsilon}\|f_{h,\varepsilon}\|_{L^2_\xi}^2$, we finally get a differential inequality for the function γ_t

$$2\varepsilon\gamma_t\partial_t\gamma_t \leq \left|i\varepsilon\partial_t\left(\gamma_t^2\right)\right| \leq \sqrt{2\varepsilon h\|\hat{G}\|_{L^1}}\,\gamma_t\,.$$

Dividing by $2\varepsilon\gamma_t$ and integrating in time, we obtain the expected result

$$\gamma_t \leq \gamma_0 + t\sqrt{\frac{h}{2\varepsilon}\|\hat{G}\|_{L^1}}\,,$$

since $\gamma_0 = C_d\sqrt{\varepsilon}$. □

Set

$$b_\chi = b\left(-hD_\xi, \xi - \mathrm{d}\Gamma_\varepsilon\left(\eta\right)\right)\chi\left(\mathrm{d}\Gamma_\varepsilon\left(\eta\right)\right)\,. \tag{2.6.1}$$

We want to control the error when we consider $\mathrm{Tr}\left[b_\chi \boldsymbol{\rho}_t^{app}\right]$ instead of $\mathrm{Tr}\left[b_\chi \boldsymbol{\rho}_t\right]$ *i.e.* we want to control $\mathrm{Tr}\left[b_\chi u_t\right]$ with

$$u_t = \boldsymbol{\rho}_t - \boldsymbol{\rho}_t^{app}\,. \tag{2.6.2}$$

Since

$$i\varepsilon\partial_t\boldsymbol{\rho}_t = \left[H_\varepsilon, \boldsymbol{\rho}_t\right]$$
$$i\varepsilon\partial_t\boldsymbol{\rho}_t^{app} = \left[H_\varepsilon, \boldsymbol{\rho}_t^{app}\right] - \left[H_\varepsilon - H_\varepsilon^{app}, \boldsymbol{\rho}_t^{app}\right]$$

the difference u_t is solution of the differential equation

$$\begin{aligned} i\varepsilon\partial_t u_t &= \left[H_\varepsilon, u_t\right] - \left[\mathrm{d}\Gamma_\varepsilon\left(\eta\right)^2 - \varepsilon\,\mathrm{d}\Gamma_\varepsilon\left(\eta^2\right), \boldsymbol{\rho}_t^{app}\right] \\ &= \left[\left(\xi - \mathrm{d}\Gamma_\varepsilon\left(\eta\right)\right)^2, u_t\right] + \left[\Phi_\varepsilon\left(f_{h,\varepsilon}\right), u_t\right] \\ &\quad - \left[\mathrm{d}\Gamma_\varepsilon\left(\eta\right)^2 - \varepsilon\,\mathrm{d}\Gamma_\varepsilon\left(\eta^2\right), \boldsymbol{\rho}_t^{app}\right] \end{aligned}$$

with initial data $u_{t=0} = 0$. We thus get an integral expression for $\mathrm{Tr}\left[b_\chi u_t\right]$,

$$\begin{aligned} \mathrm{Tr}\left[b_\chi u_t\right] &= -\frac{i}{\varepsilon}\int_0^t \mathrm{Tr}\left[b_\chi\left[\left(\xi - \mathrm{d}\Gamma_\varepsilon\left(\eta\right)\right)^2, u_s\right]\right]\mathrm{d}s \\ &\quad + \frac{i}{\varepsilon}\int_0^t \mathrm{Tr}\left[b_\chi\left[\mathrm{d}\Gamma_\varepsilon\left(\eta\right)^2 - \varepsilon\,\mathrm{d}\Gamma_\varepsilon\left(\eta^2\right), \boldsymbol{\rho}_s^{app}\right]\right]\mathrm{d}s \\ &\quad - \frac{i}{\varepsilon}\int_0^t \mathrm{Tr}\left[b_\chi\left[\Phi_\varepsilon\left(f_{h,\varepsilon}\right), u_s\right]\right]\mathrm{d}s\,. \end{aligned}$$

Remark 2.6.7. Let $\mathcal{H}$ be a Hilbert space. If A, $B \in \mathcal{L}(\mathcal{H})$ and $C \in \mathcal{L}_1(\mathcal{H})$, then

$$\mathrm{Tr}\left[A\left[B, C\right]\right] = \mathrm{Tr}\left[\left[A, B\right] C\right] .$$

Lemma 2.6.8. *There exists a constant C independent of χ such that for b_χ and u_t defined by Equations (2.6.1) and (2.6.2),*

1. $\left|\frac{1}{\varepsilon}\int_0^t \mathrm{Tr}\left[b_\chi\left[\left(\xi - \mathrm{d}\Gamma_\varepsilon\left(\eta\right)\right)^2, u_{h,\varepsilon,s}\right]\right] \mathrm{d}s\right| \le \frac{h}{\varepsilon}\int_0^t \left\|u_{h,\varepsilon,s}\right\|_{\mathcal{L}_1} \mathrm{d}s \le C\frac{h^2t^3}{\varepsilon^3}$,
2. $\frac{1}{\varepsilon}\int_0^t \mathrm{Tr}\left[b_\chi\left[\mathrm{d}\Gamma_\varepsilon\left(\eta\right)^2 - \varepsilon\,\mathrm{d}\Gamma_\varepsilon\left(\eta^2\right), \boldsymbol{\rho}^{app}\right]\right] \mathrm{d}s = 0$,
3. $\left|\frac{1}{\varepsilon}\int_0^t \mathrm{Tr}\left[b_\chi\left[\Phi_\varepsilon\left(f_{h,\varepsilon}\right), u_s\right]\right] \mathrm{d}s\right| \le C\frac{t^3h^{3/2}}{\varepsilon^{7/2}}\left(\sqrt{\varepsilon} + \sqrt{\frac{t}{2}}\sqrt{\frac{ht}{\varepsilon}}\right)$.

Proof of 1. Let us introduce $\chi_1 \succ \chi$ in order to handle only bounded operators:

$$\begin{aligned}
&\mathrm{Tr}\left[b_\chi\left[\left(\xi - \mathrm{d}\Gamma_\varepsilon\left(\eta\right)\right)^2, u_s\right]\right] \\
&\quad = \mathrm{Tr}\left[b_\chi\chi_1\left(\mathrm{d}\Gamma_\varepsilon\left(\eta\right)\right)\left[\left(\xi - \mathrm{d}\Gamma_\varepsilon\left(\eta\right)\right)^2, u_s\right]\right] \\
&\quad = \mathrm{Tr}\left[b_\chi\left[\chi_1\left(\mathrm{d}\Gamma_\varepsilon\left(\eta\right)\right)\left(\xi - \mathrm{d}\Gamma_\varepsilon\left(\eta\right)\right)^2, u_s\right]\right] \\
&\quad = \mathrm{Tr}\left[\left[b_\chi, \chi_1\left(\mathrm{d}\Gamma_\varepsilon\left(\eta\right)\right)\left(\xi - \mathrm{d}\Gamma_\varepsilon\left(\eta\right)\right)^2\right] u_s\right] \\
&\quad = \mathrm{Tr}\left[\chi\left(\mathrm{d}\Gamma_\varepsilon\left(\eta\right)\right)\frac{h}{i}\left\{b\left(x,\xi\right), \xi^2\right\}\left(-hD_\xi, \xi - \mathrm{d}\Gamma_\varepsilon\left(\eta\right)\right) u_s\right] \\
&\quad = \mathrm{Tr}\left[\frac{h}{i}\chi\left(\mathrm{d}\Gamma_\varepsilon\left(\eta\right)\right)\left(2\xi.b\right)\left(-hD_\xi, \xi - \mathrm{d}\Gamma_\varepsilon\left(\eta\right)\right) u_s\right] .
\end{aligned}$$

We can then estimate the initial trace by

$$\begin{aligned}
&\left|\mathrm{Tr}\left[b_\chi\left[\left(\xi - \mathrm{d}\Gamma_\varepsilon\left(\eta\right)\right)^2, u_s\right]\right]\right| \\
&\le h\left\|\chi\left(\mathrm{d}\Gamma_\varepsilon\left(\eta\right)\right)\left(2\xi.b\right)\left(-hD_\xi, \xi - \mathrm{d}\Gamma_\varepsilon\left(\eta\right)\right)\right\|_{\mathcal{L}L^2_\xi\otimes\Gamma L^2_\eta}\left\|u_s\right\|_{\mathcal{L}_1 L^2_\xi\otimes\Gamma L^2_\eta} \\
&\le Ch\left\|u_s\right\|_{\mathcal{L}_1 L^2_\xi\otimes\Gamma L^2_\eta}
\end{aligned}$$

and a time integration brings

$$\left|\frac{1}{\varepsilon}\int_0^t \mathrm{Tr}\left[b_\chi\left[\left(\xi - \mathrm{d}\Gamma_\varepsilon\left(\eta\right)\right)^2, u_s\right]\right] \mathrm{d}s\right| \le C\frac{h}{\varepsilon}\int_0^t \left\|u_s\right\|_{\mathcal{L}_1} \mathrm{d}s\,.$$

Then we use that both $\hat{\boldsymbol{\rho}}_t$ and $\hat{\boldsymbol{\rho}}_t^{app}$ have the same initial value $\rho_0 \otimes \mathrm{proj}\,\Omega$ with $\rho_0 = \sum_j \lambda_j \left|\psi_{0,j}\right\rangle\left\langle\psi_{0,j}\right|$, $\sum_j \lambda_j = \mathrm{Tr}\,\rho$, $\lambda_j \ge 0$, $\left\|\psi_{0,j}\right\| = 1$ to write

$$\boldsymbol{\rho}_t = \sum_j \lambda_j \left|\varphi_{t,j}\right\rangle\left\langle\varphi_{t,j}\right| , \qquad \boldsymbol{\rho}_t^{app} = \sum_j \lambda_j \left|\varphi_{t,j}^{app}\right\rangle\left\langle\varphi_{t,j}^{app}\right| ,$$

and then $u_t = \sum_j \lambda_j \big(|\Psi_{t,j} - \Psi_{t,j}^{app}\rangle\langle \Psi_{t,j}| - |\Psi_{t,j}^{app}\rangle\langle \Psi_{t,j}^{app} - \Psi_{t,j}| \big)$ and

$$\|u_t\|_{\mathcal{L}_1 L^2_\xi} \le 2 \sum_j \lambda_j \left\| \Psi_{t,j} - \Psi_{t,j}^{app} \right\| \le C \frac{ht^2}{\varepsilon^2} \,.$$

This and the integral above yield the result. □

Proof of 2. Let $\chi_1 \succ \chi$,

$$\begin{aligned}
&\mathrm{Tr}\left[b_\chi \left[\mathrm{d}\Gamma_\varepsilon(\eta)^2 - \varepsilon\, \mathrm{d}\Gamma_\varepsilon\left(\eta^2\right), u_s \right] \right] \\
&\quad = \mathrm{Tr}\left[b_\chi \left[\chi_1\left(\mathrm{d}\Gamma_\varepsilon(\eta)\right) \left(d\Gamma_\varepsilon(\eta)^2 - \varepsilon\, \mathrm{d}\Gamma_\varepsilon\left(\eta^2\right) \right), u_s \right] \right] \\
&\quad = \mathrm{Tr}\left[\left[\chi_1\left(\mathrm{d}\Gamma_\varepsilon(\eta)\right) \left(\mathrm{d}\Gamma_\varepsilon(\eta)^2 - \varepsilon\, \mathrm{d}\Gamma_\varepsilon\left(\eta^2\right) \right), b_\chi \right] u_s \right] \\
&\quad = 0
\end{aligned}$$

since

$$\left[\chi_1\left(\mathrm{d}\Gamma_\varepsilon(\eta)\right) \left(\mathrm{d}\Gamma_\varepsilon(\eta)^2 - \varepsilon\, \mathrm{d}\Gamma_\varepsilon\left(\eta^2\right) \right), b_\chi \right] = 0 \,.$$

□

Proof of 3. We have, with $r_s = \hat{\Psi}_s - \hat{\Psi}_s^{app}$,

$$\mathrm{Tr}\left[b_\chi \left[\Phi_\varepsilon(f_{h,\varepsilon}), u_s \right] \right] = \langle r_s | \left[b_\chi, \Phi_\varepsilon(f_{h,\varepsilon}) \right] \big| \hat{\Psi}_s \big\rangle + \big\langle \hat{\Psi}_s^{app} \big| \left[b_\chi, \Phi_\varepsilon(f_{h,\varepsilon}) \right] |r_s\rangle \,.$$

Taking the modulus we obtain

$$\begin{aligned}
\left| \mathrm{Tr}\left[b_\chi \left[\Phi_\varepsilon(f_{h,\varepsilon}), u_s \right] \right] \right| &\le C \|r_s\| \left\| \Phi_\varepsilon(f_{h,\varepsilon}) \hat{\Psi}_s \right\| + \|r_s\| \left\| \Phi_\varepsilon(f_{h,\varepsilon}) b_\chi \hat{\Psi}_s \right\| \\
&\quad + \|r_s\| \left\| \Phi_\varepsilon(f_{h,\varepsilon}) b_\chi^* \hat{\Psi}_s^{app} \right\| + C \|r_s\| \left\| \Phi_\varepsilon(f_{h,\varepsilon}) \hat{\Psi}_s^{app} \right\|
\end{aligned}$$

and we observe that

$$\left\| \Phi_\varepsilon(f_{h,\varepsilon}) \Psi_s^\sharp \right\| \le \|f_{h,\varepsilon}\| \left\| (\varepsilon + N_\varepsilon)^{1/2} \hat{\Psi}_s^\sharp \right\|$$

and

$$\left\| \Phi_\varepsilon(f_{h,\varepsilon}) b_\chi \hat{\Psi}_s^\sharp \right\|^2 \le C \|f_{h,\varepsilon}\|^2 \left\| (\varepsilon + N_\varepsilon)^{1/2} \hat{\Psi}_s^\sharp \right\|^2$$

and thus

$$\left| \mathrm{Tr}\left[b_\chi \left[\Phi_\varepsilon(f_{h,\varepsilon}), u_s \right] \right] \right| \le C \|r_s\| \sqrt{\frac{h}{\varepsilon} \|\hat{G}\|_{L^1}} \left(\sqrt{\varepsilon} + \frac{s}{\sqrt{2}} \|f_{h,\varepsilon}\|_{L^2_\xi} \right)$$

by our number estimate. An integration then gives

$$\left| \frac{1}{\varepsilon} \int_0^t \mathrm{Tr}\left[b_\chi \left[\Phi_\varepsilon(f_{h,\varepsilon}), u_s \right] \right] \mathrm{d}s \right| \le C \frac{t^3 h^{3/2}}{\varepsilon^{7/2}} \|\hat{G}\|_{L^1}^{1/2} \left(\sqrt{\varepsilon} + t \sqrt{\frac{h}{2\varepsilon} \|\hat{G}\|_{L^1}} \right)$$

which is the expected estimate. □

2.6.3 Step 3: Release of the truncation on the symbol

Proposition 2.6.9. *Let b be a symbol in $\mathcal{C}_0^\infty(\mathbb{R}^{2d}_{x,\xi})$ with positive values, such that $\mathrm{Supp}_\xi\, b \subset B_R - B_{1/R}$ for some $R > 1$, $\rho \in \mathcal{L}_1^+ L^2_x$, $\mathrm{Tr}\,\rho \leq 1$, with the support of $\hat{\rho}$ in B^2_{R+1} and $\chi \in \mathcal{C}_0^\infty(\mathbb{R}^d_\lambda)$ with values in $[0,1]$, $\chi(B_{3R}) = \{1\}$. There is a constant $C_{R,b,\chi}$ such that*

$$m^{app}(b,\rho,t,\chi) - m(b,\rho_t^{app}) \geq \mathcal{E}_{2.6.3}$$

with

$$\begin{aligned}\mathcal{E}_{2.6.3} &= \mathcal{E}_{2.5} + C_{R,b,\chi} h \\ &= C\frac{ht}{\varepsilon}\left(\frac{ht}{\varepsilon} + h + \left[h\left(\frac{ht}{\varepsilon}\right)^{-1}\right]^{d/2-1} + h^{\nu(d,\alpha)} + h^{\gamma\beta(d,\alpha)}\right) + C_{r,b,\chi} h\,.\end{aligned}$$

Proof. We can restrict the proof to the case of $\rho = |\psi\rangle\langle\psi|$ with $\psi \in L^2_x$ since ρ is trace class, then $\hat{\boldsymbol{\rho}}_t = |\hat{\Psi}_t^{app}\rangle\langle\hat{\Psi}_t^{app}|$. We also define a positive symbol $b_1 \in \mathcal{C}_0^\infty(\mathbb{R}^d_\xi)$ such that $\mathrm{Supp}\, b_1 \subset [R^{-2}, R^2]$ and $b_1(\xi^2) \geq b(x,\xi)$. Then

$$\begin{aligned}
&m(b,\rho_t^{app}) - m^{app}(b,\rho,t,\chi)\\
&= \mathrm{Tr}\left[b^W(-hD_\xi, \xi - \mathrm{d}\Gamma_\varepsilon(\eta))(1-\chi(\mathrm{d}\Gamma_\varepsilon(\eta)))\hat{\boldsymbol{\rho}}_t\right]\\
&= \mathrm{Tr}\left[(1-\chi(\mathrm{d}\Gamma_\varepsilon(\eta)))^{1/2} b^W(-hD_\xi, \xi - \mathrm{d}\Gamma_\varepsilon(\eta))(1-\chi(\mathrm{d}\Gamma_\varepsilon(\eta)))^{1/2}\hat{\boldsymbol{\rho}}_t\right]\\
&\leq \mathrm{Tr}\left[b_1^W\left((\xi - \mathrm{d}\Gamma_\varepsilon(\eta))^{\cdot 2}\right)^2(1-\chi(\mathrm{d}\Gamma_\varepsilon(\eta)))\hat{\boldsymbol{\rho}}_t\right] + \mathcal{O}(h)\\
&= \mathrm{Tr}\left[b_1^W\left((\xi - \mathrm{d}\Gamma_\varepsilon(\eta))^{\cdot 2}\right)(1-\chi(\mathrm{d}\Gamma_\varepsilon(\eta)))b_1^W\left((\xi - \mathrm{d}\Gamma_\varepsilon(\eta))^{\cdot 2}\right)\hat{\boldsymbol{\rho}}_t\right] + \mathcal{O}(h)
\end{aligned}$$

with $\hat{\Psi}_t^{app}(\xi) = 1_{[0,M]}(|\xi|)\,\hat{\Psi}_t^{app}(\xi)$ and $\mathrm{Supp}\, b_1 \subset [R^{-2}, R^2]$. Then we decompose

$$\begin{aligned}\hat{\Psi}_t^{app} &= 1_{[1/2R,2R]}(|\xi|)\,\hat{\Psi}_t^{app} + 1_{[0,M]\setminus[1/2R,2R]}(|\xi|)\,\hat{\Psi}_t^{app}\\ &= \hat{\Psi}_{t,1}^{app} + \hat{\Psi}_{t,2}^{app}\,.\end{aligned}$$

With $A = b_1^W\left((\xi - \mathrm{d}\Gamma_\varepsilon(\eta))^{\cdot 2}\right)(1-\chi(\mathrm{d}\Gamma_\varepsilon(\eta)))b_1^W\left((\xi - \mathrm{d}\Gamma_\varepsilon(\eta))^{\cdot 2}\right) \geq 0$ we have the estimate

$$\mathrm{Tr}\left[A\left|\hat{\Psi}_t^{app}\right\rangle\left\langle\hat{\Psi}_t^{app}\right|\right] \leq 2\,\mathrm{Tr}\left[A\left|\hat{\Psi}_{t,1}^{app}\right\rangle\left\langle\hat{\Psi}_{t,1}^{app}\right|\right] + 2\,\mathrm{Tr}\left[A\left|\hat{\Psi}_{t,2}^{app}\right\rangle\left\langle\hat{\Psi}_{t,2}^{app}\right|\right].$$

For the first term,

$$\begin{aligned}
&\mathrm{Tr}\left[b_1^W\left((\xi - \mathrm{d}\Gamma_\varepsilon(\eta))^{\cdot 2}\right)(1-\chi(\mathrm{d}\Gamma_\varepsilon(\eta)))b_1^W\left((\xi - \mathrm{d}\Gamma(\eta))^{\cdot 2}\right)\left|\hat{\Psi}_{t,1}^{app}\right\rangle\left\langle\hat{\Psi}_{t,1}^{app}\right|\right]\\
&= \mathrm{Tr}\Big[1_{[1/2R,2R]}(|\xi|)\,b_1^W\left((\xi - \mathrm{d}\Gamma_\varepsilon(\eta))^{\cdot 2}\right)(1-\chi(\mathrm{d}\Gamma_\varepsilon(\eta)))\\
&\qquad b_1^W\left((\xi - \mathrm{d}\Gamma_\varepsilon(\eta))^{\cdot 2}\right)1_{[1/2R,2R]}(|\xi|)\left|\hat{\Psi}_{t,1}^{app}\right\rangle\left\langle\hat{\Psi}_{t,1}^{app}\right|\Big]\\
&= 0
\end{aligned}$$

since $|\xi| \in [1/2R, 2R]$, $|\xi - \mathrm{d}\Gamma_\varepsilon(\eta)| \leq R$ implies $|\mathrm{d}\Gamma_\varepsilon(\eta)| \leq 3R$ and $\chi(B_{3R}) = \{1\}$. For the second term,

$$\mathrm{Tr}\left[b_1^W\left((\xi - \mathrm{d}\Gamma_\varepsilon(\eta))^{.2}\right)(1-\chi(\mathrm{d}\Gamma_\varepsilon(\eta)))\, b_1^W\left((\xi - \mathrm{d}\Gamma(\eta))^{.2}\right)\left|\hat{\Psi}^{app}_{t,2}\right\rangle\left\langle\hat{\Psi}^{app}_{t,2}\right|\right]$$
$$\leq \mathrm{Tr}\left[b_1^W\left((\xi - \mathrm{d}\Gamma_\varepsilon(\eta))^{.2}\right)^2\left|\hat{\Psi}^{app}_{t,2}\right\rangle\left\langle\hat{\Psi}^{app}_{t,2}\right|\right]$$

since $1 - \chi(d\Gamma_\varepsilon(\eta)) \leq \mathrm{Id}$. Then we use the computation of the evolution of a symbol of $|\xi|^2$ in the case of the approximated equation as in Remark 2.5.2 to get that, since $b_1 = b_1(|\xi|^2)$ it is unchanged under the evolution, and

$$\begin{aligned}
&\mathrm{Tr}\left[b_1^W\left((\xi - \mathrm{d}\Gamma_\varepsilon(\eta))^{.2}\right)^2\left|\hat{\Psi}^{app}_{t,2}\right\rangle\left\langle\hat{\Psi}^{app}_{t,2}\right|\right] \\
&\leq \mathrm{Tr}\left[b_1^W\left((\xi - \mathrm{d}\Gamma_\varepsilon(\eta))^{.2}\right)^2\left|\hat{\psi}_{0,2}\otimes\Omega\right\rangle\left\langle\hat{\psi}_{0,2}\otimes\Omega\right|\right] + \mathcal{E}_{2.5} \\
&\leq \mathrm{Tr}\left[b_1^W\left(\xi^{.2}\right)^2\left|\hat{\psi}_{0,2}\otimes\Omega\right\rangle\left\langle\hat{\psi}_{0,2}\otimes\Omega\right|\right] + \mathcal{E}_{2.5} \\
&\leq \mathcal{E}_{2.5}
\end{aligned}$$

since $\mathrm{Supp}\, b_1 \cap \mathrm{Supp}\, \hat{\psi}_{0,2} = \emptyset$. □

2.7 The derivation of the Boltzmann equation for the model

Proposition 2.7.1. *Let $b \in \mathcal{C}_0^\infty(\mathbb{R}^{2d}_{x,\xi})$ with $\mathrm{Supp}_\xi\, b \subset B_R - B_{1/R}$. Let ρ a state and $T > 0$.*

$$\liminf_{h\to 0}\left(m\left(b, \rho^h_{N,\Delta t}\right) - m\left(\mathcal{B}^T(T)\, b, \rho\right)\right) \geq 0$$

for a fixed $\alpha \in \left]\frac{3}{4}, 1\right[$, $\Delta t = \Delta t(h) = h^\alpha$ and $N(h)\,\Delta t(h) = T$.

Proof. We define for $k \in \mathbb{N}$, $\Delta t > 0$, $b_{k,\Delta t} = \left(e^{\Delta t Q} e^{2\Delta t \xi.\partial_x}\right)^k b$. We begin by looking to one step of evolution with $e^{\Delta t Q} e^{2\Delta t \xi.\partial_x}$. □

Lemma 2.7.2. *With $b_t = e^{tQ} e^{2t\xi.\partial_x} b$, and the hypotheses of Proposition 2.7.1,*

$$\begin{aligned}
&m\left(b, \rho^h_{\Delta t}\right) - m\left(b_{\Delta t}, \rho\right) \\
&\geq -C\left(h + h^{-3/2}(\Delta t)^3 + (\Delta t)^4 h^{-2} + \Delta t\left(\Delta t + h + (h/\Delta t)^{d/2-1} + h^\mu\right)\right).
\end{aligned}$$

Proof. We recall that $\rho^h_{\Delta t} = \rho^\varepsilon_{\varepsilon\Delta t/h}$ so that with $\frac{ht}{\varepsilon} = \Delta t$, from Section 2.6,

$$\begin{aligned}
&m\left(b, \rho^h_{\Delta t}\right) - m\left(b, (\rho_{\chi_2})^{h,app}_{\Delta t}\right)\\
&= m\left(b, \rho^\varepsilon_t\right) - m\left(b, (\rho_{\chi_2})^{\varepsilon,app}_t\right)\\
&\geq -C\left(h + (ht/\varepsilon)^3 h^{-3/2} + (ht/\varepsilon)^4 h^{-2} + ht/\varepsilon\left(ht/\varepsilon + h + (\varepsilon/t)^{d/2-1} + h^\mu\right)\right)\\
&\geq -C\left(h + h^{-3/2}(\Delta t)^3 + (\Delta t)^4 h^{-2} + \Delta t\left(\Delta t + h + (h/\Delta t)^{d/2-1} + h^\mu\right)\right)
\end{aligned}$$

and from Part 2.5 also used with $\frac{ht}{\varepsilon} = \Delta t$ we get

$$m\left(b, (\rho_{\chi_2})^{\varepsilon,app}_t\right) - m\left(b_t, \rho_{\chi_2}\right) \geq -\mathcal{E}_{2.5} \geq -\mathcal{E}_{2.6}$$

and this term will be in particular controlled if we control the previous one. Finally from the conservation of the support in ξ of the symbol by the approximated Boltzmann equation we get

$$m\left(b_t, \rho_{\chi_2}\right) - m\left(b_t, \rho\right) \geq -\mathcal{O}\left(h^\infty\right)$$

for χ_2 a cutoff function chosen so that $\chi_2\left(B_R\right) = \{1\}$.

Thus we fix, for $j = 1, 2$, two cutoff functions $\chi_j \in \mathcal{C}_0^\infty(\mathbb{R}^d_\lambda)$ with values in $[0,1]$, $\chi_j(B_{M_j}) = \{1\}$ for $M_1 = 3R$ and $M_2 = 1$ and with $\chi_2(\mathbb{R}^d - B_{R+1}) = \{0\}$.

Then we can iterate this $N(h)$ times and we get the estimation

$$\begin{aligned}
&m\left(b, \rho^\varepsilon_{N(h),\varepsilon\Delta t/h}\right) - m\left(b_{N,\Delta t}, \rho\right)\\
&\geq -CN\left(h + h^{-3/2}(\Delta t)^3 + (\Delta t)^4 h^{-2} + \Delta t\left(\sqrt{\Delta t} + h + (h/\Delta t)^{d/2-1} + h^\mu\right)\right)
\end{aligned}$$

with $N\Delta t = T$ and $h^\alpha \leq \frac{ht}{\varepsilon} = \Delta t \leq 1$ for some $\alpha \in]1/2, 1[$. Thus we can choose $\Delta t = \frac{th}{\varepsilon} = h^\alpha$ and thus $N = Th^{-\alpha}$. Then we get the estimate

$$\begin{aligned}
&m\left(b, \rho_{N,\varepsilon\Delta t/h}\right) - m\left(b_{N,\Delta t}, \rho\right)\\
&\geq -CTh^{-\alpha}\left(h + h^{3\alpha-3/2} + h^{4\alpha-2} + h^\alpha\left(h^{\alpha/2} + h + h^{(1-\alpha)(d/2-1)} + h^\mu\right)\right)\\
&\geq -CTo_{h\to 0}(1)\ ,
\end{aligned}$$

for $\alpha \in]\frac{3}{4}, 1[$. Finally it suffices to prove that

$$\lim_{h\to 0} m\left(b_{N(h),\Delta t(h)}, \rho\right) = m\left(b_T, \rho\right)$$

which is true since the estimates of Proposition 2.2.9 prove that, for some constant $C > 0$, $\|b_{N,\Delta t} - b_T\|_{\mathcal{L}L^2_x} \leq \frac{C}{N}$. □

2.A Stochastics

We recall some results about Gaussian random fields that can be found in [40, 45].

Definition 2.A.1. Let $(\Omega_{\mathbb{P}}, \mathcal{G}, \mathbb{P})$ be a probability space. A real-valued random field $(\mathcal{V}_\omega(x))_{(\omega,x)\in\Omega_{\mathbb{P}}\times\mathbb{R}^d}$ is a *Gaussian random field* if for all finite choices of $x_1, \ldots, x_k \in \mathbb{R}^d$, $(\mathcal{V}_\omega(x_1), \ldots, \mathcal{V}_\omega(x_k))$ is an $\mathbb{R}^k$ valued Gaussian random variable. To each such Gaussian process we can associate a *mean function* $\mu(x) = \mathbb{E}[\mathcal{V}(x)]$ $(x \in \mathbb{R}^d)$ and a *covariance function* $\Sigma(x, x') = \mathbb{E}[\mathcal{V}(x)\mathcal{V}(x')]$ $(x, x' \in \mathbb{R}^d)$. A Gaussian random field is *translation invariant* if its covariance function $\Sigma(x, x')$ only depends on the difference $x - x'$, *i.e.* if there is a function $G : \mathbb{R}^d \to \mathbb{R}$ such that $\Sigma(x, x') = G(x - x')$.

Definition 2.A.2. A function $\Sigma : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ is *symmetric* if for all x, $x' \in \mathbb{R}^d$, $\Sigma(x, x') = \Sigma(x', x)$. It is *positive definite* if for all $x_1, \ldots, x_k \in \mathbb{R}^d$ and all $\xi_1, \ldots, \xi_k \in \mathbb{R}$,

$$\sum_{i=1}^{k}\sum_{j=1}^{k} \xi_i \Sigma(x_i, x_j)\xi_j \geq 0\,.$$

A function $G : \mathbb{R}^d \to \mathbb{R}$ is *positive definite* if $\Sigma(x, x') = G(x - x')$ is positive definite.

Theorem 2.A.3. *Given an arbitrary function $\mu : \mathbb{R}^d \to \mathbb{R}$, and a symmetric, positive definite function $\Sigma : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$, there exists a Gaussian random field $\mathcal{V}(x)$ with mean μ and covariance Σ.*

See [40] for a proof of Theorem 2.A.3.

Theorem 2.A.4 (Bochner). *A function $G : \mathbb{R}^d \to \mathbb{R}$ is the Fourier transform of a positive bounded Borel measure on $\mathbb{R}^d$ if and only if it is continuous and positive definite.*

See [45] and the references therein for Bochner's theorem.

Theorem 2.A.5 (Minlos). *A function $c : \mathcal{S}(\mathbb{R}^d) \to \mathbb{C}$ is the Fourier transform*

$$c(f) = \int_{\mathcal{S}'(\mathbb{R}^d)} \exp(-i\langle f, T\rangle)\,\mathrm{d}\mu(T)$$

of a cylinder set measure μ on $\mathcal{S}'(\mathbb{R}^d)$ if and only if

1. $c(0) = 1$,
2. *$f \mapsto c(f)$ is continuous in the strong topology,*

3. for any $f_1, \dots, f_n \in \mathcal{S}(\mathbb{R}^d)$ *and* $z_1, \dots, z_n \in \mathbb{C}$,

$$\sum_{i,j=1}^{n} z_i z_j c(f_i - f_j) \geq 0\,.$$

See [45] and the references therein for Minlos' theorem.

Definition 2.A.6. We consider the probability space $(\mathcal{S}'(\mathbb{R}^d), \mu)$ (the σ-algebra is the one generated by the cylinder sets) where μ is the measure obtained by Minlos' theorem with the positive definite function

$$c(f) = \exp\left(-\frac{\|f\|_{L^2}^2}{4}\right).$$

The *white noise* is the random variable on $\left(\mathcal{S}'\left(\mathbb{R}^d\right), \mu\right)$ with values in $\mathcal{S}'\left(\mathbb{R}^d\right)$ defined by $W_\omega = \omega$.

Remark 2.A.7. Since $\|f\|_{L^2}^2 = \langle f(x_1), \delta(x_1 - x_2) f(x_2)\rangle$ we have (in a weak sense)

$$\mathbb{E}[W(x_1)W(x_2)] = \delta(x_1 - x_2)\,.$$

Proposition 2.A.8. *Let* $G : \mathbb{R}^d \to \mathbb{R}$ *positive definite, such that* $\hat{G} = |\hat{V}|^2$ *with* $\hat{V} \in \mathcal{S}(\mathbb{R}^d; \mathbb{R})$. *The translation invariant centered Gaussian random field of covariance* $G(x - x')$ *is* $\mathcal{V}_\omega = V * W_\omega$ *where* W_ω *is the white noise.*

Remark 2.A.9. Bochner's theorem justifies the form we choose for the function G as the positivity of the Fourier transform is natural for a covariance function.

Proof. After testing with elements in $\mathcal{S}(\mathbb{R}^d)$ the following calculations hold. The mean of $V * W_\omega(x)$ is zero:

$$\mathbb{E}[V * W_\omega(x)] = \int V(x - x_1)\, \mathbb{E}[W_\omega(x_1)]\, \mathrm{d}x_1 = 0$$

and its covariance is

$$\begin{aligned}
\mathbb{E}[\mathcal{V}(x)\, \mathcal{V}(x')] &= \mathbb{E}\Big[\int V(x - x_1)\, W(x_1)\, V(x' - x_2)\, W(x_2)\, \mathrm{d}x_1\, \mathrm{d}x_2\Big] \\
&= \int V(x - x_1)\, V(x' - x_1)\, \mathrm{d}x_1 \\
&= V * V(-\cdot)\,(x - x')
\end{aligned}$$

and $\mathcal{F}\left(V * V\left(-\cdot\right)\right) = |\hat{V}|^2$, so that we get the expected covariance. □

2.B Semiclassical Measures

Semiclassical measures (and microlocal defect measures) have been studied among others in [26, 32, 33, 41]. We recall here some results. The first theorem can be found in [26].

Theorem 2.B.1. *Let (u_k) be a sequence of L^2_x such that $u_k \rightharpoonup u$ weakly. For all real sequence (h_k) such that $h_k \to 0$, there exist a subsequence (u_{k_n}) of the sequence (u_k) and a measure $\mu \in \mathcal{M}_+(\mathbb{R}^{2d}_{x,\xi})$ such that for all $b \in \mathcal{C}^\infty_0(\mathbb{R}^{2d}_{x,\xi})$,*

$$\lim_{n\to+\infty} \langle b(h_{k_n}x, D_x)u_{k_n}, u_{k_n}\rangle = \int_{\mathbb{R}^{2d}_{x,\xi}} b \,\mathrm{d}\mu\,.$$

Definition 2.B.2. The measure μ above is called a *semiclassical measure* (or Wigner measure) associated with the sequence (u_k). If there is uniqueness of the "limit measure" the sequence (u_k) is said *pure* and we note $\{\mu\} = \mathcal{M}(u_k)$.

This result holds in the case of a family of states $(\rho_h)_{h\in]0,h_0]}$, *i.e.* $\rho_h \in \mathcal{L}^+_1 L^2_x$, $\mathrm{Tr}\,\rho_h = 1$.

Theorem 2.B.3. *Let $(\rho_h)_{h\in]0,h_0]}$, $h_0 > 0$ be a family of states on L^2_x. There exist a sequence $h_k \to 0$ and a measure $\mu \in \mathcal{M}_+(\mathbb{R}^{2d}_{x,\xi})$ such that*

$$\forall b \in \mathcal{C}^\infty_0(\mathbb{R}^{2d}_{x,\xi})\,, \quad \lim_{n\to+\infty} \mathrm{Tr}\left[b^W(h_{k_n}x, D_x)\rho_{h_k}\right] = \int_{\mathbb{R}^{2d}_{x,\xi}} b \,\mathrm{d}\mu\,.$$

Proof. We first take an arbitrary sequence (h_k) such that $h_k \to 0$. Then we can define positive numbers $(\lambda_{k,j})_{j,k\geq 0}$ and normed vectors $(u_{k,j})$ of L^2_x such that $\sum_j \lambda_{k,j} = 1$ and $\rho_{h_k} = \sum_j \lambda_{k,j}|u_{k,j}\rangle\langle u_{k_n,j}|$. We can extract from each sequence $(u_{k,j})_k$ a subsequence that converges weakly to a vector u_j ($\|u_j\| \leq 1$). A diagonal extraction enables those convergences to occur simultaneously. The sequence obtained this way is still denoted by $(u_{k,j})$.

Theorem 2.B.1 applies to each sequence $(u_{k,j})_k$ and yields measures μ_j such that for well chosen subsequences h_{k_n}, $\lambda_{k_n,j} \to \lambda_j$ and

$$\lim_{n\to+\infty} \mathrm{Tr}\left[b^W\left(h_{k_n}x, D_x\right)|u_{k,j}\rangle\langle u_{k_n,j}|\right] = \int_{\mathbb{R}^{2d}_{x,\xi}} b \,\mathrm{d}\mu_j\,.$$

Again we apply a diagonal extraction argument to obtain these convergences simultaneously, and we stick with the notations $u_{k,j}$, $\lambda_{k,j}$ for the extracted objects. We observe that $\|u_j\| \leq 1$ and $\sum \lambda_j \leq 1$. We can thus sum these relations to get

$$\lim_{k\to+\infty} \sum_j \lambda_{k,j}\,\mathrm{Tr}\left[b^W\left(h_k x, D_x\right)|u_{k,j}\rangle\langle u_{k_n,j}|\right] = \int_{\mathbb{R}^{2d}_{x,\xi}} b\,\mathrm{d}\Big(\sum \lambda_j\mu_j\Big)$$

which is the expected result with $\mu = \sum_j \lambda_j\mu_j$. □

2.C General results on semigroups

Some references about semigroups of operators in Banach spaces are [30, 27, 29].

In this appendix X represents a (real or complex) Banach space.

Definition 2.C.1. A *strongly continuous semigroup* on X is a mapping $G : \mathbb{R}^+ \to \mathcal{L}(X)$, such that

1. $\forall t, s \geq 0, \quad G(t+s) = G(t)\, G(s)\,,\ G(0) = I,$
2. $G(\cdot)\, x$ is continuous for all $x \in X$.

The *infinitesimal generator* A of $G(\cdot)$ is defined by

$$D(A) = \left\{ x \in X\,,\ \exists \lim_{h \to 0^+} \frac{G(h)\, x - x}{h} \right\}, \qquad Ax = \lim_{h \to 0^+} \frac{G(h)\, x - x}{h}\,.$$

Proposition 2.C.2. *Let G be a strongly continuous semigroup on X with infinitesimal generator $(A, D(A))$. Then $D(A)$ is dense in X and A is a closed operator.*

See [27] for a proof of Proposition 2.C.2.

Notation 2.C.3. For $M > 0$ and ω in $\mathbb{R}$, we denote by $\mathcal{G}(M, \omega)$ the set of all strongly continuous semigroups G such that

$$\forall t \geq 0, \quad \|G(t)\|_{\mathcal{L}(X)} \leq M e^{\omega t}\,.$$

Theorem 2.C.4 (A perturbation result). *Let $(A, D(A))$ be the infinitesimal generator of a strongly continuous semigroup in $\mathcal{G}(M,\omega)$ and $B \in \mathcal{L}(X)$. Then $(A + B, D(A))$ is the infinitesimal generator of a strongly continuous semigroup in $\mathcal{G}(M, \omega + M\, \|B\|_{\mathcal{L}(X)})$.*

See [29, 30] for a proof of Theorem 2.C.4.

Theorem 2.C.5 (Trotter). *Let A_j, $j = 1, \ldots, k$ be the infinitesimal generators of continuous semigroups $G_j \in \mathcal{G}(M_j, \omega_j)$. If $\cap_{j=1}^{k} D(A_j)$ is dense in X and*

$$\forall n \in \mathbb{N}, \quad \|(G_1(t)\, G_2(t) \cdots G_k(t))^n\|_{\mathcal{L}(X)} \leq M e^{n\omega t}$$

and if there exists p such that $\Re p > \omega$, $(pI - (A_1 + A_2 + \cdots + A_k))X$ is dense in X then

$$\overline{A_1 + A_2 + \cdots + A_k}$$

is the infinitesimal generator of a continuous semigroup in $\mathcal{G}(M, \omega)$.

In such a situation the semigroup G generated by $\overline{A_1 + A_2 + \cdots + A_k}$ satisfies

$$\forall x \in X, \quad G(t)x = \lim_{n\to\infty} \left[G_1\Big(\frac{t}{n}\Big) G_2\Big(\frac{t}{n}\Big) \cdots G_k\Big(\frac{t}{n}\Big) \right]^n x$$

with a uniform convergence on the bounded intervals $[0, T]$, with $T > 0$.

See [29] for a proof of Theorem 2.C.5.

2.D Lemmas about an approximate identity

For $\zeta > 0$, and $r \in \mathbb{R}$, let $\kappa^{\zeta}(r) = \frac{1}{\pi}\frac{\zeta}{r^2+\zeta^2}$.

Proposition 2.D.1. *Let f be a function in the Schwartz class. Then for any $\gamma \in]0,1[$, a constant $C_\gamma > 0$ exists such that*

$$\forall \zeta > 0, \ \left\| f * \kappa^{\zeta} - f \right\|_{L^\infty} \leq \max\left\{\|f\|_\infty, \|f'\|_\infty\right\} C_\gamma \zeta^\gamma .$$

Proof. We use the formula

$$f(r_0 + \zeta r) = f(r_0) + \zeta r \int_0^1 f'(r_0 + s\zeta r)\, ds$$

so that we have both

$$\begin{aligned} |f(r_0+\zeta r) - f(r_0)| &\leq 2\|f\|_\infty , \\ |f(r_0+\zeta r) - f(r_0)| &\leq \|f'\|_\infty \zeta r , \end{aligned}$$

and the interpolation of those two results gives, for $\gamma \in [0,1]$,

$$|f(r_0+\zeta r) - f(r_0)| \leq 2\max\left\{\|f\|_\infty, \|f'\|_\infty\right\} \zeta^\gamma |r|^\gamma .$$

So, for $\gamma \in [0,1[$,

$$\left| \int_{\mathbb{R}} \left[f(r_0+\zeta r) - f(r_0)\right] \frac{\mathrm{d}r}{r^2+1} \right| \leq \max\left\{\|f\|_\infty, \|f'\|_\infty\right\} C_\gamma \zeta^\gamma$$

which is the expected result. ☐

Proposition 2.D.2. *Let $f : \mathbb{R}_r \to \mathbb{R}$ continuous, vanishing on $\mathbb{R}^-$, such that $f|_{\mathbb{R}_*^+}$ is in $\mathcal{C}^\infty(\mathbb{R}_*^+)$ and rapidly decreasing towards $+\infty$. Let $0 < r_{\min} < r_{\max}$. Then, for any $\gamma \in]0,1[$, there is a constant $C_{f,\gamma}$ such that*

$$\left\| \partial_r^k \left[f * \kappa^{\zeta} - f \right]\Big|_{[r_{\min}, r_{\max}]} \right\|_{L^\infty} \leq C_\gamma \zeta^\gamma .$$

Proof. We choose A and Δr such that $0 < A < \Delta r < r_{\min}/2$. Let $f_1 = \chi_1 f$ and $f_2 = (1-\chi_1) f$ with χ_1 a $\mathcal{C}^\infty$ decreasing function such that

$$\begin{aligned} \chi_1(r) &= 1 \,\text{if}\, r \leq A/2 \\ &= 0 \,\text{if}\, A \leq r . \end{aligned}$$

Then $f = f_1 + f_2$ and

$$f * \delta^{\zeta} = f_1 \underset{\mathcal{E}', \mathcal{C}^\infty}{*} \kappa^{\zeta} + f_2 \underset{\mathcal{S}, L^1}{*} \kappa^{\zeta} .$$

The second term is the easiest to handle since $\partial_r^k\left(f_2*\kappa^\zeta\right)=\left(\partial_r^k f_2\right)*\kappa^\zeta$ and Proposition 2.D.1 can be applied to get

$$\left\|\left(\partial_r^k f_2\right)*\kappa^\zeta-\pi\partial_r^k f_2\right\|_{L^\infty}\leq C_\gamma\left(\left\|f_2^{(k)}\right\|_\infty+\left\|f_2^{(k+1)}\right\|_\infty\right)\zeta^\gamma .$$

We now recall that we are only interested in $r\in[r_{\min},r_{\max}]$ with $0<r_{\min}<r_{\max}$ when evaluating $\partial_r^k\left(f*\kappa^\zeta\right)$. We insert another cutoff function $\chi_2\in\mathcal{D}(\mathbb{R})$ such that

$$\begin{aligned}\chi_2(r) &= 0\text{ if } r\leq r_{\min}-2\Delta r\\ &= 1\text{ if } r_{\min}-\Delta r\leq r\leq r_{\max}+\Delta r\\ &= 0\text{ if } r_{\max}+2\Delta r\leq r .\end{aligned}$$

Then $f_1*\kappa^\zeta=f_1*\chi_2\kappa^\zeta+f_1*(1-\chi_2)\kappa^\zeta$ and our hypotheses on the supports give

$$\begin{aligned}\operatorname{Supp}\left\{f_1*(1-\chi_2)\kappa^\zeta\right\} &\subset \operatorname{Supp} f_1+\operatorname{Supp}(1-\chi_2)\\ &\subset \mathbb{R}-[r_{\min}-\Delta r+A,r_{\max}+\Delta r] .\end{aligned}$$

Since $A<\Delta r$ we obtain $\left[f_1*(1-\chi_2)\kappa^\zeta\right]\big|_{[r_{\min},r_{\max}]}=0$ and we can restrict ourselves to the computation of

$$f_1\underset{\mathcal{E}',\mathcal{C}_0^\infty}{*}\chi_2\kappa^\zeta .$$

More precisely we want to estimate

$$\left\|\partial_r^k\left(f_1\underset{\mathcal{E}',\mathcal{C}_0^\infty}{*}\chi_2 u_\zeta\right)\Big|_{[r_{\min},r_{\max}]}\right\|_{L^\infty}$$

since $\chi_2\delta=0$ and thus $f_1\underset{\mathcal{E}',\mathcal{E}'}{*}\chi_2\delta=0$. But the same considerations hold for the supports of the derivatives. Thus it is sufficient to observe that we have the control

$$\begin{aligned}\left\|f_1\underset{L^1,\mathcal{C}_0^\infty}{*}\partial_r^k\left(\chi_2\kappa^\zeta\right)\right\|_{L^\infty} &\leq \|f_1\|_{L^1}\left\|\partial^k\left(\chi_2\kappa^\zeta\right)\right\|_{L^\infty} ,\\ &\leq \|f_1\|_{L^1}C_{\chi_2}\sup_{r\geq r_{\min}-2\Delta r}\left|\partial^k\kappa^\zeta\right|\end{aligned}$$

where the sup can be controlled by $C\zeta$ with C only dependent on our choice of Δr and $r_{\min}$ as

$$2\partial^k\kappa^\zeta(r)=i^k k!\frac{-(ir-\zeta)^{k+1}+(ir+\zeta)^{k+1}}{\left(r^2+\zeta^2\right)^{k+1}} .$$

Consequently

$$\left\|\partial_r^k\left[f_1\underset{\mathcal{E}',\mathcal{C}_0^\infty}{*}\chi_2\kappa^\zeta-f_1\underset{\mathcal{E}',\mathcal{E}'}{*}\chi_2\delta\right]\Big|_{[r_{\min},r_{\max}]}\right\|_{L^\infty}\leq C\zeta$$

and this ends the proof. □

2.E Formulae

2.E.1 Symmetric Fock space

For f, g in a complex Hilbert space $\mathcal{H}$,

- $a_\varepsilon(f) = \langle f, z\rangle^{Wick}$, $a_\varepsilon^*(f) = \langle z, f\rangle^{Wick}$,
- $[a_\varepsilon(f), a_\varepsilon(g)] = 0$, $[a_\varepsilon^*(f), a_\varepsilon^*(g)] = 0$, $[a_\varepsilon(f), a_\varepsilon^*(g)] = \varepsilon\langle f, g\rangle$,
- $\Phi_\varepsilon(f) = (a_\varepsilon(f) + a_\varepsilon^*(f))/\sqrt{2}$,
- $W(f) = \exp i\Phi_\varepsilon(f)$, $W(f)W(g) = e^{-\frac{i\varepsilon}{2}\Im\langle f,g\rangle}W(f+g)$,
- $E(f) = W\left(\frac{\sqrt{2}}{i\varepsilon}f\right)|\Omega\rangle$.

2.E.2 Fourier transforms

Usual Fourier transform For $u \in L^2_x$, $v \in L^2_\xi$,

- $\mathcal{F}_x u(\xi) = \int_{\mathbb{R}^d_x} e^{-ix.\xi}u(x)\,\mathrm{d}x$,
- $\mathcal{F}_x^{-1}v(x) = \int_{\mathbb{R}^d_\xi} e^{ix.\xi}v(\xi)\,\text{đ}\xi$, $\text{đ}\xi = \mathrm{d}\xi/(2\pi)^d$.

Symplectic Fourier transform For $b \in L^2\left(\mathbb{R}^{2d}_P;\mathbb{C}\right)$, $P = (p_x, p_\xi)$, $\sigma(P, P') = p_\xi.p'_x - p_x.p'_\xi$,

- $\mathcal{F}^\sigma b(P) = \int_{\mathbb{R}^{2d}_{x,\xi}} e^{-i\sigma(P,P')}b(P')\,\text{đ}P'$, $\text{đ}P' = \mathrm{d}P/(2\pi)^d$,
- $\mathcal{F}^\sigma \circ \mathcal{F}^\sigma = \mathrm{Id}$.

2.E.3 Weyl quantization

- $\tau^h_{X'} = \left(e^{-i\sigma(\cdot,X')}\right)^W(hx, \mathrm{D}_x) = e^{-i\sigma(\cdot,X')^W(hx,\mathrm{D}_x)} = e^{i(\xi'\cdot hx - x'\cdot \mathrm{D}_x)}$
- $\hat{\tau}^h_{X'} = \mathcal{F}_x\tau^h_{X'}\mathcal{F}_x^{-1} = e^{-i(\xi'\cdot hD_\xi + x'\cdot\xi)}$
- $\tau^h_{X_1}\tau^h_{X_2} = e^{\frac{i}{2}h\sigma(X_1,X_2)}\tau^h_{X_1+X_2} = e^{ih\sigma(X_1,X_2)}\tau^h_{X_2}\tau^h_{X_1}$
- $\hat{\tau}^h_{X_1}\hat{\tau}^h_{X_2} = e^{\frac{i}{2}h\sigma(X_1,X_2)}\hat{\tau}^h_{X_1+X_2} = e^{ih\sigma(X_1,X_2)}\hat{\tau}^h_{X_2}\hat{\tau}^h_{X_1}$

Liste des symboles

$[A, B]$ the commutator $AB - BA$ of two operators

$b_1 \sharp b_2$ the Moyal product of two symbols

$\{f, g\}$ the poisson bracket $\partial_\xi f.\partial_x g - \partial_x f.\partial_\xi g$ of two functions on $\mathbb{R}^{2d}_{x,\xi}$

$\vee$, $\bigvee$ the symmetric tensor product

B_R the closed ball of radius R

$\mathcal{C}^0_\infty (X; \mathbb{R})$ the continuous function vanishing at infinity (on a locally compact, Hausdorff space X)

$\mathcal{C}^\infty_b$ the functions of class $\mathcal{C}^\infty$ bounded, with bounded derivatives

$\mathbb{C}$ the field of complex numbers

$D (A)$ the domain of an operator A

$\mathcal{C}^\infty_0 (X)$ with X an open subset of $\mathbb{R}^{2d}_{x,\xi}$: the real valued functions on X of class $\mathcal{C}^\infty$ with compact support

with X an open subset of $\mathbb{R}^d_x$: the complex valued functions on X of class $\mathcal{C}^\infty$ with compact support

Δ_x the Laplacian operator on L^2_x

D_x $= -i\partial_x$

$\mathcal{F}u$, $\hat{u}$ the Fourier transform,

$$\mathcal{F}u (\xi) = \int_{\mathbb{R}^d_x} e^{-ix.\xi} u (x)\, dx$$

$\mathcal{L} (\mathcal{H}_1, \mathcal{H}_2)$ the continuous linear applications between the Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$

$\mathcal{L}_1 (\mathcal{H})$ the trace class operators on a Hilbert space $\mathcal{H}$

$\mathcal{L}_1^+(\mathcal{H})$ the positive trace class operators on a Hilbert space $\mathcal{H}$

$\mathcal{L}_2(\mathcal{H})$ the Hilbert-Schmidt operators on a Hilbert space $\mathcal{H}$

L^2_x $= L^2(\mathbb{R}^d_x;\mathbb{C})$

$L^2_{x,\xi}$ $= L^2(\mathbb{R}^d_x \times \mathbb{R}^d_\xi;\mathbb{R})$

L^2_ξ $= L^2(\mathbb{R}^d_\xi;\mathbb{C})$

$\mathcal{M}_b(X;\mathbb{R})$ the set of Radon measures on locally compact, Hausdorff space X

$\mathbb{N}$ the non-negative integers

$\mathbb{R}$ the field of real numbers

$\mathbb{S}^{d-1}$ the unit sphere for the euclidean norm in $\mathbb{R}^d$

$\operatorname{Supp} f$ the support of a function f

$\tau_x f$ the translation $f(\cdot - x)$ of $x \in \mathbb{R}^d$ of a function f with variable in $\mathbb{R}^d$

Index

$\mathscr{A}_{\{,\}}$, $\mathscr{A}_{-}$, $\mathscr{A}_{+}$, 51
$\mathscr{A}^{j}_{\vec{\mu}}$, $\mathscr{B}^{j}_{\vec{\mu}}$, $\mathscr{C}^{j,\zeta}_{\vec{\mu}}$, 61
Ad, 38
$a^{*}(f)$, $a(f)$, creation, annihilation operator, 37

$\mathcal{B}(t)$, linear Boltzmann group, 32

$\mathfrak{c}$, $\mathfrak{c}^{\zeta}$, $\mathfrak{c}^{\zeta}_{P,t}$, 56
Q^{ζ}_{-}, $Q^{\zeta}_{+,t}$, 57
Q, Q_{-}, Q_{+}, collision operator, 29
Q_t, approximated collision operator, 32
$\mathcal{C}^{0}_{\infty}(X;\mathbb{R})$, continuous functions vanishing at infinity, 31

$\text{đ}X$, 49
$\Delta_{\{\cdot,\cdot\}}$, 53
Δ_{+}, Δ_{-}, 56

$\Phi(f)$, field operator, 38
$\Phi_{\varepsilon}(f)$, field operator, 42
$\Gamma\mathcal{H}$, $\Gamma_n\mathcal{H}$, $\Gamma_F\mathcal{H}$, Fock space, 41
$\Gamma(U)$, 42
$\mathrm{d}\Gamma_{\varepsilon}(A)$, 42
$\mathcal{F}^{\sigma}$, symplectic Fourier transform, 49

general centered Gaussian random field, 36

H_{ε}, 41
$\hat{H}^{app}_{h,\varepsilon}$, 43
$\hat{H}_{\varepsilon}$, 43
$\hat{\Psi}_t$, $\hat{\Psi}^{app}_t$, 43

κ^{ζ}, 56

$m(b,\rho)$, 47
$m_{\{\cdot,\cdot\}}$, m_{+}, m_{-}, 50
$\mathcal{M}_b(X;\mathbb{R})$, Radon measures, 31

$\mathcal{N}_n(b)$, 32

ω_t, 43
$[\omega]$, 49

$[\varphi]_1$, 49
$[\varphi, p_x]_2$, 49
$(\Omega_{\mathbb{P}}, \mathcal{G}, \mathbb{P})$, probability space, 79

$\mathcal{V}^{h}_{\omega}(x)$ random field, 26

$\sigma(\xi,\xi')$, 29
ρ^{h}_{t}, $\rho^{h}_{N,\Delta t}(\bar{\omega}_N)$, $\rho^{h}_{N,\Delta t}$, 26
$\boldsymbol{\rho}_t$, $\hat{\boldsymbol{\rho}}_t$, ρ^{ε}_t, $\boldsymbol{\rho}^{app}_t$, $\hat{\boldsymbol{\rho}}^{app}_t$, $\rho^{\varepsilon,app}_t$, 43

$\mathrm{Tr}_{\mathcal{H}}$, partial trace, 38

$W(f)$, Weyl operator, 42
τ^{h}_{X}, Weyl operator, 49
$\hat{\tau}^{h}_{P}$, Weyl operator, 49
$b^{W}(hx, D_x)$, Weyl quantization, 27
$: f^{n} :$, n-th Wick power, 37
Q^{Wick}, Wick quantization, 42

z_t, 43

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Chapitre 3

Termes d'ordre élevé pour l'évolution quantique d'une observable de Wick dans le cadre de la méthode de Hepp

Article rédigé en anlglais, soumis pour publication.

Higher order terms for the quantum evolution of a Wick observable within the Hepp method

Abstract: The Hepp method is the coherent state approach to the mean field dynamics for bosons or to the semiclassical propagation. A key point is the asymptotic evolution of Wick observables under the evolution given by a time-dependent quadratic hamiltonian. This article provides a complete expansion with respect to the small parameter $\varepsilon > 0$ which makes sense within the infinite-dimensional setting and fits with finite dimensional formulae.

Sommaire

3.1 Introduction **95**
3.2 Wick calculus with polynomial observables . . . **96**
3.2.1 Definitions 96
3.2.2 Some examples of Wick quantizations 98
3.2.3 Calculus 98
3.3 Main results and a simple example **99**
3.4 Classical evolution of a Wick polynomial under a quadratic evolution **103**
3.4.1 Construction of the classical flow without the α term 103
3.4.2 The strongly continuous dynamical system associated with (α_t) 104
3.4.3 Construction of the classical flow with the α term 104
3.4.4 Composition of a Wick polynomial with the classical evolution 105
3.5 Quantum evolution of a Wick polynomial **105**
3.5.1 Without the α term 105
3.5.2 With the α term 108
3.6 Removal of the α part **109**
3.7 A Dyson type expansion formula for the Wick symbol of the evolved quantum observable . . . **110**
3.8 An exponential type expansion formula for the Wick symbol of the evolved observable **110**
3.8.1 Quantum evolution as a Bogoliubov implementation 110
3.8.2 Action of Bogoliubov transformations on Wick symbols 112
3.8.3 An evolution formula for the Wick symbol 117
3.8.4 Estimates 118
3.A $\mathbb{R}$-linear symplectic transformations **119**
3.B Relations between Weyl and Wick symbols in finite dimension **123**
3.C Symplectic Fourier transform **125**

3.1 Introduction

In this article we derive two expansions with respect to a small parameter ε of quantum evolved Wick observables under a time-dependent quadratic Hamiltonian.

The Hepp method was introduced in [64] and then extended in [56, 57] in order to study the mean field dynamics of many bosons systems via a (squeezed) coherent states approach. The asymptotic analysis in the mean field limit is done with respect to a small parameter ε, where the number of particles is of order $\frac{1}{\varepsilon}$.

Remember that the mean field dynamics is obtained as a classical Hamiltonian dynamics which governs the evolution of the center $z(t)$ of the Gaussian state (squeezed coherent state). Meanwhile the covariance of this Gaussian as well as the control of the remainder term is determined by the evolution of a quadratic approximate Hamiltonian around $z(t)$.

A key point in this method is the asymptotic analysis of the evolution of a Wick quantized observable according to this quantum time-dependent quadratic Hamiltonian.

Only a few results are clearly written about the remainder terms and some possible expansions in powers of ε, see the works of Ginibre and Velo [58, 59]. In the finite-dimensional case, entering into the semiclassical theory, accurate results have been given by Combescure, Ralston and Robert in [51] and Hagedorn and Joye in [61, 62, 63]. For the mean field infinite-dimensional setting some results have been proved in [60, 55, 71] with a different approach.

We stick here with the Hepp method with the presentation of [46] which puts the stress on the similarities and differences between the infinite-dimensional bosonic mean field problem and the finite-dimensional semiclassical analysis. Nevertheless, in [46] the authors only considered the main order term although some of their formulae make possible complete expansions. In this article we derive two expansions of the quantum evolved Wick observables which are equal term by term.

Two difficulties have to be solved :

1. Unlike the time-independent finite-dimensional case, no Mehler type explicit formula (see for example [66] or [53]) is available. A general time-dependent Hamiltonian has no explicit dynamics.
2. In the infinite-dimensional framework the quantization of a linear symplectic transformation (a Bogoliubov transformation) requires some care. Useful references on this subject are [48] and [47]. Its realization in the Fock space relies on a Hilbert-Schmidt condition on the antilinear part connected with the Shale theorem (see [72] and [69, 52, 50]).

These things are well known but have to be considered accurately while writing complete expansions.

Two different methods, with apparently two different final formulae, will be used. A first one relies on a Dyson expansion approach and provides the successive terms as time-dependent integrals. The second one uses the exact formulae for the finite-dimensional Weyl quantization and after having made explicit the relationship between Wick and Weyl quantizations like in [49] or [46], the proper limit process with respect to the dimension is carried out.

The outline of this article is the following. In Section 3.2 we recall some facts and definitions about the Fock space and Wick quantization. We then present our main results in Section 3.3 in Theorems 3.3.1 and 3.3.2 and illustrate them by a simple example. Section 3.4 and Section 3.5 are devoted to the construction and properties of the classical and quantum evolution associated with a symmetric quadratic Hamiltonian. Section 3.7 and Section 3.8 contain the proofs of our two expansion formulae. For the convenience of the reader we recall some facts about real-linear symplectomorphisms and symplectic Fourier transform in the appendices.

3.2 Wick calculus with polynomial observables

3.2.1 Definitions

We recall some definitions and results about Wick quantization. More details can be found in [46].

In this paper $(\mathcal{Z}, \langle\cdot,\cdot\rangle)$ denotes a separable Hilbert space over $\mathbb{C}$, the field of complex numbers. It is also a symplectic space with respect to the symplectic form $\sigma(z_1, z_2) = \Im\langle z_1, z_2\rangle$. We use the physicists convention that all the scalar products over Hilbert spaces are linear with respect to the right variable and antilinear with respect to the left variable. We denote by $\mathcal{S}_m$ the symmetrization operator on $\bigotimes^m \mathcal{Z}$ (the completion for the natural Hilbert scalar product of the algebraic tensor product $\bigotimes^{m,\,alg}\mathcal{Z}$) defined by

$$\mathcal{S}_m(z_1\otimes\cdots\otimes z_m) = \frac{1}{m!}\sum_{\sigma\in\mathfrak{S}_m} z_{\sigma_1}\otimes\cdots\otimes z_{\sigma_m}\,,$$

where the z_j are vectors in $\mathcal{Z}$ and $\mathfrak{S}_m$ denotes the set of the permutations of $\{1,\ldots,m\}$. We will use the notation $z_1\vee\cdots\vee z_m$ for $\mathcal{S}_m(z_1\otimes\cdots\otimes z_m)$, and $z^{\vee m}$ for $z\vee\cdots\vee z$ when the m terms of this product are equal to z. We call *monomial* of *order* $(p,q)\in\mathbb{N}^2$ a complex-valued application defined on $\mathcal{Z}$ of the form

$$b(z) = \left\langle z^{\vee q}, \tilde{b} z^{\vee p}\right\rangle\,,$$

with $\widetilde{b}\in\mathcal{L}(\bigvee^p\mathcal{Z}, \bigvee^q\mathcal{Z})$ where $\bigvee^n\mathcal{Z}$ (or $\mathcal{Z}^{\vee n}$) denotes the Hilbert completion of the n-fold symmetric tensor product, and for two Banach spaces E and F, the space of continuous linear applications from E to F is denoted by $\mathcal{L}(E,F)$. We then write $b\in\mathcal{P}_{p,q}(\mathcal{Z})$. The *total order* of b is the integer $m = p+q$. The finite linear combinations of monomials are called *polynomials*. The set of all polynomials of this type is denoted by $\mathcal{P}(\mathcal{Z})$. Subsets of particular interest of $\mathcal{P}(\mathcal{Z})$ are $\mathcal{P}_m(\mathcal{Z})$ and $\mathcal{P}_{\leq m}(\mathcal{Z})$, the finite linear combinations of monomials of total order equal to m and not greater than m.

The Hilbert space

$$\mathcal{H} := \bigoplus_{n\in\mathbb{N}} \bigvee^{n} \mathcal{Z}$$

is called the symmetric *Fock space* associated with $\mathcal{Z}$, where tensor products and sum completions are made with respect to the natural Hilbert scalar products inherited from $\mathcal{Z}$. We also consider the dense subspace $\mathcal{H}_{\text{fin}}$ of $\mathcal{H}$ of states with a finite number of particles

$$\mathcal{H}_{\text{fin}} := \bigoplus_{n\in\mathbb{N}}^{\text{alg}} \bigvee^{n} \mathcal{Z}\,,$$

where the tensor products are completed but the sum is algebraic.

The *Wick quantization* of a monomial $b \in \mathcal{P}_{p,q}(\mathcal{Z})$ is the operator defined on $\mathcal{H}_{\text{fin}}$ by its action on $\bigvee^n \mathcal{Z}$ as an element of $\mathcal{L}(\bigvee^n \mathcal{Z}, \bigvee^{n+q-p} \mathcal{Z})$,

$$b^{Wick}\Big|_{\bigvee^n \mathcal{Z}} = 1_{[p,+\infty)}(n)\,\frac{\sqrt{n!\,(n+q-p)!}}{(n-p)!}\,\varepsilon^{\frac{p+q}{2}}\left(\tilde{b} \vee I_{\bigvee^{n-p}\mathcal{Z}}\right)\,,$$

where I_X denotes the identity map on the space X and for $A_j \in \mathcal{L}\left(\mathcal{Z}^{\vee p_j}, \mathcal{Z}^{\vee q_j}\right)$, $A_1 \vee A_2 = \mathcal{S}_{q_1+q_2} A_1 \otimes A_2 \mathcal{S}_{p_1+p_2}$. The Wick quantization is extended by linearity to polynomials.

We have a notion of *derivative* of a polynomial, first defined on the monomials and then extended by linearity. For $b \in \mathcal{P}_{p,q}(\mathcal{Z})$ and for any given $z \in \mathcal{Z}$, the operator

$$\partial_{\bar{z}}^{j}\partial_{z}^{k} b(z) := \frac{p!}{(p-k)!}\frac{q!}{(q-j)!}\left(\left\langle z^{\vee(q-j)}\right| \vee I_{\bigvee^{j}\mathcal{Z}}\right)\tilde{b}\left(z^{\vee(p-k)} \vee I_{\bigvee^{k}\mathcal{Z}}\right) \tag{3.2.1}$$

is an element of $\mathcal{L}\left(\bigvee^k \mathcal{Z}, \bigvee^j \mathcal{Z}\right)$. We use the "bra" and "ket" notations of the physicists for vectors and forms in Hilbert spaces. Then we can define the *Poisson bracket* of order k of two polynomials b_1, b_2, by

$$\{b_1, b_2\}^{(k)} = \partial_z^k b_1.\partial_{\bar{z}}^k b_2 - \partial_z^k b_2.\partial_{\bar{z}}^k b_1$$

since, for any polynomial b, $\partial_z^k b(z)$ is a k-form (on $\mathcal{Z}$) and $\partial_{\bar{z}}^k b(z)$ is a k-vector.

Remark 3.2.1. The product denoted by a dot in the definition of the Poisson bracket is a $\mathbb{C}$-bilinear duality-product between k-forms and k-vectors. As an example consider the polynomials

$$b_1(z) = \left\langle z^{\vee 3}, \xi_1^{\vee 3}\right\rangle \left\langle \eta_1^{\vee 2}, z^{\vee 2}\right\rangle \quad \text{and} \quad b_2(z) = \left\langle z^{\vee 3}, \xi_2^{\vee 3}\right\rangle \left\langle \eta_2, z\right\rangle\,.$$

The Poisson bracket of order 2 of b_1 and b_2 is

$$\{b_1, b_2\}^{(2)}(z) = 2 \times 6 \times \left\langle z^{\vee 3}, \xi_1^{\vee 3} \right\rangle \left\langle \eta_1^{\vee 2} \vee z, \xi_2^{\vee 3} \right\rangle \langle \eta_2, z \rangle - 0.$$

3.2.2 Some examples of Wick quantizations

Here is a quick review of the notations used for some useful examples of Wick quantization. A vector of $\mathcal{Z}$ is denoted by ξ, A is a bounded operator and z is the variable of the polynomials. In the next table, the first column describes the polynomial and the second the corresponding Wick quantization (as an operator on $\mathcal{H}_{fin}$).

$\langle z, Az \rangle$	$\leftrightarrow$	$\mathrm{d}\Gamma(A)$
$\lvert z \rvert^2$	$\leftrightarrow$	N
$\langle z, \xi \rangle$	$\leftrightarrow$	$a^*(\xi)$
$\langle \xi, z \rangle$	$\leftrightarrow$	$a(\xi)$
$\sqrt{2}\Re \langle z, \xi \rangle$	$\leftrightarrow$	$\Phi(\xi)$

The operator $\mathrm{d}\Gamma(A)$ is the usual second quantization of an operator restricted to $\mathcal{H}_{fin}$ multiplied by a factor ε. If $A = I_{\mathcal{Z}}$ we obtain N the usual number operator multiplied by a factor ε. The operators a, a^* and Φ are the usual annihilation, creation and field operators of quantum field theory with an additional $\sqrt{\varepsilon}$ factor. The real and imaginary parts of a complex number ζ are denoted by $\Re\zeta$ and $\Im\zeta$. The field operators $\Phi(\xi)$ are essentially self-adjoint and this enables us to define the (ε-dependent) Weyl operators

$$W(\xi) = e^{i\Phi(\xi)}.$$

3.2.3 Calculus

Here are some calculation rules for Wick quantizations of polynomials in $\mathcal{P}(\mathcal{Z})$. The proofs can be found in [46].

Proposition 3.2.2. *For every polynomial $b \in \mathcal{P}(\mathcal{Z})$,*

- $b_1^{Wick} b_2^{Wick} = \left(\sum_{k=0}^{\min\{p_1,q_2\}} \frac{\varepsilon^k}{k!} \partial_z^k b_1 . \partial_{\bar{z}}^k b_2 \right)^{Wick}$ *in $\mathcal{H}_{fin}$ for any $b_i \in \mathcal{P}_{p_i,q_i}(\mathcal{Z})$,*
- b^{Wick} *is closable and the domain of the closure contains*

  $$\mathcal{H}_0 = Vect\{W(z)\varphi, \varphi \in \mathcal{H}_{fin}, z \in \mathcal{Z}\},$$

  (we still denote by b^{Wick} the closure of b^{Wick}),
- $\left(b^{Wick}\right)^* = \bar{b}^{Wick}$ *on $\mathcal{H}_{fin}$ (where the bar denotes the usual conjugation on complex numbers),*
- *for any z_0 in $\mathcal{Z}$, $W\left(\frac{\sqrt{2}}{i\varepsilon} z_0\right)^* b^{Wick} W\left(\frac{\sqrt{2}}{i\varepsilon} z_0\right) = (b(z_0 + z))^{Wick}$ holds on $\mathcal{H}_0$ where $b(z_0 + \cdot) \in \mathcal{P}(\mathcal{Z})$.*

3.3 Main results and a simple example

Our two hypotheses are:

H1 Let $(\alpha_t)_{t\in\mathbb{R}}$ be a one parameter family of self-adjoint operators on $\mathcal{Z}$ defining a strongly continuous dynamical system $u_\alpha(t,s)$.

H1' Assume **H1** and additionally that the dynamical system preserves a dense set D such that, for any $\psi \in D$, $u_\alpha(\cdot,\cdot)\,\psi$ belongs to $\mathcal{C}^1\left(\mathbb{R}^2,\mathcal{Z}\right)\cap \mathcal{C}^0\left(\mathbb{R}^2,D\right)$.

H2 Let β be in $\mathcal{C}^0\left(\mathbb{R};\mathcal{Z}^{\vee 2}\right)$, ($\beta_t$ defines a $\mathbb{C}$-antilinear Hilbert-Schmidt operator by $z\mapsto \left(I_{\mathcal{Z}}\vee\langle z|\right)\beta_t$).

With **H1'** and **H2**, the *classical flow* associated with a family $Q_t(z) = \langle z,\alpha_t z\rangle + \Im\left\langle \beta_t, z^{\vee 2}\right\rangle$ of quadratic polynomials is the solution $\varphi(t,s)$ to the equation

$$\left\{\begin{array}{rcl} i\partial_t\varphi(t,0)[z] & = & \partial_{\bar z}Q_t\left(\varphi(t,0)[z]\right)\\ \varphi(0,0) & = & I_{\mathcal{Z}}\end{array}\right. \tag{3.3.1}$$

where $\partial_{\bar z}Q_t(z) = \alpha z + i\left(I_{\mathcal{Z}}\vee\langle z|\,\beta\right)$, written in a weak sense.

Although things are better visualized by writing a differential equation, the hypotheses **H1** and **H2** suffice to define the dynamical system $\varphi(t,s)$. Details about this point are given in Section 3.4. Actually $\varphi(t,s)$ is a family of symplectomorphisms of $(\mathcal{Z},\sigma)$ which are naturally decomposed into their $\mathbb{C}$-linear and $\mathbb{C}$-antilinear parts:

$$\varphi = L + A\,,\quad L\in\mathcal{L}(\mathcal{Z})\,,\quad AA^*\in\mathcal{L}_1(\mathcal{Z})\,.$$

See Appendix 3.A for more details about symplectomorphisms and this decomposition.

Similarly, the *quantum flow* associated with Q_t is the solution $U(t,s)$ to

$$\left\{\begin{array}{rcl} i\varepsilon\partial_t U(t,0) & = & Q_t^{Wick}U(t,0)\\ U(0,0) & = & I_{\mathcal{H}}\end{array}\right.\,. \tag{3.3.2}$$

The precise meaning of the solutions to this equation is specified in Section 3.5.

We are ready to state our two main results dealing with the evolution of a Wick observable b^{Wick}, $b\in\mathcal{P}(\mathcal{Z})$, under the quantum flow, that is to say the quantity $U(0,t)\,b^{Wick}U(t,0)$. (We use the usual notation $\langle N\rangle = \sqrt{N^2+1}$.)

Theorem 3.3.1. *Assume **H1** and **H2**. Let $b\in\mathcal{P}_{\le m}(\mathcal{Z})$ be a polynomial. Then, for any time $t\ge 0$, the formula*

$$U(0,t)\,b^{Wick}U(t,0) = \left(b^{(0),t}\right)^{Wick} + \sum_{k=1}^{\lfloor m/2\rfloor}\left(\frac{\varepsilon}{2}\right)^k\int_{\Delta_t^k}\left(b^{(k)t,\bar s^k}\right)^{Wick}d\bar s^k \tag{3.3.3}$$

holds as an equality of continuous operators from $\mathcal{D}\left(\langle N\rangle^{m/2}\right)$ to $\mathcal{H}$, where

- $\bar{s}^k = (s_1, \ldots, s_k) \in \mathbb{R}_+^k$ *and* $\Delta_t^k = \left\{\bar{s}^k \in \mathbb{R}_+^k,\ \sum_{j=1}^k s_j \leq t\right\}$,
- *the polynomials* $b^{(k)t,\bar{s}^k}$ *are defined recursively by*

$$\left\{\begin{array}{rcl} b^{(0)t}(z) & = & b(\varphi(t,0)z) \\ b^{(k+1)t,\bar{s}^{k+1}} & = & \lambda^{s_{k+1}} b^{(k)t,\bar{s}^k} \end{array}\right. ,$$

with $\lambda^s c = -i\left\{c \circ \varphi(0,s), Q_s\right\}^{(2)} \circ \varphi(s,0)$ *for any polynomial* c.

Theorem 3.3.2. *Assume* ***H1*** *and* ***H2****. Let* $m \geq 2$ *and* $b \in \mathcal{P}_{\leq m}(\mathcal{Z})$ *a polynomial. Then introducing*

- *the vector* $v_t \in \bigotimes^2 \mathcal{Z}$ *such that for all* $z_1, z_2 \in \mathcal{Z}$,

$$\langle z_1 \otimes z_2, v_t \rangle = \langle z_1, L^*(t,0) A(t,0) z_2 \rangle ,$$

- *the operator on* $\mathcal{P}(\mathcal{Z})$

$$\Lambda^t c(z) = \mathrm{Tr}\left[-2A^*(t,0) A(t,0) \partial_{\bar{z}} \partial_z c(z)\right] + \langle v_t| \,.\, \partial_{\bar{z}}^2 c(z) + \partial_z^2 c(z) \,.\, |v_t\rangle ,$$

the formula

$$U(0,t) b^{Wick} U(t,0) = \left(e^{\frac{\varepsilon}{2}\Lambda^t}(b \circ \varphi(t,0))\right)^{Wick} \tag{3.3.4}$$

holds as an equality of continuous operators from $\mathcal{D}\left(\langle N\rangle^{m/2}\right)$ *to* $\mathcal{H}$.

Remark 3.3.3. The derivative $\partial_{\bar{z}}\partial_z c(z)$ is in $\mathcal{L}(\mathcal{Z})$ and Tr denotes the trace on the subset of trace class operators of $\mathcal{L}(\mathcal{Z})$.

Remark 3.3.4. For $m \geq 2$ the operators λ^t and Λ^t send $\mathcal{P}_m(\mathcal{Z})$ into $\mathcal{P}_{m-2}(\mathcal{Z})$.

Remark 3.3.5. The exponential is intended in the sense

$$e^{\frac{\varepsilon}{2}\Lambda^t} b = \sum_{k=0}^{\lfloor m/2 \rfloor} \frac{1}{k!}\left(\frac{\varepsilon}{2}\Lambda^t\right)^k b$$

for a polynomial b in $\mathcal{P}_{\leq m}(\mathcal{Z})$.

Example 3.3.6. To give an idea of the behavior of these formulae we apply them in the simplest (non trivial) possible situation, with $\mathcal{Z} = \mathbb{C}$ and $Q_t(z) = \Im\left(z^2\right)$. As Q_t is time-independent the classical evolution equation is autonomous and thus we can write $\varphi(t,s) = \varphi(t-s)$ and $i\partial_t \varphi(t) z = \partial_{\bar{z}} Q(\varphi(t) z) = i\overline{\varphi(t) z}$. The solution is $\varphi(t) z = z\cosh t + \bar{z}\sinh t$. We can then compute both

$$\int_0^t b^{(1)t,s} ds \qquad \text{and} \qquad \Lambda^t(b \circ \varphi(t)) .$$

The first one is easily computed as $\partial_z^2 Q(z) = -i$, $\partial_{\bar{z}}^2 Q(z) = i$ and, with $c = b \circ \varphi(t)$,

$$\begin{aligned} -i\{c \circ \varphi(-s), Q(z)\}^{(2)} &= \left(\partial_z^2 + \partial_{\bar{z}}^2\right)(c \circ \varphi(-s)) \\ &= \left[\cosh(-2s)\left(\partial_z^2 + \partial_{\bar{z}}^2\right) c \right. \\ &\qquad \left. + 2\sinh(-2s)\, \partial_{\bar{z}} \partial_z c\right] \circ \varphi(-s) \end{aligned}$$

and thus

$$\begin{aligned} \int_0^t b^{(1)t,s} ds &= \int_0^t \left(\cosh(-2s)\left(\partial_z^2 + \partial_{\bar{z}}^2\right) + 2\sinh(-2s)\, \partial_{\bar{z}} \partial_z\right) ds\, (b \circ \varphi(t)) \\ &= \left(\frac{1}{2}\sinh(2t)\left(\partial_z^2 + \partial_{\bar{z}}^2\right) + (1 - \cosh(2t))\, \partial_{\bar{z}} \partial_z\right)(b \circ \varphi(t)) \; . \end{aligned}$$

Now we compute the second one. Since $L(t,0)\, z = L^*(t,0)\, z = z\cosh t$ and $A(t,0)\, z = A^*(t,0)\, z = \bar{z}\sinh t$, we get $v_t = \cosh t \sinh t$ and then obtain directly

$$\Lambda^t = (1 - \cosh(2t))\, \partial_{\bar{z}} \partial_z + \frac{1}{2}\sinh(2t)\left(\partial_z^2 + \partial_{\bar{z}}^2\right) \; .$$

We thus obtain the same result with the two computations for the term of order 1 in ε.

Then we can show that

$$\int_{\Delta_t^k} b^{(k)t,\bar{s}^k} d\bar{s}^k = \frac{1}{k!}\left(\Lambda^t\right)^k (b \circ \varphi(t))$$

since

$$\begin{aligned} &\int_{\Delta_t^k} \prod_{j=1}^k \left(2\sinh(-2s_j)\, \partial_{\bar{z}} \partial_z + \cosh(-2s_j)\left(\partial_z^2 + \partial_{\bar{z}}^2\right)\right) d\bar{s}^k \\ &\qquad = \frac{1}{k!}\left((1 - \cosh(-2t))\, \partial_{\bar{z}} \partial_z - \frac{1}{2}\sinh(-2t)\left(\partial_z^2 + \partial_{\bar{z}}^2\right)\right)^k \end{aligned}$$

because

$$\begin{aligned} &\frac{d}{ds}\left[(1 - \cosh(-2s))\, \partial_{\bar{z}} \partial_z - \frac{1}{2}\sinh(-2s)\left(\partial_z^2 + \partial_{\bar{z}}^2\right)\right] \\ &\qquad = 2\sinh(-2s)\, \partial_{\bar{z}} \partial_z + \cosh(-2s)\left(\partial_z^2 + \partial_{\bar{z}}^2\right) \; . \end{aligned}$$

Remark 3.3.7. Since these two formulae will be proven independently and the identification of each term of order k in ε in the expansion of the symbol is clear, we carry out a computation only on the formal level for the convenience of the reader to show the link between the two formulae in the general case.

We show (formally) that

$$\frac{d}{ds}\Lambda^s = \lambda^s .$$

Then it is simple to show that

$$\int_{\bar{s}^k \in \Delta_t^k} \lambda^{s_k} \lambda^{s_{k-1}} \cdots \lambda^{s_1} d\bar{s}^k = \frac{1}{k!} \left(\Lambda^t\right)^k$$

as operators on $\mathcal{P}(\mathcal{Z})$ once the case $k = 2$ is understood:

$$\begin{aligned} 2 \int_{\bar{s}^2 \in \Delta_t^2} \lambda^{s_2} \lambda^{s_1} d\bar{s}^2 &= \int_0^t \int_0^{s_1} \lambda^{s_2} \lambda^{s_1} ds_2 ds_1 + \int_0^t \int_0^{s_2} \lambda^{s_2} \lambda^{s_1} ds_1 ds_2 \\ &= \int_0^t \Lambda^{s_1} \lambda^{s_1} ds_1 + \int_0^t \lambda^{s_2} \Lambda^{s_2} ds_2 \\ &= \left(\Lambda^t\right)^2 . \end{aligned}$$

In this computation we have used that $\Lambda^0 = 0$ as $A(0,0) = 0$.

We first give λ^s in a more explicit way. As $\partial_{\bar{z}}^2 Q = i\,|\beta\rangle$ and $\partial_z^2 Q = -i\,\langle\beta|$ we first get

$$\lambda c = \left[\partial_z^2 \left(c \circ \varphi^{-1}\right).|\beta\rangle + \langle\beta|\,.\partial_{\bar{z}}^2 \left(c \circ \varphi^{-1}\right)\right] \circ \varphi$$

with $\varphi = \varphi(t,0)$ and omitting the time dependence everywhere. Then with $\varphi = L + A$ (and thus $\varphi^{-1} = L^* - A^*$) and $\langle z_1, Az_2\rangle = \langle z_1 \otimes z_2, w_A\rangle$ we obtain

$$\begin{aligned} \lambda c(z) = \partial_z^2 c(z).\left|\left(L^{*\vee 2} + A^{*\vee 2}\right)\beta\right\rangle + \left\langle\left(L^{*\vee 2} + A^{*\vee 2}\right)\beta\right|.\partial_{\bar{z}}^2 c(z) \\ - 2\left(\langle\left(I_{\mathcal{Z}} \otimes \partial_{\bar{z}}\partial_z c(z)^* L^*\right)\beta, w_A\rangle + \langle w_A, \left(I_{\mathcal{Z}} \otimes \partial_{\bar{z}}\partial_z c(z) L^*\right)\beta\rangle\right) . \end{aligned}$$

Then we compute $\frac{d}{ds}\Lambda^s$ in several parts. The linear and antilinear parts of the equation $i\partial_s\varphi(s,0)\,z = \partial_{\bar{z}}Q_s\left(\varphi(s,0)\,z\right)$ give

$$\begin{aligned} \partial_s Lz &= -i\alpha Lz + \left(\langle Az| \vee I_{\mathcal{Z}}\right)|\beta\rangle \\ \partial_s Az &= -i\alpha Az + \left(\langle Lz| \vee I_{\mathcal{Z}}\right)|\beta\rangle . \end{aligned}$$

We now show that $\partial_s v_s = \left|\left(L^{*\vee 2} + A^{*\vee 2}\right)\beta\right\rangle$,

$$\begin{aligned} \partial_s \langle z_1 \otimes z_2, v_s\rangle &= \partial_s \langle Lz_1, Az_2\rangle \\ &= \langle -i\alpha Lz_1, Az_2\rangle + \langle\beta, Az_2 \vee Az_1\rangle \\ &\qquad + \langle Lz_1, -i\alpha Az_2\rangle + \left(\langle Lz_2| \vee \langle Lz_1|\right)|\beta\rangle \\ &= \langle\beta, (A \vee A)(z_1 \vee z_2)\rangle + \langle(L \vee L)(z_1 \vee z_2), \beta\rangle \\ &= \left\langle z_1 \vee z_2, \left(L^{*\vee^2} + A^{*\vee^2}\right)\beta\right\rangle . \end{aligned}$$

And thus $\partial_s\left(\partial_z^2.\left|v\right\rangle+\left\langle v\right|.\partial_{\bar z}^2\right)=\partial_z^2.\left|\left(L^{*\vee 2}+A^{*\vee 2}\right)\beta\right\rangle+\left\langle\left(L^{*\vee 2}+A^{*\vee 2}\right)\beta\right|.\partial_{\bar z}^2$.

We then show that

$$\partial_s\mathrm{Tr}\left[A^*A\partial_{\bar z}\partial_z c\left(z\right)\right]=\left\langle\beta,\left(I_{\mathcal{Z}}\otimes L\partial_{\bar z}\partial_z c\left(z\right)\right)w_A\right\rangle+\left\langle w_A,\left(I_{\mathcal{Z}}\otimes\partial_{\bar z}\partial_z c\left(z\right)L^*\right)\beta\right\rangle\ .$$

We first observe that $\mathrm{Tr}\left[A^*A\partial_{\bar z}\partial_z c\left(z\right)\right]=\left\langle w_A,\left(I_{\mathcal{Z}}\otimes\partial_{\bar z}\partial_z c\left(z\right)\right)w_A\right\rangle$. A simple calculation using $\partial_s Az=-i\alpha Az+\left(\left\langle Lz\right|\vee I_{\mathcal{Z}}\right)\left|\beta\right\rangle$ shows that $\partial_s w_A=\left(-i\alpha\otimes I_{\mathcal{Z}}\right)w_A+\left(I_{\mathcal{Z}}\otimes L^*\right)\beta$ and this immediately gives the result.

3.4 Classical evolution of a Wick polynomial under a quadratic evolution

The adjoint of a $\mathbb{C}$-antilinear operator is defined in Appendix 3.A.

Definition 3.4.1. A $\mathbb{C}$-antilinear operator A on $\mathcal{Z}$ is said of *Hilbert-Schmidt class* if $\left\|A\right\|_{\mathcal{L}_2^a(\mathcal{Z})}:=\left\|AA^*\right\|_{\mathcal{L}_1(\mathcal{Z})}^{1/2}$ is finite, where $\left\|\cdot\right\|_{\mathcal{L}_1(\mathcal{Z})}$ is the usual trace norm for $\mathbb{C}$-linear operators. The set of Hilbert-Schmidt antilinear operators is denoted by $\mathcal{L}_2^a\left(\mathcal{Z}\right)$.

Let $\mathcal{X}\left(\mathcal{Z}\right)=\mathcal{L}\left(\mathcal{Z}\right)+\mathcal{L}_2^a\left(\mathcal{Z}\right)$ with norm

$$\left\|T\right\|_{\mathcal{X}(\mathcal{Z})}=\left\|L\right\|_{\mathcal{L}(\mathcal{Z})}+\left\|A\right\|_{\mathcal{L}_2^a(\mathcal{Z})}$$

for $T=L+A$, where L and A are respectively $\mathbb{C}$-linear and $\mathbb{C}$-antilinear. The space $\mathcal{X}\left(\mathcal{Z}\right)$ is a Banach algebra.

Remark 3.4.2. The norm $\left\|T\right\|_{\mathcal{X}(\mathcal{Z})}$ is well defined as the decomposition $T=L+A$ is unique ($L=\frac{1}{2}\left(T-iTi\right)$ and $A=\frac{1}{2}\left(T+iTi\right)$).

3.4.1 Construction of the classical flow without the α term

Let $\beta\in\mathcal{C}^0\left(\mathbb{R};\mathcal{Z}^{\vee 2}\right)$ and $Q_t=\Im\left\langle\beta_t,z^{\vee 2}\right\rangle$. Observe that $\partial_{\bar z}Q\left(t\right)\left(z\right)=i\left(I_{\mathcal{Z}}\vee\left\langle z\right|\right)\beta_t$ and so $\left(\partial_{\bar z}Q_t\right)_t$ is a continous one parameter family of $\mathcal{X}\left(\mathcal{Z}\right)$, so that the theory of ordinary differential equations in Banach algebras (see for example [65]) asserts that there exists a unique two parameters family $\varphi\left(t_2,t_1\right)$ of elements of $\mathcal{X}\left(\mathcal{Z}\right)$ such that

$$\left\{\begin{array}{rcl} i\partial_t\varphi\left(t,0\right) & = & \partial_{\bar z}Q_t\,\varphi\left(t,0\right)\\ \varphi\left(0,0\right) & = & I_{\mathcal{Z}}\end{array}\right.,$$

with φ of $\mathcal{C}^1$ class in both parameters such that for all r, s and t,

$$\varphi\left(t,s\right)\varphi\left(s,r\right)=\varphi\left(t,r\right)\ .$$

The classical flow $\varphi\left(t,s\right)$ is a symplectomorphism with respect to the symplectic form $\sigma\left(z_1,z_2\right)=\Im\left\langle z_1,z_2\right\rangle$. It can be checked deriving

$$\sigma\left(\varphi\left(t,s\right)z_1,\varphi\left(t,s\right)z_2\right)$$

with respect to t.

3.4.2 The strongly continuous dynamical system associated with (α_t)

We first state a proposition which is a direct consequence of Theorem X.70 in [70] in the unitary case. This proposition provides a set of assumptions ensuring the existence of a strongly continuous dynamical system associated with a family $(\alpha_t)_t$ of self-adjoint operators. Other more general situations can be considered as in [67, 68] for example.

Proposition 3.4.3. *Let $(\alpha_t)_{t\in\mathbb{R}}$ be a family of self-adjoint operators on the Hilbert space $\mathcal{Z}$ satisfying the following conditions.*

1. *The α_t have a common domain D (from which it follows by the closed graph theorem that $c(t,s) = (\alpha_t - i)(\alpha_s - i)^{-1}$ is bounded).*

2. *For each $z \in \mathcal{Z}$, $(t-s)^{-1} c(t,s) z$ is uniformly strongly continuous and uniformly bounded in s and t for $t \neq s$ lying in any fixed compact interval.*

3. *For each $z \in \mathcal{Z}$, $c(t) z = \lim_{s\nearrow t} (t-s)^{-1} c(t,s) z$ exists uniformly for t in each compact interval and $c(t)$ is bounded and strongly continuous in t.*

The approximate propagator u_k is defined by $u_k(t,s) = \exp(-(t-s) i\alpha_{\frac{j-1}{k}})$ if $\frac{j-1}{k} \leq s \leq t \leq \frac{j}{k}$ and $u_k(t,r) = u_k(t,s) u_k(s,r)$.

Then for all s, t in a compact interval and any $z \in \mathcal{Z}$,

$$u(t,s) z = \lim_{k\to+\infty} u_k(t,s) z$$

exists uniformly in s and t. Further, if $z \in D$, then $u(t,s) z$ is in D for all s, t and satisfies

$$\begin{cases} i\frac{d}{dt} u(t,s) z &= \alpha_t u(t,s) z \\ u(s,s) z &= z \end{cases}.$$

3.4.3 Construction of the classical flow with the α term

Assume **H1** and **H2**. Let $\hat{\varphi}$ be the solution of

$$\begin{cases} i\partial_t \hat{\varphi}(t,0) &= \partial_{\bar{z}} \hat{Q}_t \, \hat{\varphi}(t,0) \\ \hat{\varphi}(0,0) &= I_{\mathcal{Z}} \end{cases},$$

with $\hat{Q}_t(z) = \Im \left\langle \hat{\beta}_t, z^{\vee 2} \right\rangle$, $\hat{\beta}_t = u_\alpha(t,0)^{*\vee 2} \beta_t$. What we call here the solution of

$$\begin{cases} i\partial_t \varphi(t,0) &= \partial_{\bar{z}} Q_t \, \varphi(t,0) \\ \varphi(0,0) &= I_{\mathcal{Z}} \end{cases}, \tag{3.4.1}$$

with $Q_t = \langle z, \alpha_t z\rangle + \Im \left\langle \beta_t, z^{\vee 2}\right\rangle$ is

$$\varphi(t,0) = u_\alpha(t,0) \circ \hat{\varphi}(t,0) \ .$$

Depending on the assumptions on (α_t) it will be possible to precise if φ sloves Equation (3.4.1) in a usual sense (strongly, weakly, on some dense subset...).

With the particular set of assumptions of Theorem 3.4.3 we get that for all $z_1 \in D$ and $z_2 \in \mathcal{Z}$,

$$\left\{ \begin{array}{rcl} i\partial_t \langle z_1, \varphi(t,0) z_2\rangle & = & \langle \alpha z_1, \varphi(t,0) z_2\rangle + i \langle z_1 \vee \varphi(t,0) z_2, \beta\rangle \\ \varphi(0,0) & = & I_{\mathcal{Z}} \end{array} \right. .$$

3.4.4 Composition of a Wick polynomial with the classical evolution

The composition of a polynomial with the classical flow defines a time-dependent polynomial.

Definition 3.4.4. We define a norm on $\mathcal{P}(\mathcal{Z})$ by

$$\|b\|_{\mathcal{P}(\mathcal{Z})} = \sum_{p,\,q} \|b_{p,q}\|_{q\leftarrow p}$$

where $b = \sum_{p,\,q} b_{p,q}$ is a polynomial with $b_{p,q} \in \mathcal{P}_{p,q}(\mathcal{Z})$ and $\|b_{p,q}\|_{q\leftarrow p}$ is a shorthand for $\|\tilde{b}_{p,q}\|_{\mathcal{L}(\bigvee^p \mathcal{Z}, \bigvee^q \mathcal{Z})}$. For a polynomial b in $\mathcal{P}_m(\mathcal{Z})$, we will sometimes write $\|b\|_{\mathcal{P}_m(\mathcal{Z})}$.

Proposition 3.4.5. *Let $b \in \mathcal{P}_m(\mathcal{Z})$ be a polynomial, and $\varphi \in \mathcal{X}(\mathcal{Z})$. Then $b \circ \varphi \in \mathcal{P}_m(\mathcal{Z})$ and we have the estimate*

$$\|b \circ \varphi\|_{\mathcal{P}_m(\mathcal{Z})} \leq \|\varphi\|^m_{\mathcal{X}(\mathcal{Z})} \|b\|_{\mathcal{P}_m(\mathcal{Z})} \ .$$

Proof. The proof is essentially the same as in Proposition 2.12 of [46]. □

3.5 Quantum evolution of a Wick polynomial

3.5.1 Without the α term

Definition 3.5.1. Let $\beta \in \mathcal{C}^0\left(\mathbb{R}; \mathcal{Z}^{\vee 2}\right)$ and $Q_t(z) = \Im \left\langle \beta_t, z^{\vee 2}\right\rangle$. A family $U(t,s)$ of unitary operators on $\mathcal{H}$ defined for s, t real is a *solution* of

$$\left\{ \begin{array}{rcl} i\partial_t U(t,0) & = & \frac{Q_t^{Wick}}{\varepsilon} U(t,0) \\ U(0,0) & = & I_{\mathcal{H}} \end{array} \right. \qquad (3.5.1)$$

if

1. $U(t,s)$ is strongly continuous in $\mathcal{H}$ with respect to s, t with $U(s,s) = I$,
2. $U(t,r) = U(t,s)\,U(s,r)$, $r \le s \le t$,
3. $i\frac{d}{dt}U(t,s)\,y$ exists for almost every t (depending on s) and is equal to $Q_t^{Wick}U(t,s)\,y$,
4. $i\varepsilon\frac{d}{ds}U(t,s)\,y = -U(t,s)\,Q_s^{Wick}y$, $y \in \mathcal{D}(N+1)$, $0 \le s \le t$.

This definition is made to fit the general framework of Theorems 4.1 and 5.1 of [67]. More precisely we may check the following theorem.

Theorem 3.5.2. *Let $\beta \in \mathcal{C}^0\left(\mathbb{R}; \mathcal{Z}^{\vee 2}\right)$ and $Q_t(z) = \Im\left\langle \beta_t, z^{\vee 2}\right\rangle$.*

Then the quantum flow equation (3.5.1) associated to the family $\frac{1}{\varepsilon}Q_t$ has a unique solution. This solution preserves the sets $\mathcal{D}(\langle N\rangle^{k/2})$ for $k \ge 2$.

To establish this theorem we will use the following estimates.

Lemma 3.5.3. *Let $\beta \in \mathcal{Z}^{\vee 2}$ and $Q(z) = \Im\left\langle \beta, z^{\vee 2}\right\rangle$. Then, on $\mathcal{H}_{fin}$, and for $k \ge 1$, Q^{Wick} satisfies the estimates*

$$\left\| Q^{Wick}/\varepsilon \Psi \right\| \le \frac{3}{2}\,\|\beta\|_{\mathcal{Z}^{\vee 2}}\,\|(N/\varepsilon + 1)\,\Psi\| \tag{3.5.2}$$

and

$$\pm i\left[Q^{Wick}/\varepsilon, (N/\varepsilon + 1)^k\right] \le 3^k\sqrt{2}\,\|\beta\|_{\mathcal{Z}^{\vee 2}}\,(N/\varepsilon + 1)^k\,. \tag{3.5.3}$$

The second estimate is in the sense of quadratic forms, for all $\Psi \in \mathcal{H}_{fin}$,

$$\pm\, i\left(\left\langle \frac{1}{\varepsilon}Q^{Wick}\Psi, (N/\varepsilon + 1)^k\,\Psi\right\rangle - \left\langle (N/\varepsilon + 1)^k\,\Psi, \frac{1}{\varepsilon}Q^{Wick}\Psi\right\rangle\right) \le \frac{3^k}{\sqrt{2}}\,\|\beta\|_{\mathcal{Z}^{\vee 2}}\left\langle \Psi, (N/\varepsilon + 1)^k\,\Psi\right\rangle\,.$$

Proof. The first estimate is a consequence of $n + 2 \le 2\,(n+1)$ associated to

$$\frac{2i}{\varepsilon}\,Q^{Wick}\Big|_{\mathcal{Z}^{\vee n}} = \sqrt{n\,(n-1)}\,\langle\beta| \vee I_{\bigvee^{n-2}\mathcal{Z}} - \sqrt{(n+2)\,(n+1)}\,|\beta\rangle \vee I_{\bigvee^{n}\mathcal{Z}}\,.$$

For the second estimate, consider $\frac{2i}{\varepsilon}\left\langle \Psi, \left[(1 + N/\varepsilon)^k, Q^{Wick}\right]\Psi\right\rangle$. The first term of this commutator is

$$\sum_n (n+1)^k\left(\sqrt{(n+2)\,(n+1)}\left\langle \Psi^{(n)} \vee \langle\beta|\,, \Psi^{(n+2)}\right\rangle - \sqrt{n\,(n-1)}\left\langle \Psi^{(n)}, |\beta\rangle \vee \Psi^{(n-2)}\right\rangle\right)\,.$$

Then we deduce easily the second term and a reindexation gives the following form for the whole commutator:

$$\sum_n \left[(n+1)^k - ((n+2)+1)^k\right] \sqrt{(n+2)(n+1)}$$
$$\times \left(\left\langle \Psi^{(n)} \vee \langle\beta| , \Psi^{(n+2)} \right\rangle + \left\langle \Psi^{(n+2)}, |\beta\rangle \vee \Psi^{(n)} \right\rangle \right) .$$

Newton's binomial formula and the inequalities $\sum_{l=0}^{k-1} \binom{k}{l} 2^{k-l} \leq 3^k$ and $(n+1)^l \leq (n+1)^{k-1}$ yield

$$(n+1)^k - ((n+2)+1)^k \leq 3^k (n+1)^{k-1} .$$

Using also $n+2 \leq 2(n+1)$ to control $\sqrt{(n+2)(n+1)}$ we obtain

$$\pm i \left\langle \Psi, \left[(1+N/\varepsilon)^k, \frac{Q^{Wick}}{\varepsilon}\right] \Psi \right\rangle$$
$$\leq \frac{1}{2} \sum_n 3^k (n+1)^{k-1} \sqrt{2} (n+1) \left\| \Psi^{(n)} \right\| \|\beta\|_{\mathcal{Z}^{\vee 2}} \left\| \Psi^{(n+2)} \right\| .$$

Cauchy-Schwarz's inequality gives the claimed estimate. □

Lemma 3.5.4. *Let $\beta \in \mathcal{Z}^{\vee 2}$ and $Q(z) = \Im \langle \beta, z^{\vee 2} \rangle$. Then Q^{Wick} is essentially self-adjoint on $\mathcal{H}_{fin}$ and its closure is essentially self-adjoint on any other core for $N/\varepsilon + 1$. Inequalities (3.5.2) and (3.5.3) still hold on $\mathcal{D}(N/\varepsilon + 1)$.*

We still denote by Q^{Wick} this self-adjoint extension.

Proof. We apply the commutators Theorem X.37 of [70] with the estimates of Lemma 3.5.3 for $k = 1$. □

Lemma 3.5.5. *If a solution of the quantum flow equation (3.5.1) exists then it leaves $\mathcal{Q}((N/\varepsilon+1)^k) = \mathcal{D}((N/\varepsilon+1)^{k/2})$ invariant for any integer $k \geq 2$.*

In the time-independent case the estimate

$$\|U(t,0)\|_{\mathcal{L}\left(\mathcal{D}\left((N/\varepsilon+1)^{k/2}\right)\right)} \leq \exp\left(3^k \sqrt{2} \|\beta\| |t|\right)$$

holds.

Proof. From Lemma 3.5.4, for any $k \geq 2$, $\mathcal{D}((N/\varepsilon+1)^{k/2}) \subset \mathcal{D}(Q^{Wick})$. We can adapt the proof of Theorem 2 of [54] to the case of the quantization of a continuous one parameter family of quadratic polynomials with the estimates of Lemma 3.5.3. □

Proof of theorem 3.5.2 . We use Theorems 4.1 and 5.1 of [67] with the family of operators $iQ(t)^{Wick}/\varepsilon$ (here we directly consider the self-adjoint extension of Q_t^{Wick}/ε). We set $Y = \mathcal{D}((N/\varepsilon+1)^{k/2})$.

1. This family is stable in the sense that $\| \prod_{j=1}^{k} e^{-is_j Q(t_j)^{Wick}/\varepsilon} \|_{\mathcal{L}(\mathcal{H})} \leq 1$ (we actually have an equality here).

2. The space Y is admissible for this family in the sense that for each t, $(iQ_t^{Wick}/\varepsilon+\lambda)^{-1}$ leaves Y invariant and
$$\left\| \left(iQ_t^{Wick}/\varepsilon + \lambda \right)^{-1} \right\|_{\mathcal{L}(Y)} \leq \left(\lambda - 3^k\sqrt{2}\,\|\beta\| \right)^{-1}$$
for $\Re\lambda > 3^k\sqrt{2}\,\|\beta\|$.

   This is true because, as we have seen in Lemma 3.5.5, $(e^{-isQ_t^{Wick}/\varepsilon})_{s\in\mathbb{R}}$ leaves Y invariant and, thanks to the estimate of the same lemma, we can apply the resolvent formula
$$\left(iQ_t^{Wick}/\varepsilon + \lambda \right)^{-1} = \int_0^{+\infty} e^{-\lambda s} e^{-isQ_t^{Wick}/\varepsilon} ds$$
and obtain the desired estimate.

3. $Y \subset \mathcal{D}\left(Q_t^{Wick}/\varepsilon\right)$ so that $Q_t^{Wick}/\varepsilon \in \mathcal{L}(Y, \mathcal{H})$ for each t, and the map $t \to Q_t^{Wick}/\varepsilon \in \mathcal{L}(Y,\mathcal{H})$ is continuous.

4. $Y = \mathcal{D}((N/\varepsilon+1)^{k/2})$ is reflexive.

Theorems 4.1 and 5.1 of [67] thus apply and give the existence of an evolution operator.

The preservation of the set $\mathcal{D}((N/\varepsilon+1)^{k/2})$ comes from the application of Lemma 3.5.5 to the solution of the time-dependent problem. To conclude it is then enough to observe that the domains $\mathcal{D}(\langle N\rangle^{k/2})$ and $\mathcal{D}((N/\varepsilon+1)^{k/2})$ are the same and have equivalent norms. □

3.5.2 With the α term

Assume **H1** and **H2**. Let $\hat{U}$ be the solution of
$$\left\{ \begin{array}{rcl} i\partial_t \hat{U}(t,0) & = & \frac{\hat{Q}_t^{Wick}}{\varepsilon} \hat{U}(t,0) \\ \hat{U}(0,0) & = & I_{\mathcal{H}} \end{array} \right. \tag{3.5.4}$$
with $\hat{Q}_t(z) = \Im\left\langle \hat{\beta}_t, z^{\vee 2} \right\rangle$, $\hat{\beta}_t = u_\alpha(t,0)^{*\vee 2}\beta_t$. What we call here the solution of
$$\left\{ \begin{array}{rcl} i\partial_t U(t,0) & = & \frac{Q_t^{Wick}}{\varepsilon} U(t,0) \\ U(0,0) & = & I_{\mathcal{H}} \end{array} \right. \tag{3.5.5}$$
with $Q_t = \langle z, \alpha_t z\rangle + \Im\left\langle \beta_t, z^{\vee 2}\right\rangle$ is
$$U(t,0) = \Gamma(u_\alpha(t,0)) \circ \hat{U}(t,0)\ .$$

3.6 Removal of the α part

Proposition 3.6.1. *Assume* ***H1*** *and* ***H2****. Suppose Theorems 3.3.1 and 3.3.2 hold with a null one parameter family of self-adjoint operators on* $\mathcal{Z}$*, and* $\hat{\beta}_t = u_\alpha(t,0)^{*\vee 2}\beta_t$*. We denote with a hat the quantities associated with this solution. Then Theorems 3.3.1 and 3.3.2 hold.*

Proof. For Equation 3.3.3, we forget during the proof the $(t,0)$ dependency in our notations and write

$$\int_{\Delta_t^0} b^{(0)t,\bar{s}^0} d\bar{s}^0$$

instead of $b^{(0),t}$. Then

$$\begin{aligned}
U^* b^{Wick} U &= \hat{U}^* \Gamma(u_\alpha^*) b^{Wick} \Gamma(u) \hat{U} \\
&= \hat{U}^* (b \circ u_\alpha)^{Wick} \hat{U} \\
&= \sum_{k=0}^{\lfloor \frac{m}{2} \rfloor} \left(\frac{\varepsilon}{2}\right)^k \int_{\Delta_t^k} \left(\widehat{b \circ u_\alpha}^{(k)t,\bar{s}^k}\right)^{Wick} d\bar{s}^k
\end{aligned}$$

where the $\hat{b}^{(k)t,\bar{s}^k}$ are defined recursively by

$$\left\{\begin{array}{rcl}
\hat{b}^{(0)t}(z) &=& b \circ \hat{\varphi} \\
\hat{b}^{(k+1)t,\bar{s}^{k+1}} &=& \hat{\lambda}^{s_{k+1}} \hat{b}^{(k)t,\bar{s}^k}
\end{array}\right.$$

with $\hat{\lambda}^s c = -i\left\{c \circ \hat{\varphi}(0,s), \hat{Q}_s\right\}^{(2)} \circ \hat{\varphi}(s,0)$ for any polynomial c. Thus it suffices to prove that

$$\widehat{b \circ u_\alpha}^{(k)t,\bar{s}^k} = b^{(k)t,\bar{s}^k}.$$

This is clear for $k = 0$ as $u_\alpha \circ \hat{\varphi} = \varphi$. Then we observe that

$$\begin{aligned}
\hat{\lambda}^s c &= -i\left\{c \circ \hat{\varphi}^{-1}, \hat{Q}\right\}^{(2)} \circ \hat{\varphi} \\
&= -i\left\{c \circ \varphi^{-1} \circ u_\alpha, \hat{Q}\right\}^{(2)} \circ u_\alpha^{-1} \circ \varphi \\
&= -i\left\{c \circ \varphi^{-1}, Q\right\}^{(2)} \circ \varphi
\end{aligned}$$

where we used that $\partial_z^2 \langle z, \alpha z\rangle = 0$, $\partial_{\bar{z}}^2 \langle z, \alpha z\rangle = 0$ and $\beta_t = u_\alpha(t,0)^{\vee 2}\hat{\beta}_t$. □

We can thus restrict our proof to the case of a polynomial Q_t of the form $Q_t(z) = \Im\langle \beta_t, z^{\vee 2}\rangle$ with $\beta_t \in \mathcal{C}^0(\mathbb{R}; \mathcal{Z}^{\vee 2})$ and no (α_t) term.

3.7 A Dyson type expansion formula for the Wick symbol of the evolved quantum observable

In this section we prove Theorem 3.3.1.

Proof. We first prove that the formula, for $c \in \mathcal{P}_{\leq m}(\mathcal{Z})$,

$$U(0,s)\left(c\circ\varphi(0,s)\right)^{Wick}U(s,0) = c^{Wick} - \frac{i\varepsilon}{2}\int_0^s U(0,\sigma)\left\{c\circ\varphi(0,\sigma),Q_\sigma\right\}^{(2)Wick}U(\sigma,0)\,d\sigma$$

holds as an equality of continuous operators from $\mathcal{D}(\langle N\rangle^{m/2})$ to $\mathcal{H}$, with $\langle N\rangle = (N^2+1)^{1/2}$. This is a consequence of the fact that the derivative of the left hand term as a function of s is $-\frac{i\varepsilon}{2}U(0,s)\left\{c\circ\varphi(0,s),Q_s\right\}^{(2)Wick}U(s,0)$ as it can be seen from the relation

$$i\partial_\sigma\left(c\circ\varphi(0,\sigma)\right) = -\partial_z\left(c\circ\varphi(0,\sigma)\right).\partial_{\bar z}Q_\sigma + \partial_z Q_\sigma.\partial_{\bar z}\left(c\circ\varphi(0,\sigma)\right)$$

and Proposition 3.2.2. Applying the previous formula with $c = b^{(K)t,\bar s^K}$ we get recursively

$$\begin{aligned} &U(0,t)\,b^{Wick}U(t,0) \\ &= \sum_{k=0}^{K-1}\left(\frac{\varepsilon}{2}\right)^k\int_{\bar s^k\in\Delta_t^k}\left(b^{(k)t,\bar s^k}\right)^{Wick}d\bar s^k \\ &\quad + \left(\frac{\varepsilon}{2}\right)^K\int_{\bar s^K\in\Delta_t^K}U(0,s_K)\left(b^{(K)t,\bar s^K}\circ\varphi(0,s_K)\right)^{Wick}U(s_K,0)\,d\bar s^K\,. \end{aligned}$$

This process gives a null remainder as soon as $K > m/2$ as for $K \leq \lfloor m/2\rfloor$, since the polynomial $b^{(K)\bar s^K}$ is of total order $m-2K$. □

3.8 An exponential type expansion formula for the Wick symbol of the evolved observable

In this section we prove Theorem 3.3.2.

3.8.1 Quantum evolution as a Bogoliubov implementation

Some basic facts about symplectomorphisms are recalled in Appendix 3.A.

Definition 3.8.1. A symplectomorphism T is called *implementable* if and only if there exists a unitary operator U on $\mathcal{H}$, called a *Bogoliubov implementer* of T, such that

$$\forall\xi\in\mathcal{Z},\ U^*W(\xi)\,U = W(T\xi)\ .$$

Proposition 3.8.2. *Assume* $\alpha_t \equiv 0$ *and* ***H2***. *Let* $Q_t = \Im \left\langle \beta_t, z^{\vee 2} \right\rangle$, $\varphi(t,s)$ *the associated classical evolution (see Section 3.4) and* $U(t,s)$ *the associated quantum evolution (see Section 3.5). Then for all* t *in* $\mathbb{R}$, $U(t,0)$ *is a Bogoliubov implementer of* $-i\varphi(0,t)\,i$.

Proof. We begin with a formal computation which will be justified further. It suffices to show that

$$i\varepsilon\partial_t \left[U(0,t)\, W(-i\varphi(t,0)\, i\xi)\, U(t,0)\right] = 0\,.$$

Computing this derivative and omitting the time and $-i\varphi(t,0)\,i\xi$ dependencies in our notations, we get with $U(t,0) = U$

$$U^* W \left\{ -W^* Q^{Wick} W + Q^{Wick} + W^* i\varepsilon\partial_t W \right\} U\,.$$

Then from Proposition 2.10 (iii) in [46], the differential formula of Weyl operators recalled in Proposition 3.8.3 below and with $f_t = -i\varphi(t,0)\,i\xi$ it suffices to show that

$$Q\left(z + \frac{i\varepsilon}{\sqrt{2}} f_t\right) = Q(z) + i\varepsilon\left(\frac{i\varepsilon}{2}\Im\left\langle f_t, \partial_t f_t\right\rangle + i\sqrt{2}\Re\left\langle \partial_t f_t, z\right\rangle\right)$$

to get the result. This equality results from the expansion of $Q(z) = \Im\left\langle \beta, z^{\vee 2}\right\rangle$, recalling that $i\partial_t\varphi(t,0)\,\xi = \partial_{\bar z} Q(\varphi(t,0)\,\xi)$, and observing that $\partial_{\bar z} Q(z) = i\left(\left(\langle z| \vee I_{\mathcal{Z}}\right)|\beta\rangle\right)$. We now need to clarify the meaning of this computation. It suffices to show that the quantity

$$\left\langle \Phi, U(0,t)\, W(-i\varphi(t,0)\, i\xi)\, U(t,0)\, \Psi\right\rangle$$

is constant for Ψ, Φ in $\mathcal{D}(N+1)$. Since this domain is preserved by the operators $U(t,s)$, the Weyl operators are weakly derivable on this domain (see next proposition), and $U(t,s)$ is derivable on this domain, then we get the justification of the previous formal computation. □

Proposition 3.8.3. *Let* z, h *be vectors in* $\mathcal{Z}$, t *be a real parameter and* φ, ψ *be in the domain of* $\Phi(h)$. *Then*

$$\begin{aligned}\lim_{t\to 0}\frac{1}{t}\left(\left\langle \varphi, \left[W(z+th) - W(z)\right]\psi\right\rangle\right) &= \left\langle \varphi, W(z)\left[i\Phi(h) + \frac{i\varepsilon}{2}\Im\langle z, h\rangle +\right]\psi\right\rangle \\ &= \left\langle \varphi, \left[i\Phi(h) - \frac{i\varepsilon}{2}\Im\langle z, h\rangle\right] W(z)\,\psi\right\rangle\,.\end{aligned}$$

Proof. For the first equality. The Weyl commutation relations give

$$\begin{aligned}\frac{1}{t}\langle\varphi,[W(z+th)-W(z)]\psi\rangle &= \frac{1}{t}\left\langle W(-z)\varphi,\left[e^{\frac{i\varepsilon}{2}\Im\langle z,th\rangle}W(th)-I_{\mathcal{Z}}\right]\psi\right\rangle\\ &= \left\langle W(-z)\varphi,e^{\frac{i\varepsilon}{2}\Im\langle z,th\rangle}\frac{1}{t}(W(th)-I_{\mathcal{Z}})\psi\right\rangle\\ &\quad+\frac{1}{t}\left(e^{\frac{i\varepsilon}{2}\Im\langle z,th\rangle}-1\right)\langle W(-z)\varphi,\psi\rangle\\ &\underset{t\to 0}{\longrightarrow}\left\langle\varphi,W(z)\left[i\Phi(h)+\frac{i\varepsilon}{2}\Im\langle z,h\rangle\right]\psi\right\rangle.\end{aligned}$$

The convergence of the first term is due to the continuous one parameter group structure of $W(th)$. The other equality is obtained in the same way. □

3.8.2 Action of Bogoliubov transformations on Wick symbols

A theorem due to Shale (see [72]) characterizes implementable symplectomorphisms. We quote here a version of this theorem fitting our needs.

Theorem 3.8.4 (Shale, 1962). *A symplectomorphism T is implementable if and only if the $\mathbb{C}$-linear part of T^*T-Id is trace class.*

We can now quote the main result of this part.

Theorem 3.8.5. *Let $T=L+A$ with L $\mathbb{C}$-linear and A $\mathbb{C}$-antilinear, be an implementable symplectomorphism with a Bogoliubov implementer U preserving $\mathcal{D}(\langle N\rangle^{k/2})$ for any integer $k\geq 2$, then for any polynomial b in $\mathcal{P}_{\leq m}(\mathcal{Z})$ with $m\geq 2$,*

$$U^*b^{Wick}U=\left(e^{\frac{\varepsilon}{2}\Lambda[T]}\left[b\left(T^*\cdot\right)\right]\right)^{Wick} \tag{3.8.1}$$

as an equality of continuous operators from $\mathcal{D}(\langle N\rangle^{m/2})$ to $\mathcal{H}$, with $\langle N\rangle=(N^2+1)^{1/2}$, where

- *the exponential is a finite expansion whose rank depends on the degree of the polynomial b,*
- *the operator $\Lambda[T]$ is defined on any polynomial c by*

  $$\Lambda[T]\,c(z)=Tr[-2AA^*\partial_{\bar z}\partial_z c(z)]+\langle v|\,.\partial_{\bar z}^2 c(z)+\partial_z^2 c(z)\,.\,|v\rangle$$

  with $v\in\bigotimes^2\mathcal{Z}$ the vector such that for all z_1, $z_2\in\mathcal{Z}$, $\langle z_1\otimes z_2,v\rangle=\langle z_1,LA^*z_2\rangle$.

In order to prove this result, we use intermediate steps.

1. We prove that $U^*b^{Weyl}U=b\left(T^*\cdot\right)^{Weyl}$ in finite dimension.

2. We use the Fourier transform and the formula

$$b^{Weyl} = \frac{1}{(\pi\varepsilon/2)^d}\left(b * e^{-\frac{|z|^2}{\varepsilon/2}}\right)^{Wick}$$

   to get the result in finite dimension.

3. We extend the result to infinite dimension.

3.8.2.1 Action of Bogoliubov transformations on Weyl quantizations of polynomials in finite dimension

Definition 3.8.6. In a finite-dimensional Hilbert space $\mathcal{Z}$ identified with $\mathbb{C}^d$, the *symplectic Fourier transform* is defined by

$$\mathcal{F}^\sigma[f](z) = \int_{\mathcal{Z}} e^{2\pi i\sigma(z,z')} f(z')\, L(dz')$$

where L denotes the Lebesgue measure, and f is any Schwartz tempered distribution. We associate with each polynomial $b \in \mathcal{P}_{p,q}(\mathcal{Z})$ a Weyl observable by

$$b^{Weyl} = \int_{\mathcal{Z}} \mathcal{F}^\sigma[b](z)\, W\left(-i\sqrt{2}\pi z\right) L(dz)\ . \tag{3.8.2}$$

This formula has a meaning as an equality of quadratic forms on $\mathcal{S}(\mathcal{Z})$ since for any Φ, Ψ in $\mathcal{S}(\mathcal{Z})$, $z \mapsto \langle \Phi, W(-i\sqrt{2}\pi z)\Psi\rangle$ and its derivative are continuous bounded functions and $\mathcal{F}^\sigma[b]$ is made of derivatives of the delta function.

Proposition 3.8.7. *Let $b \in \mathcal{P}_{\le m}(\mathcal{Z})$ with $m \ge 2$ be a polynomial on a finite-dimensional Hilbert space $\mathcal{Z}$. Let T be an implementable symplectomorphism with implementation U preserving the domain $\mathcal{D}(\langle N\rangle^{m/2})$. Then*

$$U^* b^{Weyl} U = b(T^* \cdot)^{Weyl}$$

as a continuous operator from $\mathcal{D}(\langle N\rangle^{m/2})$ to $\mathcal{H}$.

Proof. We compute, in the sense of quadratic forms on $\mathcal{S}(\mathcal{Z})$,

$$\begin{aligned}
U^* b^{Weyl} U &= \int \mathcal{F}^\sigma[b](z)\, W\left(-\sqrt{2}\pi T i z\right) L(dz) \\
&= \int \mathcal{F}^\sigma[b](T^* z)\, W\left(-i\sqrt{2}\pi z\right) L(dz) \\
&= \int \mathcal{F}^\sigma[b(T^* \cdot)](z)\, W\left(-i\sqrt{2}\pi z\right) L(dz) \\
&= b(T^* \cdot)^{Weyl}
\end{aligned}$$

where we made use of the relation $Ti = i(T^*)^{-1}$, the volume preservation of T^* in $\mathcal{Z}$ seen as a $\mathbb{R}$-vector space and the property of composition of a symplectic Fourier transform by a symplectomorphism (see Appendix 3.C). The boundedness from $\mathcal{D}(\langle N\rangle^{m/2})$ to $\mathcal{H}$ is deduced from the facts that the Fourier transform of b involves only derivatives of the delta function of order smaller or equal to m and that a derivation of the Weyl operator gives at worse a field factor which is controlled by $\langle N\rangle^{1/2}$. □

3.8.2.2 Action of Bogoliubov transformations on Wick quantization of polynomials in finite dimension

Proposition 3.8.8. *Let $b \in \mathcal{P}_{\leq m}(\mathcal{Z})$ with $m \geq 2$ be a polynomial on a finite-dimensional Hilbert space $\mathcal{Z}$. Let T be an implementable symplectomorphism with implementation Upreserving the domain $\mathcal{D}(\langle N\rangle^{m/2})$. Then*

$$U^* b^{Wick} U = \left(e^{\frac{\varepsilon}{2}\Lambda[T]}\left[b\left(T^* \cdot\right)\right]\right)^{Wick}, \tag{3.8.3}$$

as a continuous operator from $\mathcal{D}(\langle N\rangle^{m/2})$ to $\mathcal{H}$, where $\Lambda[T]$ is defined as in Theorem 3.8.5.

Proof. We search the polynomial c such that $U^* b^{Wick} U = c^{Wick}$. In finite dimension for polynomials we can use the well known deconvolution formula

$$c^{Wick} = \left(c * \frac{1}{(\pi\varepsilon/2)^d} e^{\frac{|z|^2}{\varepsilon/2}}\right)^{Weyl}.$$

By Proposition 3.8.7 we boil down to search for a polynomial c such that

$$\left(b * \frac{1}{(\pi\varepsilon/2)^d} e^{\frac{|z|^2}{\varepsilon/2}}\right)(T^* \cdot) = c * \frac{1}{(\pi\varepsilon/2)^d} e^{\frac{|z|^2}{\varepsilon/2}}.$$

Using symplectic Fourier transform (see appendix 3.C) and its properties with respect to convolution, composition with symplectomorphisms and Gaussians, we get

$$\begin{aligned}\mathcal{F}^\sigma c &= \left[\mathcal{F}^\sigma b\left(T^* \cdot\right)\right] \times \left[\mathcal{F}^\sigma\left(\frac{e^{\frac{|z|^2}{\varepsilon/2}}}{(\pi\varepsilon/2)^d}\right)(T^* \cdot)\right] \times \left[\mathcal{F}^\sigma\left(\frac{e^{-\frac{|z|^2}{\varepsilon/2}}}{(\pi\varepsilon/2)^d}\right)\right] \\ &= e^{\frac{\pi^2\varepsilon\left(|T^* \cdot|^2 - |\cdot|^2\right)}{2}} \times \mathcal{F}^\sigma b\left(T^* \cdot\right).\end{aligned}$$

Writting $T = L + A$ with L the $\mathbb{C}$-linear and A the $\mathbb{C}$-antilinear part of T we obtain

$$\begin{aligned}|T^* z|^2 - |z|^2 &= \langle L^* z, L^* z\rangle + \langle A^* z, A^* z\rangle + \langle L^* z, A^* z\rangle + \langle A^* z, L^* z\rangle - \langle z, z\rangle \\ &= \langle z, LL^* z\rangle + \langle z, AA^* z\rangle + \langle LA^* z, z\rangle + \langle z, LA^* z\rangle - \langle z, z\rangle \\ &= \langle z, 2AA^* z\rangle + \left\langle v, z^{\vee 2}\right\rangle + \left\langle z^2, v\right\rangle\end{aligned}$$

with $v \in \bigotimes^2 \mathcal{Z}$ the vector such that for all $z_1, z_2 \in \mathcal{Z}$, $\langle z_1 \otimes z_2, v\rangle = \langle z_1, LA^* z_2\rangle$. By Fourier transforming again, we get

$$\pi^2 \mathcal{F}^\sigma \left[\left(|T^* \cdot|^2 - |\cdot|^2\right) \times \cdot\right] \mathcal{F}^\sigma c = \mathrm{Tr}\left[-2AA^* \partial_{\bar{z}} \partial_z c\,(z)\right] + \langle v|\, \partial_{\bar{z}}^2 c\,(z) + \partial_z^2 c\,(z)\, |v\rangle$$

as the $\mathbb{C}$-linear and $\mathbb{C}$-antilinear parts behave differently under Fourier transform (the $\mathbb{C}$-linear part has a minus sign added, see appendix 3.C). We then obtain the claimed result. □

3.8.2.3 Extension to infinite dimension on a "cylindrical" class of polynomials

Theorem 3.8.9. *Let $\hat{T}$ be symplectomorphism of the form $\hat{T} = e^{c\rho}$, with c a conjugation and ρ a positive, self-adjoint, Hilbert-Schmidt operator commuting with c. Let $(\xi_j)_{j\in\mathbb{N}}$ a Hilbert basis in which ρ is diagonal. Let π_K be the orthogonal projection on the finite-dimensional space $\mathcal{Z}_K = Vect(\{\xi_j\}_{j\leq K})$.*

Then for any polynomial b in $\mathcal{P}_m(\mathcal{Z})$ with $m \geq 2$ and any integer K

$$\hat{U}^* b_K^{Wick} \hat{U} = \left(e^{\frac{\varepsilon}{2}\Lambda[\hat{T}]}\left[b_K\left(\hat{T}^* \cdot\right)\right]\right)^{Wick}$$

as continuous operators from $\mathcal{D}(\langle N\rangle^{\frac{m}{2}})$ to $\mathcal{H}$ where $b_K(z) = b(\pi_K z)$.

Proof. We first remark that, with $Q(z) = \Im\langle c\rho z, z\rangle$, $e^{-iQ^{Wick}/\varepsilon}$ is a Bogoliubov implementer of $\hat{T}$ as it can be seen using Proposition 3.8.2 and the Hilbert-Schmidt property of ρ. We define $\rho_L = \rho\pi_L$, $\hat{T}_L = \hat{T}\pi_L$ and the operator $Q_L(z)^{Wick} = \Im\langle c\rho_L z, z\rangle^{Wick}$. We use the identification $\mathcal{H} = \Gamma_s(\mathcal{Z}_L) \otimes \Gamma_s(\mathcal{Z}_L^\perp)$ and observe that on $\Gamma_s(\mathcal{Z}_L) \otimes \{\Omega^{\mathcal{Z}_L^\perp}\}$, $e^{-iQ^{Wick}/\varepsilon} = e^{-iQ_L^{Wick}/\varepsilon}$. For $K \leq L$ we obtain on $\Gamma_s(\mathcal{Z}_L) \otimes \{\Omega^{\mathcal{Z}_L^\perp}\}$

$$\hat{U}_L^* b_K^{Wick} \hat{U}_L = \left(e^{\frac{\varepsilon}{2}\Lambda[\hat{T}_L]}\left[b_K\left(\hat{T}_L^* \cdot\right)\right]\right)^{Wick}$$

by Proposition 3.8.8, with $\hat{U}_L = e^{-iQ_L^{Wick}/\varepsilon}$. But on this domain it is the same as

$$\hat{U}^* b_K^{Wick} \hat{U} = \left(e^{\frac{\varepsilon}{2}\Lambda[\hat{T}]}\left[b_K\left(\hat{T}^* \cdot\right)\right]\right)^{Wick}$$

with $\hat{U} = e^{-iQ^{Wick}/\varepsilon}$. We thus get an equality on $\cup_L \Gamma_s(\mathcal{Z}_L)$, and by continuity of the involved operators from $\mathcal{D}(\langle N\rangle^{\frac{m}{2}})$ to $\mathcal{H}$ we get the expected result. □

We will first show that Formula (3.8.1) apply in particular to a well chosen class of cylindrical polynomials, and then extend it by density to every polynomial.

3.8.2.4 Extension to general polynomials

We split the proof of Formula (3.8.1) for general polynomials into several lemmata and propositions.

Lemma 3.8.10. *Let $(\xi_j)_{j\in\mathbb{N}}$ be a Hilbert basis of $\mathcal{Z}$, π_m be the orthogonal projector on $\mathcal{Z}_m = Vect(\{\xi_j\}_{j\leq m})$. Let b be a polynomial in $\mathcal{P}_{p,q}(\mathcal{Z})$ and define $b_K = b(\pi_K\cdot)$. Then $(\widetilde{b_K})_{K\in\mathbb{N}}$ is bounded and*

$$\tilde{b} = w - \lim_{j\to\infty} \widetilde{b_K}\,.$$

To formulate more clearly some convergence results we need some extra definitions.

Definition 3.8.11. We define the spaces

$$\mathcal{L}^{\vee}_{p,q}(\mathcal{Z}) = \mathcal{L}\left(\mathcal{Z}^{\vee p}, \mathcal{Z}^{\vee q}\right)\,, \quad \mathcal{L}^{\vee}_{m} = \bigoplus_{p+q=m} \mathcal{L}^{\vee}_{p,q} \quad \text{and} \quad \mathcal{L}^{\vee}_{\leq m} = \bigoplus_{m'\leq m} \mathcal{L}^{\vee}_{m'}$$

corresponding to $\mathcal{P}_{p,q}(\mathcal{Z})$, $\mathcal{P}_m(\mathcal{Z})$ and $\mathcal{P}_{\leq m}(\mathcal{Z})$.

Let $b = \sum_{p,q} b_{p,q}$ be a polynomial, with $b_{p,q} \in \mathcal{P}(\mathcal{Z})$. We note $\tilde{b} = (\widetilde{b_{p,q}}) \in \bigoplus_{p,q} \mathcal{L}^{\vee}_{p,q}(\mathcal{Z})$.

The norm of $\tilde{b} = (\widetilde{b_{p,q}}) \in \mathcal{L}^{\vee}_{\leq m}(\mathcal{Z})$ is $\|\tilde{b}\|_{\mathcal{L}^{\vee}_{\leq m}(\mathcal{Z})} = \sum_{p,q} \|\widetilde{b_{p,q}}\|_{\mathcal{L}(\bigvee^p \mathcal{Z}, \bigvee^q \mathcal{Z})}\,.$

A sequence $(\tilde{b}_K)_{K\in\mathbb{N}}$ of elements of $\mathcal{L}_{\leq m}(\mathcal{Z})$ *converges weakly* to $\tilde{b}$ in $\mathcal{L}_{\leq m}(\mathcal{Z})$ if $\tilde{b}_{K_{p,q}}$ converges weakly to $\tilde{b}_{p,q}$ for every p and q as $K \to +\infty$.

Lemma 3.8.12. *Let T be an operator in $\mathcal{X}(\mathcal{Z})$, $(b_K)_{K\in\mathbb{N}}$ and b be polynomials in $\mathcal{P}_m(\mathcal{Z})$ such that $(\tilde{b}_K)_{K\in\mathbb{N}}$ converges weakly to $\tilde{b}$. Then $b_K(T\cdot)$ and $b(T\cdot)$ are in $\mathcal{P}_m(\mathcal{Z})$ and $\widetilde{b_K(T\cdot)}$ converges weakly to $\widetilde{b(T\cdot)}$.*

Lemma 3.8.13. *Let T be an operator in $\mathcal{X}(\mathcal{Z})$, $(b_K)_{K\in\mathbb{N}}$ and b be polynomials in $\mathcal{P}_m(\mathcal{Z})$ such that $(\tilde{b}_K)_{K\in\mathbb{N}}$ is bounded and converges weakly to $\tilde{b}$. Then $(\widetilde{e^{\frac{\varepsilon}{2}\Lambda[T]}b_K})_{K\in\mathbb{N}}$ converges weakly to $\widetilde{e^{\frac{\varepsilon}{2}\Lambda[T]}b}$.*

Proof. It is enough to show that weak convergence is preserved by the action of $\Lambda[T]$. But, for any polynomial b,

$$\widetilde{\Lambda[T]\,b} = \operatorname*{Tr}_1\left[(-2A^*A\otimes I_{\mathcal{Z}^{\vee q-1}})\,\tilde{b}\right] + (\langle v|\vee I_{\mathcal{Z}^{\vee q-2}})\,\tilde{b} + \tilde{b}\,(|v\rangle\vee I_{\mathcal{Z}^{\vee p-2}})\,,$$

where Tr_1 is the partial trace on the first $\mathcal{Z}$ subspace on the left and any direction on the right (so that if $\tilde{b}\in\mathcal{L}^{\vee}_{p,q}(\mathcal{Z})$, then $\mathrm{Tr}_1[(-2A^*A\otimes I_{\mathcal{Z}^{\vee q-1}})\tilde{b}]$ is in $\mathcal{L}^{\vee}_{p-1,q-1}(\mathcal{Z})$). With this formula the preservation of the weak convergence is clear. □

Proposition 3.8.14. *Let* b *and* $(b_K)_{K\in\mathbb{N}}$ *be Wick polynomials in* $\mathcal{P}_{p,q}(\mathcal{Z})$ *such that* $w-\lim \tilde{b}_K = \tilde{b}$. *Then*

$$w-\lim_K (b_K - b)^{Wick} \langle N\rangle^{-\frac{p+q}{2}} = 0\,.$$

Proposition 3.8.15. *Let* b *and* $(b_K)_{K\in\mathbb{N}}$ *be Wick polynomials in* $\mathcal{P}_{p,q}(\mathcal{Z})$ *such that* $w-\lim \tilde{b}_K = \tilde{b}$. *Let* U *be a unitary operator on the Fock space* $\mathcal{H}$ *such that, for all* $k\geq 2$, $\langle N\rangle^{\frac{k}{2}} U \langle N\rangle^{-\frac{k}{2}}$ *is a bounded operator. Then*

$$w-\lim_K U^* (b_K - b)^{Wick} U \langle N\rangle^{-\frac{m'}{2}} = 0$$

with $m' = \max(m,2)$, $m = p+q$.

Proposition 3.8.16. *Let* T *be an implementable symplectomorphism with Bogoliubov implementer* U. *Then for any polynomial* b *in* $\mathcal{P}_{\leq m}(\mathcal{Z})$, $m\geq 2$,

$$U^* b^{Wick} U = \left(e^{\frac{\varepsilon}{2}\Lambda[T]}\left[b\left(T^*\cdot\right)\right]\right)^{Wick}$$

as continuous operators from $\mathcal{D}(\langle N\rangle^{\frac{m}{2}})$ *to* $\mathcal{H}$.

Proof. From the results 3.8.10 to 3.8.15 we deduce the result for symplectomorphisms of the form $\hat{T} = e^{c\rho}$, with c a conjugation and ρ a positive, self-adjoint, Hilbert-Schmidt operator commuting with c. Then we observe that the hypothesis on the form of $\hat{T}$ is not restrictive as, if T is of the form $ue^{c\rho}$ with u unitary, then, with $\hat{U}$ a Bogoliubov implementer for $\hat{T}$, $\hat{U}\Gamma(u^*)$ is a Bogoliubov implementer for T and

$$\Gamma(u)\left(e^{\frac{\varepsilon}{2}\Lambda[\hat{T}]}\left[b\left(\hat{T}^*\cdot\right)\right]\right)^{Wick}\Gamma(u^*) = \left(e^{\frac{\varepsilon}{2}\Lambda[T]}\left[b\left(T^*\cdot\right)\right]\right)^{Wick}.$$

Indeed for any polynomial c, and operator φ in $\mathcal{X}(\mathcal{Z})$, $\Gamma(\varphi)\, c^{Wick}\Gamma(\varphi^*) = c(\varphi^*\cdot)^{Wick}$ and

$$\Lambda\left[\hat{T}\right]^k\left[b\left(\hat{T}^*\cdot\right)\right](u^*\cdot) = \Lambda\left[u\hat{T}\right]^k\left[b\left(\hat{T}^*u^*\cdot\right)\right]$$

as can be checked by an explicit computation and using the fact that $L = u\hat{L}$ and $A = u\hat{A}$ with the L, $\hat{L}$ and A, $\hat{A}$ denoting respectively the $\mathbb{C}$-linear and $\mathbb{C}$-antilinear parts of T and $\hat{T}$. This achieves the proof. □

3.8.3 An evolution formula for the Wick symbol

We can now prove Theorem 3.3.2.

Proof. We only need to apply propositions 3.8.2 and 3.8.16 with $T = -i\varphi(0,t)\, i = L^*(t,0) + A^*(t,0)$ (with $\varphi(t,0) = L(t,0) + A(t,0)$). We remark that for any symplectomorphism T, $(-iTi)^* = T^{-1}$ so that $(-i\varphi(0,t)\, i)^* = \varphi(t,0)$ and thus we get the result. □

3.8.4 Estimates

We now give estimates for the different terms of the expansion of the symbol.

Proposition 3.8.17. *Let $T = L + A$ be an implementable symplectomorphism with L $\mathbb{C}$-linear and A $\mathbb{C}$-antilinear. Then the operator $\Lambda[T]$ defined on $\mathcal{P}(\mathcal{Z})$ by*

$$\Lambda[T]\,c(z) = Tr\left[-2AA^*\partial_{\bar{z}}\partial_z c\right] + \langle v|\,\partial_{\bar{z}}^2 c(z) + \partial_z^2 c(z)\,|v\rangle\ ,$$

with $v \in \bigotimes^2 \mathcal{Z}$ the vector such that for all $z_1, z_2 \in \mathcal{Z}$, $\langle z_1 \otimes z_2, v\rangle = \langle z_1, LA^* z_2\rangle$ is such that, for c in $\mathcal{P}_m(\mathcal{Z})$

$$\|\Lambda[T]\,c\|_{\mathcal{P}_{m-2}(\mathcal{Z})} \leq 2\,\|T\|_{\mathcal{X}(\mathcal{Z})}\,\|A\|_{\mathcal{L}_2^a(\mathcal{Z})}\,\|c\|_{\mathcal{P}_m(\mathcal{Z})}\ .$$

Proof. We only have to remark that for any polynomial c in $\mathcal{P}_{p,q}(\mathcal{Z})$ the following estimates hold

$$\|Tr\left[B\partial_{\bar{z}}\partial_z c(z)\right]\|_{q-1\leftarrow p-1} \leq \|B\|_{\mathcal{L}_1(\mathcal{Z})}\,\|c\|_{q\leftarrow p}$$

for any trace class operator B, and

$$\left\|\langle v|\,\partial_{\bar{z}}^2 c(z)\right\|_{q-2\leftarrow p} \leq \|v\|_{\bigvee^2 \mathcal{Z}}\,\|c\|_{q\leftarrow p}$$

and that $\|v\|_{\bigvee^2 \mathcal{Z}} = \|LA^*\|_{\mathcal{L}_2^a(\mathcal{Z})} \leq \|L\|_{\mathcal{L}(\mathcal{Z})}\,\|A\|_{\mathcal{L}_2^a(\mathcal{Z})}$. The same estimate holds for $\partial_z^2 c(z)\,|v\rangle$. □

We apply this result to the expression given in the theorem 3.3.2.

Proposition 3.8.18. *Let $(Q_t)_t$ be a continuous one parameter family of quadratic polynomials, φ the classical flow associated to $(Q_t)_t$, and Λ^t the operator defined in theorem 3.3.2. Then, for b in $\mathcal{P}_{\leq m}(\mathcal{Z})$*

$$\left\|e^{\frac{\varepsilon}{2}\Lambda^t}\left(b\circ\varphi(t,0)\right)\right\|_{\mathcal{P}(\mathcal{Z})} \leq \|b\|_{\mathcal{P}(\mathcal{Z})}\,\|\varphi(t,0)\|_{\mathcal{X}(\mathcal{Z})}^m \sum_{k=0}^{m} \frac{1}{k!}\left(\varepsilon\,\|\varphi(t,0)\|_{\mathcal{X}(\mathcal{Z})}\,\|A(t,0)\|_{\mathcal{L}_2^a(\mathcal{Z})}\right)^k$$

where A is the $\mathbb{C}$-antilinear part of φ.

Proof. It is enough to combine the propositions 3.4.5 and 3.8.17. □

Remark 3.8.19. The norm $\|\varphi(t,0)\|_{\mathcal{X}(\mathcal{Z})}$ is bigger than 1 as for any symplectic transformation $T = L + A$ with L $\mathbb{C}$-linear and A $\mathbb{C}$-antilinear, $L^*L = I_{\mathcal{Z}} + A^*A \geq I_{\mathcal{Z}}$ (see proposition 3.A.4) and thus $\|T\|_{\mathcal{X}(\mathcal{Z})} \geq \|L\|_{\mathcal{L}(\mathcal{Z})} \geq 1$.

Appendix

3.A ℝ-linear symplectic transformations

In this part we adapt and recall some results of [69] to fit our needs.

Let $(\mathcal{Z}, \langle\cdot,\cdot\rangle)$ be a separable Hilbert space over the complex numbers field $\mathbb{C}$. The scalar products is linear with respect to the right variable and antilinear with respect to the left variable. We note $\mathrm{Aut}_{\mathbb{R}}(\mathcal{Z})$ the group of $\mathbb{R}$-linear continuous automorphisms on $\mathcal{Z}$. We define a symplectic form σ on $\mathcal{Z}$ by

$$\sigma(z_1, z_2) := \Im \langle z_1, z_2\rangle \ .$$

Definition 3.A.1. A $\mathbb{R}$-linear automorphism T is a *symplectomorphism* if it preserves the symplectic form, i.e. if

$$\forall z_1, z_2 \in \mathcal{Z}, \quad \sigma(Tz_1, Tz_2) = \sigma(z_1, z_2) \ .$$

We note $\mathrm{Sp}_{\mathbb{R}}(\mathcal{Z})$ the set of symplectic transformations over the Hilbert space $\mathcal{Z}$. It is a subgroup of $\mathrm{Aut}_{\mathbb{R}}(\mathcal{Z})$.

Proposition 3.A.2. *A $\mathbb{R}$-linear application $T : \mathcal{Z} \to \mathcal{Z}$ can be written as a sum of two applications respectively $\mathbb{C}$-linear and $\mathbb{C}$-antilinear in a unique way :*

$$T = \frac{T - iTi}{2} + \frac{T + iTi}{2} \, .$$

Definition 3.A.3. Let A be a (bounded) $\mathbb{C}$-antilinear operator on the Hilbert space $\mathcal{Z}$. We define its *adjoint* A^* as the only antilinear operator such that

$$\forall z_1, z_2 \in \mathcal{Z}, \quad \langle z_1, Az_2\rangle = \langle z_2, A^* z_1\rangle \ .$$

Let $T = L + A = \mathcal{Z} \to \mathcal{Z}$ be a $\mathbb{R}$-linear application with L $\mathbb{C}$-linear and A $\mathbb{C}$-antilinear. The *adjoint* T^* of T is defined by $T^* = L^* + A^*$.

Proposition 3.A.4. *Let $T = L + A$ be a $\mathbb{R}$-linear automorphism with L $\mathbb{C}$-linear and A $\mathbb{C}$-antilinear, then the following conditions are equivalent.*

1. *$L + A$ is a symplectomorphism.*
2. *$(L^* - A^*)(L + A) = I_{\mathcal{Z}}$.*
3. *$(L^* + A^*)(L - A) = I_{\mathcal{Z}}$.*
4. *$L^*L - A^*A = I_{\mathcal{Z}}$ and $L^*A = A^*L$.*
5. *$L^* - A^*$ is a symplectomorphism.*
6. *$L - A$ is a symplectomorphism.*
7. *$LL^* - AA^* = I_{\mathcal{Z}}$ and $A^*L = L^*A$.*

Proof. (1) ⇔ (2) Let $T = L + A$ a symplectomorphism, for all $z_1, z_2 \in \mathcal{Z}$,

$$\begin{aligned}\sigma(z_1, z_2) = \Im\langle z_1, z_2\rangle &= \Im\langle (L+A) z_1, T z_2\rangle \\ &= \Im\left(\langle z_1, L^* T z_2\rangle + \overline{\langle z_1, A^* T z_2\rangle}\right) \\ &= \Im\langle z_1, (L^* - A^*) T z_2\rangle \ .\end{aligned}$$

Replacing z_1 by iz_1 we get the same relation with a real part instead of an imaginary part and finally

$$\langle z_1, [(L^* - A^*)(L+A) - I_{\mathcal{Z}}] z_2\rangle = 0$$

and this in turn implies $(L^* - A^*)(L+A) = I_{\mathcal{Z}}$. We can reverse the order of these calculations in order to obtain the first equivalence.

(2) ⇔ (3) The $\mathbb{C}$-linearity and antilinearity properties of L and A give

$$(L^* - A^*)(L+A)\, i = i\,(L^* + A^*)(L - A)$$

so that we get the equivalent condition (3).

((2) and (3)) ⇔ (4) The sum and the difference of the equations of (2) and (3) give (4) and the sum and difference of the equations in (4) give (2) and (3).

(1) ⇔ (5) From (1) and (3) we know that the inverse of a symplectomorphism $T = L + A$ is $T^{-1} = L^* - A^*$ which is necessarily a symplectomorphism too, and thus (1) ⇒ (5). We get (5) ⇒ (1) exchanging T and T^{-1}.

(1) ⇔ (6) ⇔ (7) is easily deduced from the previous equivalences. □

Proposition 3.A.5. *Let $T = L + A$ be a symplectomorphism with L $\mathbb{C}$-linear and A $\mathbb{C}$-antilinear, then L is invertible.*

Proof. From Proposition 3.A.4 we get

$$L^* L = I_{\mathcal{Z}} + A^* A \geq I_{\mathcal{Z}} \quad \text{and} \quad L L^* = I_{\mathcal{Z}} + A A^* \geq I_{\mathcal{Z}}$$

and thus L and L^* are injective. From the injectivity of L^* we get $\overline{\mathrm{Ran} L} = (\mathrm{Ker} L^*)^{\perp} = \{0\}^{\perp} = \mathcal{Z}$.

It is now enough to show that the range of L is closed. Pick a vector $y \in \mathcal{Z}$, there is a sequence $(x_n) \in \mathcal{Z}^{\mathbb{N}}$ such that $L x_n \to y$. The relation $L^* L \geq I_{\mathcal{Z}}$ gives $|L x_m - L x_n| \geq |x_n - x_m|$. The left hand part of the inequality goes to 0 for $m, n \to \infty$, so that (x_n) is a Cauchy sequence and thus converges to a limit x. By continuity of L, $Lx = y$ and L is indeed one to one. □

Definition 3.A.6. An application c from $\mathcal{Z}$ to $\mathcal{Z}$ is a *conjugation* if and only if it satisfies the following conditions.

1. c si $\mathbb{R}$-linear.
2. $c^2 = I_{\mathcal{Z}}$.

3. For all z_1, z_2 in $\mathcal{Z}$, $\langle cz_1, z_2\rangle = \langle cz_2, z_1\rangle$.

Remark 3.A.7. It follows from the third condition in this definition that a conjugation is antilinear.

One may define different conjugations on the same Hilbert space over $\mathbb{C}$ (even for a one dimensional Hilbert space). As an example one can consider a Hilbert basis (e_j) and define the application $c : \sum_j \alpha_j e_j \mapsto \sum_j \overline{\alpha_j} e_j$.

Definition 3.A.8. Let c be a conjugation on the Hilbert space $\mathcal{Z}$. The *real* and *imaginary* parts of a vector $z \in \mathcal{Z}$ (with respect to the conjugation c) are defined as

$$\Re z := \frac{z + cz}{2} \quad \text{and} \quad \Im z := \frac{z - cz}{2i} \,.$$

They verify $z = \Re z + i\Im z$. The space $E^c_{\mathbb{R}} := \Re\mathcal{Z} = \Im\mathcal{Z}$ is a subspace of $\mathcal{Z}$ as $\mathbb{R}$-vector space, $\langle\cdot,\cdot\rangle$ restricted to $E^c_{\mathbb{R}}$ is a real scalar product and $E = E^c_{\mathbb{R}} \oplus iE^c_{\mathbb{R}}$.

Let f be a $\mathbb{R}$-linear application on $\mathcal{Z}$, then we can define the applications from $E^c_{\mathbb{R}}$ to itself

$$\begin{aligned} \alpha &: z \mapsto \Re f(z) \,, \qquad & \gamma &: z \mapsto \Re f(iz) \,, \\ \beta &: z \mapsto \Im f(z) \,, \qquad & \delta &: z \mapsto \Im f(iz) \,. \end{aligned}$$

Then, if a, $b \in E^c_{\mathbb{R}}$, then $f(a + ib) = \alpha(a) + i\beta(a) + \gamma(ib) + i\delta(ib)$, and f can be represented as an application on $E^c_{\mathbb{R}} \times E^c_{\mathbb{R}}$ by the matrix

$$\begin{pmatrix} \alpha & \gamma \\ \beta & \delta \end{pmatrix} .$$

The following relations hold with the above sign if f is $\mathbb{C}$-linear and with the below sign if f is $\mathbb{C}$-antilinear: $\beta = \mp\gamma$ and $\alpha = \pm\delta$ and f^* is represented by the matrix $\left(\begin{smallmatrix} \alpha^T & \mp\beta^T \\ \beta^T & \pm\alpha^T \end{smallmatrix}\right)$.

We want to show a reduction result for the symplectomorphisms in the spirit of the polar decomposition, in the case of an implementable symplectomorphism (see Definition 3.8.1 and Theorem 3.8.4).

Theorem 3.A.9. *Let T be an implementable symplectomorphism. Then*

$$T = ue^{c\rho}$$

where

- *u is a unitary operator,*
- *c is a conjugation,*
- *ρ is a Hilbert-Schmidt, self-adjoint, non-negative operator commuting with c.*

Remark 3.A.10. The operator u is the unitary operator of the polar decomposition $L = u\,|L|$ of the $\mathbb{C}$-linear part of T. The conjugation c is a specific conjugation associated with L and will be constructed during the proof and $\rho = \arg\cos|L|$.

Proof. Let us write $T = L + A$ with L $\mathbb{C}$-linear and A $\mathbb{C}$-antilinear. With $L = u\,|L|$ the polar decomposition of L we get $T = u\,(|L| + u^*A)$ so that it is enough to show the two next lemmas. □

Lemma 3.A.11. *Let $(E, \langle\cdot,\cdot\rangle)$ be a finite-dimensional Hilbert space over $\mathbb{C}$. Let $f : E \to E$ be a $\mathbb{C}$-antilinear application such that*

$$ff^* = I_E \qquad \textit{and} \qquad f = f^*\,.$$

Then there exists an orthonormal basis (u_j) of E such that

$$\forall j,\ f\,(u_j) = u_j\,.$$

Proof. Let us consider an arbitrary conjugation c_0 on E and the $\begin{pmatrix} \alpha & \beta \\ \beta & -\alpha \end{pmatrix}$ "matrix" of f (as a $\mathbb{R}$-linear operator) on $E = E_{\mathbb{R}}^{c_0} \oplus iE_{\mathbb{R}}^{c_0}$ identified with $E_{\mathbb{R}}^{c_0} \times E_{\mathbb{R}}^{c_0}$. The matrix associated to f^* is $\begin{pmatrix} \alpha^T & \beta^T \\ \beta^T & -\alpha^T \end{pmatrix}$ so that the relation $f = f^*$ gives $\alpha = \alpha^T$ and $\beta = \beta^T$. From $ff^* = I_E$ we deduce $\alpha^2 + \beta^2 = \mathrm{Id}$ and $\alpha\beta = \beta\alpha$. We can thus diagonalize simultaneously α and β, and so in a convenient basis of $E_{\mathbb{R}}^{c_0}$ the matrix of f is of the form

$$\left(\begin{array}{ccc|ccc} \ddots & & 0 & \ddots & & 0 \\ & \lambda_j^\alpha & & & \lambda_j^\beta & \\ 0 & & \ddots & 0 & & \ddots \\ \hline \ddots & & 0 & \ddots & & 0 \\ & \lambda_j^\beta & & & -\lambda_j^\alpha & \\ 0 & & \ddots & 0 & & \ddots \end{array}\right).$$

We can thus confine ourself to the case of a space E of complex dimension 1 and of f with a matrix of the form $\begin{pmatrix} \alpha & \beta \\ \beta & -\alpha \end{pmatrix}$ with α and β real numbers. We search a normalized vector $z = \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix} = \begin{pmatrix} x \\ y \end{pmatrix}$ and a real λ such that $f\,(z) = \lambda z$, i.e.

$$\begin{aligned} \lambda \begin{pmatrix} x \\ y \end{pmatrix} &= \begin{pmatrix} \alpha x + \beta y \\ -\alpha y + \beta x \end{pmatrix} = \begin{pmatrix} x & y \\ -y & x \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \\ &= \sqrt{\alpha^2 + \beta^2} \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} \cos\phi \\ \sin\phi \end{pmatrix} = \sqrt{\alpha^2 + \beta^2} \begin{pmatrix} \cos(\phi-\theta) \\ \sin(\phi-\theta) \end{pmatrix} \end{aligned}$$

so that if we choose θ such that $\phi - \theta = \theta$ we get the desired result with $\lambda = \sqrt{\alpha^2 + \beta^2}$. Finally, from $ff^* = I_E$ we deduce that $\lambda = 1$ and the result follows. □

Lemma 3.A.12. *Let $T = L + A$ be an implementable symplectomorphism with L $\mathbb{C}$-linear self-adjoint and positive, A $\mathbb{C}$-antilinear.*

Then L and A commute, there exist a conjugation c commuting with L and A such that Ac is self-adjoint and non-negative and

$$T = e^{c\rho}$$

with $\rho = \arg\cosh L = \arg\sinh (Ac)$ a Hilbert-Schmidt, non-negative and self-adjoint operator commuting with c.

Proof. As $AA^* \in \mathcal{L}_1(\mathcal{Z})$, $AA^* = \sum_j \lambda_j^2 |e_j\rangle\langle e_j|$, with $\lambda_j \in \mathbb{R}$ and $\sum_j \lambda_j^2 < \infty$, from $L^2 = I_{\mathcal{Z}} + AA^*$ we deduce $L^2 = \sum_j \mu_j^2 |e_j\rangle\langle e_j|$ with $\mu_j = \sqrt{1+\lambda_j^2}$ and thus $L = \sum_j \mu_j |e_j\rangle\langle e_j|$.

From the equivalent characterizations of a symplectomorphism we get

$$L^2 - AA^* = I_{\mathcal{Z}} \quad \text{and} \quad L^2 - A^*A = I_{\mathcal{Z}}$$

multiplying the first equality on the right and the second on the left by A and computing the difference we get $\left[L^2, A\right] = 0$. As L is self-adjoint and positive one can use the functional calculus and $L = \sqrt{L^2}$ to obtain $[L, A] = 0$.

From $[L, A] = 0$, $L = L^*$ and the characterizations of a symplectomorphism, we also get $AL = LA = L^*A = A^*L$ so that $(A - A^*)\, L = 0$ and from the invertibility of L one deduces $A = A^*$.

The proper subspaces associated with L and $\ker(L - \mu I_{\mathcal{Z}})$, are thus stable by the action of A (and finite-dimensional). We also remark that on $\ker(L - \mu I_{\mathcal{Z}})$, $AA^* = L^2 - I_{\mathcal{Z}} = (\mu^2 - 1) I_{\mathcal{Z}}$, so that two cases are possible:

$$\mu = 1\,, \text{ then } A = 0 \qquad \text{or} \qquad \mu > 1\,, \text{ then } \frac{1}{\sqrt{\mu^2-1}} A \frac{1}{\sqrt{\mu^2-1}} A^* = I_{\mathcal{Z}}\,.$$

We apply Lemma 3.A.11 to the $\mathbb{C}$-antilinear applications induced by the applications $A/\sqrt{\mu^2-1}$ on the Hilbert spaces $\ker(L - \mu I_{\mathcal{Z}})$. This provides us with a Hilbert basis (e_j) of $\mathcal{Z}$ which diagonalizes both L and A. We can also define a conjugation $c\left(\sum_j \alpha_j e_j\right) = \sum_j \overline{\alpha_j} e_j$. This conjugation commutes with L and A, and Ac is clearly a non-negative self-adjoint operator and so is necessarily $\sqrt{AA^*}$. We finally get for every vector e_j of the basis the relations $Le_j = \mu_j e_j$ and $Ae_j = \lambda_j e_j$ with $\mu_j^2 - \lambda_j^2 = 1$, and thus one can define $\rho_j = \arg\cosh \mu_j$ ($\rho_j = \arg\sinh \lambda_j$ as $\lambda_j \geq 0$) and so we can define $\rho = \arg\cosh L = \arg\sinh Ac$ so that $T = e^{c\rho}$. □

3.B Relations between Weyl and Wick symbols in finite dimension

We want to use the relation between the Weyl and Wick symbols associated to a same Wick polynomial in finite dimension, working with $\mathcal{Z} = \mathbb{C}^r$ we have

$$b = \frac{1}{(\pi\varepsilon/2)^r} \breve{b} * e^{-\frac{|z|^2}{\varepsilon/2}}$$

where b is the Wick symbol and $\breve{b}$ is the Weyl symbol and $b^{Wick} = \breve{b}^{Weyl}$. We want to get rid of the convolution and for this we use the Fourier transform

$$\mathcal{F}f\left(x'\right) = \frac{1}{(2\pi)^r} \int_{\mathbb{R}^{2r}} e^{-ix.x'} f(x)\, dx$$

where $x, x' \in \mathbb{R}^{2r} \cong \mathbb{C}^r$. The inverse Fourier transform is then

$$\mathcal{F}^{-1} f(x) = \frac{1}{(2\pi)^r} \int_{\mathbb{R}^{2r}} e^{ix.x'} f\left(x'\right) dx' .$$

We can use the formulae

$$\begin{aligned} \mathcal{F}(f * g) &= (2\pi)^r \mathcal{F}f.\mathcal{F}g \\ \mathcal{F}\left[e^{-\alpha\frac{|x|^2}{2}}\right]\left(x'\right) &= \frac{1}{\alpha^r} e^{-\frac{|x'|^2}{2\alpha}} \\ \mathcal{F}^{-1}(x \times \cdot)\,\mathcal{F} &= D_x . \end{aligned}$$

We then obtain with $m = 2n$

$$\begin{aligned} \mathcal{F}b\left(z'\right) &= \frac{(2\pi)^r}{(\pi\varepsilon/2)^r} \mathcal{F}\left[e^{-\frac{|z|^2}{\varepsilon/2}}\right] \mathcal{F}\breve{b}\left(z'\right) \\ &= \left(\frac{4}{\varepsilon}\right)^r \left(\frac{\varepsilon}{4}\right)^r e^{-\frac{\varepsilon}{8}|z'|^2} \mathcal{F}\breve{b}\left(z'\right) \\ &= e^{-\frac{\varepsilon}{8}|z'|^2} \mathcal{F}\breve{b}\left(z'\right) \end{aligned}$$

and

$$\begin{aligned} b &= \mathcal{F}^{-1} e^{-\frac{\varepsilon}{8}|z'|^2} \mathcal{F}\breve{b} \\ &= e^{-\frac{\varepsilon}{8}\mathcal{F}^{-1}|z'|^2\mathcal{F}} \breve{b} \\ &= e^{\frac{\varepsilon}{2}\partial_z.\partial_{\bar{z}}} \breve{b} \end{aligned}$$

using the fact that

$$\mathcal{F}^{-1}\left|z'\right|^2 \mathcal{F} = D^2_{(x,\xi)} = -4 \times \frac{1}{2}(\partial_x - i\partial_\xi) . \frac{1}{2}(\partial_x + i\partial_\xi) = -4\partial_z.\partial_{\bar{z}} .$$

It is clear that if $\breve{b}$ is a polynomial in $\mathcal{P}_{\leq m}(\mathcal{Z})$, then b is in this class of polynomials, as we can see deriving the convolution product. We want to show that the application

$$\begin{aligned} \mathcal{P}_{\leq m}(\mathcal{Z}) &\to \mathcal{P}_{\leq m}(\mathcal{Z}) \\ \breve{b} &\mapsto b = \frac{1}{(\pi\varepsilon/2)^n} \breve{b} * e^{-\frac{|z|^2}{\varepsilon/2}} \end{aligned}$$

is a bijection. As the dimension of $\mathcal{Z}$ is finite, the dimension of $\mathcal{P}_{\leq m}(\mathcal{Z})$ is finite and it is enough to show the injectivity of this application. For this we want to justify that on the part of main degree this application is the identity. This is obvious from the following facts:

- $\partial_{\bar{z}}^q \partial_z^p b = \frac{1}{(\pi\varepsilon/2)^r} \partial_{\bar{z}}^q \partial_z^p \breve{b} * e^{-\frac{|z|^2}{\varepsilon/2}}$
- this application is the identity on the constants.

Thus we can also consider the reverse application that we will improperly note

$$\breve{b} = e^{-\frac{\varepsilon}{2}\partial_z.\partial_{\bar{z}}} b\,.$$

3.C Symplectic Fourier transform

Let us then consider the symplectic Fourier transform on $L^2\left(\mathbb{C}^d;\mathbb{C}\right) \equiv L^2\left(\mathbb{R}^{2d}\right)$ with $z = x + iy$, defined by

$$\mathcal{F}^\sigma(f)(z) = \int e^{i2\pi\sigma(z,z')} f\left(z'\right) L\left(dz'\right)$$

with $\sigma(z,z') = \Im\langle z,z'\rangle = \Im\left[\langle x,x'\rangle + \langle y,y'\rangle + i\langle x,y'\rangle - i\langle y,x'\rangle\right]$ and L denotes the Lebesgue measure. We list here some properties of the symplectic Fourier transform.

1. Inverse.
$$\left(\mathcal{F}^\sigma\right)^{-1} = \mathcal{F}^\sigma$$
2. Convolution.
$$\mathcal{F}^\sigma(f * g) = \mathcal{F}^\sigma f.\mathcal{F}^\sigma g$$
3. Composition with a symplectic transformation. Let T be a symplectomorphism, then
$$\mathcal{F}^\sigma\left[f(T\cdot)\right](z) = \mathcal{F}^\sigma[f](Tz)\ .$$
4. Gaussians. For $a > 0$,
$$\mathcal{F}^\sigma\left[e^{-a|\cdot|^2}\right](z) = \left(\frac{\pi}{a}\right)^d e^{-\pi^2|z|^2/a}\,.$$
5. Derivation. We consider the derivations $\partial_z = \frac{1}{2}\left(\partial_x - i\partial_y\right)$ and $\partial_{\bar{z}} = \frac{1}{2}\left(\partial_x + i\partial_y\right)$ then
$$-\frac{1}{\pi}\partial_z.z_0 = \mathcal{F}^\sigma\left(\bar{z}.z_0\times\right)\mathcal{F}^\sigma \quad \text{and} \quad \frac{1}{\pi}\bar{z}_0.\partial_{\bar{z}} = \mathcal{F}^\sigma\left(\bar{z}_0.z\times\right)\mathcal{F}^\sigma\,.$$

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Chapitre 4

Propagation du chaos pour des systèmes constitués d'un grand nombre de bosons en dimension un avec une interaction ponctuelle entre deux bosons.

Article rédigé en anglais, à paraître dans Asymptotic Analysis.

Propagation of chaos for many-boson systems in one dimension with a point pair-interaction.

Joint work with Zied Ammari.

Abstract: We consider the semiclassical limit of nonrelativistic quantum many-boson systems with delta potential in one dimensional space. We prove that time evolved coherent states behave semiclassically as squeezed states by a Bogoliubov time-dependent affine transformation. This allows us to obtain properties analogous to those proved by Hepp and Ginibre-Velo ([95], [90, 91]) and also to show propagation of chaos for Schrödinger dynamics in the mean field limit. Thus, we provide a derivation of the cubic NLS equation in one dimension.

Sommaire

4.1 Introduction 131
4.2 Preliminaries and main results 135
4.3 Many-boson system 140
4.4 The cubic NLS equation 143
4.5 Time-dependent quadratic dynamics 144
4.6 Propagation of coherent states 150
4.7 Propagation of chaos 164
4.A Elementary estimate 167
4.B Commutator theorems 169
4.C Non-autonomous Schrödinger equation 171

4.1 Introduction

We consider a non-relativistic quantum system of $\mathbf{N}$ bosons moving in d-dimensional space in the mean field scaling with a two-body point interaction. The heuristic Hamiltonian of the system is given by

$$\mathrm{H}_{\mathbf{N}} := \sum_{i=1}^{\mathbf{N}} -\Delta_{x_i} + \frac{1}{\mathbf{N}} \sum_{1 \le i < j \le \mathbf{N}} \delta(x_i - x_j)\,, \quad x_i, x_j \in \mathbb{R}^d\,. \tag{4.1.1}$$

Here δ stands for the Dirac distribution and the Hamiltonian $\mathrm{H}_{\mathbf{N}}$ formally acts on the space of symmetric square-integrable functions $L^2_s(\mathbb{R}^{d\mathbf{N}})$. This model is widely studied in the physical literature, particulary in the one dimension case $d = 1$ (see [89]). There are at least two subjects in which such a Hamiltonian is of interest, namely in nuclear physics and in quantum statistical mechanics. The Hamiltonian (4.1.1) indeed describes a simplified model of stripping reaction in nuclear physics where the main motivation is the calculation of cross-section and scattering matrix. In quantum statistical mechanics, (4.1.1) is related to Bose gases with hard-sphere interaction and Fermi pseudopotential (see [99]).

To the best of our knowledge there are, from a mathematical point of view, only few results available in dimension $d = 2, 3$. They are mainly restricted to the three-body problem. In contrast, the one dimensional case $d = 1$ is quite simple. For instance, we can prove selfadjointness of $\mathrm{H}_{\mathbf{N}}$ by standard quadratic form technics. Consequently, the dynamic of the system is well defined in this case and it is given by the time-dependent Schrödinger equation

$$i\partial_t \Psi^t_{\mathbf{N}} = \mathrm{H}_{\mathbf{N}} \Psi^t_{\mathbf{N}}\,. \tag{4.1.2}$$

Beyond the simplicity of the one dimensional case, the delta interaction in (4.1.1) is only form-bounded with respect to the kinetic energy. This means that the potential is quite singular. It is even not a Lebesgue measurable function. As we will explain it later, this feature of the model motivates our analysis.

Our goal in this paper is the justification of the chaos conservation hypothesis for the quantum many-body Hamiltonian (4.1.1) in one dimension $d = 1$. This well-know hypothesis finds its roots in statistical physics of classical many-particle systems (see [94] and references therein). Roughly speaking, we want to show that if the initial state of the system is uncorrelated

$$\Psi^0_{\mathbf{N}} = \varphi_0^{\otimes \mathbf{N}} \in L^2_s(\mathbb{R}^{d\mathbf{N}}) \quad \text{with} \quad \|\varphi_0\|_{L^2(\mathbb{R}^d)} = 1\,,$$

then the evolved state, at any fixed time t, is in a certain sense asymptotically uncorrelated, i.e.,

$$\Psi^t_{\mathbf{N}} \simeq \varphi_t^{\otimes \mathbf{N}} \quad \text{when} \quad \mathbf{N} \to \infty$$

and φ_t solves the one particle nonlinear cubic Schrödinger equation

$$\begin{cases} i\partial_t\varphi = -\Delta\varphi + |\varphi|^2\varphi \\ \varphi_{|t=0} = \varphi_0\,. \end{cases} \tag{4.1.3}$$

More precisely, consider the k-particle correlation functions of the state $\Psi^t_{\mathbf{N}}$

$$\gamma^t_{k,\mathbf{N}}(x_1,\cdots,x_k;y_1,\cdots,y_k) \\ = \int_{\mathbb{R}^{d(\mathbf{N}-k)}} \Psi^t_{\mathbf{N}}(x_1,\cdots,x_k;z)\,\overline{\Psi^t_{\mathbf{N}}(y_1,\cdots,y_k;z)}\,dz\,. \tag{4.1.4}$$

The kernel $\gamma^t_{k,\mathbf{N}}$ is symmetric with respect to any permutation over the variables $(x_1,\cdots,x_k)$ or $(y_1,\cdots,y_k)$. Furthermore, it defines a positive trace class operator over $L^2(\mathbb{R}^{dk})$, which we still denote by $\gamma^t_{k,\mathbf{N}}$. The chaos conservation hypothesis (also called propagation of chaos) is the property of convergence in the trace norm of $\gamma^t_{k,\mathbf{N}}$ to the projector $|\varphi_t^{\otimes k}\rangle\langle\varphi_t^{\otimes k}|$, i.e.,

$$\lim_{\mathbf{N}\to\infty} \mathrm{Tr}\left|\gamma^t_{k,\mathbf{N}} - |\varphi_t^{\otimes k}\rangle\langle\varphi_t^{\otimes k}|\right| = 0\,.$$

By duality, this convergence of correlation functions $\gamma^t_{k,\mathbf{N}}$ is also equivalent to the statement:

$$\lim_{\mathbf{N}\to\infty} \langle\Psi^t_{\mathbf{N}},\ A\otimes 1^{(\mathbf{N}-k)}\ \Psi^t_{\mathbf{N}}\rangle = \langle\varphi_t^{\otimes k},\ A\,\varphi_t^{\otimes k}\rangle\,, \tag{4.1.5}$$

for any bounded operator $A : L^2(\mathbb{R}^{dk}) \to L^2(\mathbb{R}^{dk})$. Here $1^{(\mathbf{N}-k)}$ denotes the identity operator acting on $L^2(\mathbb{R}^{d(\mathbf{N}-k)})$.

In the recent years, mainly motivated by the study of Bose-Einstein condensates, there is a renewed and growing interest in the analysis of many-body quantum dynamics in the mean field limit (see [73], [77], [78], [84], [82], [83], [86], [87], [88], [100], [105], etc).

A statement similar to (4.1.5) was first proved in [105] for bounded potentials (i.e., where δ in (4.1.1) is replaced by a real-valued function V in $L^\infty(\mathbb{R}^d)$ and the cubic Schrödinger equation (4.1.3) by a nonlinear Hartree equation). Then it was extended in [78, 84] to the Coulomb potential using the so-called BBGKY hierarchy method. This approach (named after Bogoliubov, Born, Green, Kirkwood, and Yvon) is based on the analysis of the Heisenberg equation,

$$\begin{cases} \partial_t\rho_t = i[\rho_t, \mathrm{H}_{\mathbf{N}}], \\ \rho_{|t=0} = |\varphi_0^{\otimes\mathbf{N}}\rangle\langle\varphi_0^{\otimes\mathbf{N}}|\,, \end{cases} \tag{4.1.6}$$

together with the finite chain of equations obtained from (4.1.6) by taking partial traces on k variables with $0 \le k \le \mathbf{N}$. For a general presentation on this method and its connection to the mean field problem for classical particles, we refer the reader to the reviews [105, 93]. More recently, other approaches have emerged (e.g. [75],[86],[98],[103]) and error estimates were also derived.

One of the alternative approaches to the chaos conservation hypothesis uses the second quantization framework (details on this notions are recalled in Section 4.2). We consider the Hamiltonian,

$$H_\varepsilon = \varepsilon \int_{\mathbb{R}^d} \nabla a^*(x) \nabla a(x)\ dx + \frac{\varepsilon^2}{2} \int_{\mathbb{R}^{2d}} a^*(x) a^*(y) \delta(x-y) a(x) a(y)\ dxdy\,, \tag{4.1.7}$$

where a,a^* are the usual creation-annihilation operator-valued distributions in the Fock space over $L^2(\mathbb{R}^d)$. Recall that a and a^* satisfy the canonical commutation relations

$$[a(x), a^*(y)] = \delta(x-y)\,, \quad [a^*(x), a^*(y)] = 0 = [a(x), a(y)]\,.$$

A simple computation leads to the following identity

$$\varepsilon^{-1} H_{\varepsilon_{|L^2_s(\mathbb{R}^{d\mathbf{N}})}} = \mathrm{H}_{\mathbf{N}}, \quad \text{if} \quad \varepsilon = \frac{1}{\mathbf{N}}\,.$$

Thus, the statement (4.1.5) on propagation of chaos can be written (up to an unessential factor) as

$$\lim_{\varepsilon \to 0} \langle e^{-it\varepsilon^{-1} H_\varepsilon} \Psi^0_{\mathbf{N}}\,, b^{Wick} e^{-it\varepsilon^{-1} H_\varepsilon} \Psi^0_{\mathbf{N}} \rangle = \langle \varphi_t^{\otimes k}, A \varphi_t^{\otimes k} \rangle\,, \quad (\varepsilon = \frac{1}{\mathbf{N}}),$$

where b^{Wick} denotes ε-dependent Wick observables defined by

$$b^{Wick} = \varepsilon^k \int_{\mathbb{R}^{2kd}} \prod_{i=1}^k a^*(x_i)\ \ A(x_1, \cdots, x_k; y_1, \cdots, y_k) \prod_{j=1}^k a(y_j)\ dx_1 \cdots dx_k dy_1 \cdots dy_k\,. \tag{4.1.8}$$

Here $A(x_1, \cdots, x_k; y_1, \cdots, y_k)$ denotes the distribution kernel of the bounded operator A on $L^2(\mathbb{R}^{kd})$. Therefore, the mean field limit ($\mathbf{N} \to \infty$) for the Hamiltonian $\mathrm{H}_{\mathbf{N}}$ can be related to the semiclassical limit ($\varepsilon \to 0$) for H_ε. The study of the semiclassical limit for many-boson systems started with the work of Hepp [95]. It was subsequently improved by Ginibre and Velo [90, 91]. This analysis uses coherent states

$$\Psi^0_\varepsilon = e^{-\frac{|\varphi|^2}{2\varepsilon}} \sum_{n=0}^\infty \varepsilon^{-n/2} \frac{\varphi^{\otimes n}}{\sqrt{n!}}\,, \quad \varphi \in L^2(\mathbb{R}^d)\,,$$

instead of chaos states $\Psi^0_{\mathbf{N}} = \varphi_0^{\otimes \mathbf{N}}$. However, a clever argument in the work of Rodnianski and Schlein [103] shows that propagation of chaos can be deduced form the semiclassical analysis with coherent states. They also provided error estimates on the k-particle correlation functions.

In this context, our purpose in considering this problem is to weaken the assumptions on the two-body potential. We expect that the statement (4.1.5) holds true for the general situation where δ is replaced by a quadratic form Q which is infinitesimally form bounded with respect to $-\Delta$. As one steep forward, we look at the specific problem of delta potential in one dimension which fits the above setting. The best available result in this direction, at our knowledge, is the work of Ginibre and Velo [91]. However, it is only valid for coherent states and dimension $d \geq 3$. The recent work of [98] apply to potentials V in $L^2(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$ while the work [103] assumes $(-\Delta+1)^{1/2}$-bounded potential (i.e., $V(-\Delta+1)^{-1/2}$ is bounded operator). Some other works are specific for the Coulomb potential (e.g., [81],[88]). To briefly enlighten the comparison, we consider, in three dimension, the potential

$$V(x) = \frac{1}{|x|^\alpha}\,.$$

Then the work [103] apply for $\alpha \leq 1$ and [98] for $\alpha < 3/2$ while V is $-\Delta$-form bounded for $\alpha < 2$. So far, the Hamiltonian (4.1.1) has not been considered to our knowledge, except in [73] where a partial result is proved (i.e., convergence of BBGKY hirearchy is proved but not the uniqueness).

Another point of view consists of replacing the delta interaction in (4.1.1) by a smooth scaled potential $V_{\mathbf{N}}(x) = \mathbf{N}^{d\beta} V(\mathbf{N}^\beta x)$ with $\beta \in (0,1)$. In this case, propagation of chaos was proved (under some assumptions) in [74] for $d = 1$ and in [82] for $d = 3$. Although, $V_{\mathbf{N}}$ converges in a distribution sense to $\delta \int V(x)dx$, it is not clear how this can be related to our problem. We remark that the case $\beta = 1$ is related to the Gross-Pitaevskii equation derived in [83].

For reader convenience we give a glimpse of our main results. Essentially, our work is divided into three parts:
(i) Propagation of coherent states,
(ii) Propagation of chaos,
(iii) Non-autonomous abstract Schrödinger equation.
In (i) we give a semiclassical approximation of the evolved coherent states $e^{-it\varepsilon^{-1}H_\varepsilon}\Psi_\varepsilon^0$ using the unitary propagator $U_2(t,s)$ of a time-dependent quadratic Hamiltonian $A_2(t)$ related to H_ε. It is the most technical part of the paper where subtle points about form domains come into the play. The main result is Theorem 4.6.1 which is actually slightly stronger than the usual formulation of the semiclassical approximation in [95],[90, 91]. This will be helpful to achieve part (ii). We also identify $U_2(t,s)$ as a time-dependent Bogoliubov transformation in Proposition 4.6.7. Once Theorem 4.6.1 is proved, the part (ii) follows from an argument in [103] which can be

made abstract. For completeness we provide a proof for this fact (see Theorem 4.2.3). In part (iii) we establish some abstract results on the existence of unitary propagator for non-autonomous Schrödinger equations which may have their own interest. For instance, we prove in Corollary 4.C.4 a result which can be considered as time-dependent counterpart of the well-known Nelson commutator theorem [101] (see Appendix 4.C). This is a key point which allows to construct the unitary propagator $U_2(t,s)$ with crucial estimates (see Proposition 4.5.5).

For the sake of clarity, we restricted ourselves in this paper to the specific case of point interaction potential in one dimension. We hope that this will be helpful for further improvement. We believe indeed that such simple example sums up the principal difficulties on the problem. We also remark that the results here can be easily extended to the case $V(x) = -\delta(x)$ by working locally in time.

Finally, we outline the content of this article. We recall the basic definitions for the Fock space framework in Section 4.2 and state two of our main results (Theorem 4.2.3 and Proposition 4.2.4). Then we accurately introduce the quantum dynamics of the considered many-boson system and its classical counterpart, namely the cubic NLS equation. The study of the semiclassical limit through Hepp's method is carried out in Section 4.6 where we use results on the time-dependent quadratic approximation derived in Section 4.5. In the last Section 4.7 we apply the argument of [103] to prove the chaos propagation result.

4.2 Preliminaries and main results

Let $\mathfrak{H}$ be a Hilbert space. We denote by $\mathcal{L}(\mathfrak{H})$ the space of all linear bounded operators on $\mathfrak{H}$. For a linear unbounded operator L acting on $\mathfrak{H}$, we denote by $\mathcal{D}(L)$ (respectively $\mathcal{Q}(L)$) the operator domain (respectively form domain) of L. Let D_{x_j} denotes the differential operator $-i\partial_{x_j}$ on $L^2(\mathbb{R}^n)$ where $(x_1, \cdots, x_n) \in \mathbb{R}^n$. Let $H^s(\mathbb{R}^m)$ denotes the Sobolev spaces.

In the following we recall the second quantization framework. We denote by $L^2_s(\mathbb{R}^{nd})$ the space of symmetric square integrable functions, i.e.,

$$\Psi_n \in L^2_s(\mathbb{R}^{nd}) \text{ iff } \Psi_n \in L^2(\mathbb{R}^{nd}) \text{ and } \Psi_n(x_1, \cdots, x_n) = \Psi_n(x_{\sigma_1}, \ldots, x_{\sigma_n}) \text{ a.e.,}$$

for any permutation σ on the symmetric group $\mathrm{Sym}(n)$. We can see $L^2_s(\mathbb{R}^{nd})$ as a closed subspace of $L^2(\mathbb{R}^{nd})$ characterized by the orthogonal projection $\mathfrak{S}_n$, given by

$$\mathfrak{S}_n \Psi_n(x_1, \cdots, x_n) = \frac{1}{n!} \sum_{\sigma \in \mathrm{Sym}(n)} \Psi_n(x_{\sigma(1)}, \cdots, x_{\sigma(n)}), \quad \Psi_n \in L^2(\mathbb{R}^{nd}).$$

The symmetric Fock space over $L^2(\mathbb{R})$ is defined as the Hilbert space,

$$\mathcal{F} = \bigoplus_{n=0}^{\infty} L_s^2(\mathbb{R}^{nd}),$$

endowed with the inner product

$$\langle \Psi, \Phi \rangle = \sum_{n=0}^{\infty} \int_{\mathbb{R}^{nd}} \overline{\Psi_n(x_1, \cdots, x_n)}\, \Phi_n(x_1, \cdots, x_n)\, dx_1 \cdots dx_n\,,$$

where $\Psi = (\Psi_n)_{n\in\mathbb{N}}$ and $\Phi = (\Phi_n)_{n\in\mathbb{N}}$ are two arbitrary vectors in $\mathcal{F}$. The vacuum is the vector $\Omega_0 = (1, 0, \cdots)$ in $\mathcal{F}$. We will use the notation

$$\mathcal{S}_s(\mathbb{R}^{nd}) := \mathfrak{S}_n \mathcal{S}(\mathbb{R}^{nd})$$

where $\mathcal{S}(\mathbb{R}^{nd})$ is the Schwartz space on $\mathbb{R}^{nd}$. A convenient subspace of $\mathcal{F}$ is given by the algebraic direct sum

$$\mathcal{S} := \bigoplus_{n=0}^{\text{alg}} \mathcal{S}_s(\mathbb{R}^{nd})\,.$$

The most common operators on $\mathcal{F}$ are determined by their action on the family of vectors

$$\varphi^{\otimes n}(x_1, \dots, x_n) = \prod_{i=1}^{n} \varphi(x_i)\,, \quad \varphi \in L^2(\mathbb{R}^d)\,,$$

which spans the space $L_s^2(\mathbb{R}^{nd})$ thanks to the polarization identity,

$$\mathfrak{S}_n \prod_{i=1}^{n} \varphi_i(x_i) = \frac{1}{2^n n!} \sum_{\varepsilon_i=\pm 1} \varepsilon_1 \cdots \varepsilon_n \prod_{i=1}^{n} \Big(\sum_{j=1}^{n} \varepsilon_j \varphi_j(x_i)\Big)\,.$$

For example, the creation and annihilation operators $a^*(f)$ and $a(f)$, parameterized by $\varepsilon > 0$, are defined by

$$\begin{aligned} a(f)\varphi^{\otimes n} &= \sqrt{\varepsilon n}\ \langle f, \varphi\rangle \varphi^{\otimes(n-1)} \\ a^*(f)\varphi^{\otimes n} &= \sqrt{\varepsilon(n+1)}\ \mathfrak{S}_{n+1}(\, f \otimes \varphi^{\otimes n})\,, \quad \forall \varphi, f \in L^2(\mathbb{R}^d). \end{aligned}$$

They can also by written as

$$a(f) = \sqrt{\varepsilon} \int_{\mathbb{R}^d} \overline{f(x)}\, a(x)\, dx, \quad a^*(f) = \sqrt{\varepsilon} \int_{\mathbb{R}^d} f(x)\, a^*(x)\, dx,$$

where $a^*(x), a(x)$ are the canonical creation-annihilation operator-valued distributions. Recall that for any $\Psi = (\Psi^{(n)})_{n\in\mathbb{N}} \in \mathcal{S}$, we have

$$[a(x)\Psi]^{(n)}(x_1, \cdots, x_n) = \sqrt{(n+1)}\Psi^{(n+1)}(x, x_1, \cdots, x_n),$$

$$[a^*(x)\Psi]^{(n)}(x_1, \cdots, x_n) = \frac{1}{\sqrt{n}} \sum_{j=1}^{n} \delta(x - x_j)\Psi^{(n-1)}(x_1, \cdots, \hat{x}_j, \cdots, x_n)\,,$$

where δ is the Dirac distribution at the origin and $\hat{x}_j$ means that the variable x_j is omitted. The Weyl operators are given for $f \in L^2(\mathbb{R}^d)$ by

$$W(f) = e^{\frac{i}{\sqrt{2}}[a^*(f)+a(f)]},$$

and they satisfy the Weyl commutation relations,

$$W(f_1)W(f_2) = e^{-\frac{i\varepsilon}{2}\mathrm{Im}\langle f_1, f_2\rangle}\, W(f_1+f_2), \tag{4.2.1}$$

with $f_1, f_2 \in L^2(\mathbb{R}^d)$.

The interaction term in the Hamiltonian (4.1.7) is a quartic Wick product which we shall consider as a quadratic form on $\mathcal{S}$. From a general point view, this is better understood as a Wick quantization of a polynomial symbol. Let us briefly recall this Wick quantization procedure.

Definition 4.2.1. We say that a function $b : \mathcal{S}(\mathbb{R}^d) \to \mathbb{C}$ is a continuous (p,q)-homogenous polynomial on $\mathcal{S}(\mathbb{R}^d)$ iff it satisfies:
(i) $b(\lambda z) = \bar{\lambda}^q \lambda^p b(z)$ for any $\lambda \in \mathbb{C}$ and $z \in \mathcal{S}(\mathbb{R}^d)$,
(ii) there exists a (unique) continuous hermitian form $\mathfrak{Q} : \mathcal{S}_s(\mathbb{R}^{dq}) \times \mathcal{S}_s(\mathbb{R}^{dp}) \to \mathbb{C}$ such that

$$b(z) = \mathfrak{Q}(z^{\otimes q}, z^{\otimes p}).$$

We denote by $\mathcal{E}$ the vector space spanned by all those polynomials.

The Schwartz kernel theorem ensures for any continuous (p,q)-homogenous polynomial b, the existence of a kernel $\tilde{b}(.,.) \in \mathcal{S}'(\mathbb{R}^{d(p+q)})$ such that

$$b(z) = \int_{\mathbb{R}^{d(p+q)}} \tilde{b}(k_1', \cdots, k_q'; k_1, \cdots, k_p)\, \overline{z(k_1')\cdots z(k_q')}\, z(k_1)\cdots z(k_p)\; dk'dk\,,$$

in the distribution sense. The set of (p,q)-homogenous polynomials $b \in \mathcal{E}$ such that the kernel $\tilde{b}$ defines a bounded operator from $L^2_s(\mathbb{R}^{dp})$ into $L^2_s(\mathbb{R}^{dq})$ will be denoted by $\mathcal{P}_{p,q}(L^2(\mathbb{R}^d))$. Those classes of polynomial symbols are studied and used in [76, 75].

Definition 4.2.2. The Wick quantization is the map which associate to each continuous (p,q)-homogenous polynomial $b \in \mathcal{E}$, a quadratic form b^{Wick} on $\mathcal{S}$ given by

$$\begin{aligned}
&\langle \Psi, b^{Wick}\Phi\rangle \\
&= \varepsilon^{\frac{p+q}{2}} \int_{\mathbb{R}^{d(p+q)}} \tilde{b}(k',k)\, \langle a(k_1')\cdots a(k_q')\Psi, a(k_1)\cdots a(k_p)\Phi\rangle_{\mathcal{F}} dk dk' \\
&= \sum_{n=p}^{\infty} \varepsilon^{\frac{p+q}{2}} \frac{\sqrt{n!(n-p+q)!}}{(n-p)!} \\
&\qquad \int_{\mathbb{R}^{d(n-p)}} dx \int_{\mathbb{R}^{d(p+q)}} dk dk'\, \tilde{b}(k',k)\, \overline{\Psi^{(n)}(k,x)}\Phi^{(n-p+q)}(k',x),
\end{aligned}$$

for any $\Phi, \Psi \in \mathcal{S}$.

We have, for example,

$$a^*(f) = \langle z, f\rangle^{Wick} \quad \text{and} \quad a(f) = \langle f, z\rangle^{Wick}.$$

Furthermore, for any self-adjoint operator A on $L^2(\mathbb{R}^d)$ such that $\mathcal{S}(\mathbb{R}^d)$ is a core for A, the Wick quantization

$$\mathrm{d}\Gamma(A) := \langle z, Az\rangle^{Wick},$$

defines a self-adjoint operator on $\mathcal{F}$. In particular, if A is the identity we get the ε-dependent number operator

$$N := \langle z, z\rangle^{Wick}.$$

We recall the standard number estimate (see, *e.g.*, [76, Lemma 2.5]),

$$\left|\langle \Psi, b^{Wick}\Phi\rangle\right| \leq ||\tilde{b}||_{\mathcal{L}(L^2_s(\mathbb{R}^{dp}),L^2_s(\mathbb{R}^{dq}))}\, ||N^{q/2}\Psi|| \times ||N^{p/2}\Phi||, \tag{4.2.2}$$

which holds uniformly in $\varepsilon \in (0,1]$ for $b \in \mathcal{P}_{p,q}(L^2(\mathbb{R}^d))$ and any $\Psi, \Phi \in \mathcal{D}(N^{max(p,q)/2})$.

In this section, we state two of our main results. Other results as Corollary 4.6.5 and 4.6.6 are not less interesting, in our opinion, but they are postponed to Section 4.6 to keep the presentation fairly simple. The rigorous meaning of the Hamiltonian (4.1.7) is explained in Section 4.3, while the existence and uniqueness of solutions for the nonlinear Schrödinger equation (4.1.3) are recalled in Section 4.4. The first result is propagation of chaos.

Theorem 4.2.3. *For any $\varphi_0 \in H^2(\mathbb{R})$ such that $||\varphi_0||_{L^2(\mathbb{R})} = 1$ and any $b \in \mathcal{P}_{p,p}(L^2(\mathbb{R}))$, we have*

$$\lim_{n\to\infty} \langle \varphi_0^{\otimes n}, e^{it/\varepsilon_n H_{\varepsilon_n}}\, b^{Wick}\, e^{-it/\varepsilon_n H_{\varepsilon_n}} \varphi_0^{\otimes n}\rangle = b(\varphi_t),$$

where $n\varepsilon_n = 1$ and φ_t solves the NLS equation (4.1.3) with initial data φ_0.

The proof is given in Section 4.7 and follows the argument of [103]. In fact, we express $\varphi_0^{\otimes n}$ in terms of coherent states,

$$\varphi_0^{\otimes n} = \frac{e^{n/2}\sqrt{n!}}{2\pi n^{n/2}} \int_0^{2\pi} e^{-i\theta n}\, W(\frac{\sqrt{2}}{i\varepsilon_n} e^{i\theta}\varphi_0)\Omega_0\, d\theta \quad \text{with} \quad \varepsilon_n = 1/n$$

and then use the semiclassical propagation estimate for coherent states given in the proposition below.

Proposition 4.2.4. *For any $\varphi_0 \in H^2(\mathbb{R})$ there exists $c > 0$ depending only on φ_0 such that*

$$\left\| e^{-it/\varepsilon H_\varepsilon} W(\frac{\sqrt{2}}{i\varepsilon}\varphi_0)\Omega_0 - e^{i\omega(t)/\varepsilon} W(\frac{\sqrt{2}}{i\varepsilon}\varphi_t) U_2(t,0)\Omega_0 \right\|_{\mathcal{F}} \leq e^{ce^{c|t|}}\, \varepsilon^{1/8},$$

holds for any $t \in \mathbb{R}$ *. Here* φ_t *solves the NLS equation (4.1.3) with the initial condition* φ_0*,* $\omega(t) = \frac{1}{2}\int_0^t ||\varphi_s^2||_{L^2}^2 \, ds$ *and* $U_2(t,s)$ *is the unitary propagator given by Proposition 4.5.5.*

Actually, we will prove a stronger result in Section 4.6 (see Theorem 4.6.1). This part of the paper is the most technical. However, the idea behind Proposition 4.2.4 is rather simple. In fact, we write a Taylor expansion of the Hamiltonian H_ε around the classical solution φ_t and consider only the terms of order less or equal to ε. Such quantity defines a time-dependent quadratic Hamiltonian which provides an approximation for the evolution of coherent states. If we attempt to show Proposition 4.2.4, we formally differentiate the quantity

$$\mathcal{Y}(t) = e^{i\frac{t}{\varepsilon}H_\varepsilon} e^{i\omega(t)/\varepsilon} W(\frac{\sqrt{2}}{i\varepsilon}\varphi_t) U_2(t,0) \,.$$

So, we obtain

$$\begin{aligned} & -i\varepsilon\partial_t \mathcal{Y}(t) \\ & \quad = e^{i\frac{t}{\varepsilon}H_\varepsilon} e^{i\omega(t)/\varepsilon} W(\frac{\sqrt{2}}{i\varepsilon}\varphi_t) \left[\tilde{H}_\varepsilon - A_0(t) - \sqrt{\varepsilon}A_1(t) - \varepsilon A_2(t)\right] U_2(t,0) \,, \end{aligned}$$

where $\tilde{H}_\varepsilon = W(\frac{\sqrt{2}}{i\varepsilon}\varphi_t)^* H_\varepsilon W(\frac{\sqrt{2}}{i\varepsilon}\varphi_t)$ and $A_0(t), A_1(t), A_2(t)$ are ε-independent operators. It is possible to expand $\tilde{H}_\varepsilon$ in the form $\tilde{H}_\varepsilon = \sum_{k=0}^4 \varepsilon^{k/2} A_k(t)$, where again $A_k(t)$ are ε-independent operators, so that

$$\begin{aligned} \mathcal{Y}(t)\Omega_0 - \mathcal{Y}(0)\Omega_0 = i\varepsilon^{1/2} \int_0^t & e^{i\frac{s}{\varepsilon}H_\varepsilon} e^{i\omega(s)/\varepsilon} W(\frac{\sqrt{2}}{i\varepsilon}\varphi_s) \\ & \times [A_3(s) + \sqrt{\varepsilon}A_4(s)] U_2(s,0)\Omega_0 \, ds \,. \end{aligned} \tag{4.2.3}$$

Then, we estimate the left hand side of (4.2.3), for $t > 0$, by

$$\begin{aligned} & \left\| \mathcal{Y}(t)\Omega_0 - W(\frac{\sqrt{2}}{i\varepsilon}\varphi_0)\Omega_0 \right\|_{\mathcal{F}} \\ & \qquad \le \sqrt{\varepsilon} \int_0^t \left\| [A_3(s) + \sqrt{\varepsilon}A_4(s)] U_2(s,0)\Omega_0 \right\|_{\mathcal{F}} ds \,. \end{aligned} \tag{4.2.4}$$

Hence, we get the coherent state estimate when the integrand in the right hand side of (4.2.4) is bounded uniformly in ε. This holds true if we replace the δ interaction in (4.3.1) by a bounded potential V. But, in our case we end up with the problem that $U_2(s,0)\Omega_0$ is not in the domain of $A_3(s) + \sqrt{\varepsilon}A_4(s)$. So, we can not proceed in this way. Instead, we use a careful decomposition by means of appropriate cutoffs (see Lemma 4.6.4) and exploit a crucial uniform estimates derived in Lemma 4.6.3 and Proposition 4.5.5. Other results concerning abstract non-autonoumous Schrödinger equation are stated in Appendix 4.C. They may be considered as an improvement of Kisynski's work [97]. In particular, Corollary 4.C.4 is used to prove Lemma 4.6.3 and Proposition 4.5.5.

4.3 Many-boson system

In nonrelativistic many-body theory, boson systems are described by the second quantized Hamiltonian in the symmetric Fock space $\mathcal{F}$ formally given by

$$H_\varepsilon = -\varepsilon \int_{\mathbb{R}^d} a^*(x)\Delta a(x)dx + \frac{\varepsilon^2}{2}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} a^*(x)a^*(y)\delta(x-y)a(x)a(y)\,dxdy\,. \tag{4.3.1}$$

The rigorous meaning of formula (4.3.1) is as a quadratic form on $\mathcal{S}$, which we denote by h^{Wick}, obtained by Wick quantization of the classical energy functional

$$h(z) = \int_{\mathbb{R}^d} |\nabla z(x)|^2\,dx + P(z), \text{ where } P(z) = \frac{1}{2}\int_{\mathbb{R}^d} |z(x)|^4\,dx, \quad z \in \mathcal{S}(\mathbb{R}^d)\,. \tag{4.3.2}$$

More explicitly, we have for $\Psi \in \mathcal{S}$

$$\begin{aligned}\langle \Psi, h^{Wick}\Psi\rangle &= \varepsilon\sum_{n=1}^{\infty} n\int_{\mathbb{R}^{dn}} \left|\partial_{x_1}\Psi^{(n)}(x_1,\cdots,x_n)\right|^2 dx_1\cdots dx_n \\ &+ \varepsilon^2\sum_{n=2}^{\infty}\frac{n(n-1)}{2}\int_{\mathbb{R}^{d(n-1)}}\left|\Psi^{(n)}(x_2,x_2,\cdots,x_n)\right|^2 dx_2\cdots dx_n\,.\end{aligned}$$

Moreover, in one dimensional space (i.e., $d=1$) one can show the existence of a unique self-adjoint operator bounded from below, which we denote by H_ε, such that

$$\langle \Psi, H_\varepsilon\Psi\rangle = \langle \Psi, h^{Wick}\Psi\rangle, \qquad \text{for any } \Psi\in\mathcal{S}.$$

This is proved in Proposition 4.3.3.

In all the sequel we restrict our analysis to space <u>dimension $d = 1$</u> and consider the small parameter ε such that <u>$\varepsilon \in (0, 1]$</u>. The ε-independent self-adjoint operator,

$$S_\mu\Psi := \Psi + \sum_{n=1}^{\infty}\left[n^\mu\,\Psi^{(n)} + \sum_{j=1}^{n} -\Delta_{x_j}\Psi^{(n)}\right] = \left(\varepsilon^{-1}\mathrm{d}\Gamma(-\Delta) + \varepsilon^{-\mu}N^\mu + 1\right)\Psi\,,$$

with $\mu > 0$, defines the Hilbert space $\mathcal{F}_+^\mu$ given as the linear space $\mathcal{D}(S_\mu^{1/2})$ equipped with the inner product

$$\langle \Psi, \Phi\rangle_{\mathcal{F}_+^\mu} := \langle S_\mu^{1/2}\Psi, S_\mu^{1/2}\Phi\rangle_{\mathcal{F}}.$$

We denote by $\mathcal{F}_-^\mu$ the completion of $\mathcal{D}(S_\mu^{-1/2})$ with respect to the norm associated to the following inner product

$$\langle \Psi, \Phi\rangle_{\mathcal{F}_-^\mu} := \langle S_\mu^{-1/2}\Psi, S_\mu^{-1/2}\Phi\rangle_{\mathcal{F}}.$$

Therefore, we have the Hilbert rigging

$$\mathcal{F}_+^\mu \subset \mathcal{F} \subset \mathcal{F}_-^\mu.$$

Note that the form domain of the ε-dependent self-adjoint operator $\mathrm{d}\Gamma(-\Delta)+N^\mu$ with $\mu > 0$ is

$$\mathcal{Q}(\mathrm{d}\Gamma(-\Delta) + N^\mu) = \mathcal{F}_+^\mu \quad \text{for any } \varepsilon \in (0,1]\,.$$

Lemma 4.3.1. *For any* $\Psi, \Phi \in \mathcal{S}$,

$$\left|\langle \Psi, P^{Wick}\Phi\rangle\right| \leq \frac{1}{4}\,||[\mathrm{d}\Gamma(-\Delta) + N^3]^{1/2}\Psi|| \;\times\; ||[\mathrm{d}\Gamma(-\Delta) + N^3]^{1/2}\Phi||\,.$$

Proof. A simple computation yields for any $\Psi, \Phi \in \mathcal{S}$

$$\langle \Psi, P^{Wick}\Phi\rangle = \sum_{n=2}^{\infty} \varepsilon^2 \frac{n(n-1)}{2} \int_{\mathbb{R}^{n-1}} \overline{\Psi^{(n)}(x_2, x_2, x_3, \cdots, x_n)} \times \Phi^{(n)}(x_2, x_2, x_3, \cdots, x_n)\, dx_2 \cdots dx_n\,. \quad (4.3.3)$$

Cauchy-Schwarz inequality yields

$$\begin{aligned}
&\left|\langle \Psi, P^{Wick}\Phi\rangle\right| \\
\leq\; &\left[\sum_{n=2}^{\infty} \varepsilon^2 \frac{n(n-1)}{2} \int_{\mathbb{R}^{n-1}} |\Psi^{(n)}(x_2, x_2, x_3, \cdots, x_n)|^2\, dx_2 \cdots dx_n\right]^{1/2} \\
&\times \left[\sum_{n=2}^{\infty} \varepsilon^2 \frac{n(n-1)}{2} \int_{\mathbb{R}^{n-1}} |\Phi^{(n)}(x_2, x_2, x_3, \cdots, x_n)|^2\, dx_2 \cdots dx_n\right]^{1/2}.
\end{aligned}$$

Using Lemma 4.A.1, we get for any $\alpha(n) > 0$

$$\begin{aligned}
&\left|\langle \Psi, P^{Wick}\Phi\rangle\right| \\
\leq\; &\left[\sum_{n=2}^{\infty} \varepsilon^2 \frac{n(n-1)}{2\sqrt{2}} \left(\alpha(n)\langle D_{x_1}^2 \Psi^{(n)}, \Psi^{(n)}\rangle + \frac{\alpha(n)^{-1}}{2}\langle \Psi^{(n)}, \Psi^{(n)}\rangle\right)\right]^{1/2} \\
&\times \left[\sum_{n=2}^{\infty} \varepsilon^2 \frac{n(n-1)}{2\sqrt{2}} \left(\alpha(n)\langle D_{x_1}^2 \Phi^{(n)}, \Phi^{(n)}\rangle + \frac{\alpha(n)^{-1}}{2}\langle \Phi^{(n)}, \Phi^{(n)}\rangle\right)\right]^{1/2}.
\end{aligned}$$

Hence, by choosing $\alpha(n) = \frac{1}{\sqrt{2}\varepsilon(n-1)}$, it follows that

$$\begin{aligned}
&\left|\langle\Psi, P^{Wick}\Phi\rangle\right| \\
\leq\ & \frac{1}{4}\left[\sum_{n=2}^{\infty}\varepsilon n\langle D_{x_1}^2\Psi^{(n)}, \Psi^{(n)}\rangle + \sum_{n=2}^{\infty}\varepsilon^3 n(n-1)^2\langle\Psi^{(n)}, \Psi^{(n)}\rangle\right]^{1/2} \\
&\times\left[\sum_{n=2}^{\infty}\varepsilon n\langle D_{x_1}^2\Phi^{(n)}, \Phi^{(n)}\rangle + \sum_{n=2}^{\infty}\varepsilon^3 n(n-1)^2\langle\Phi^{(n)}, \Phi^{(n)}\rangle\right]^{1/2} \\
\leq\ & \frac{1}{4}\sqrt{\langle\Psi, [\mathrm{d}\Gamma(-\Delta) + N^3]\Psi\rangle} \times \sqrt{\langle\Phi, [\mathrm{d}\Gamma(-\Delta) + N^3]\Phi\rangle}\,.
\end{aligned}$$

This leads to the claimed estimate. □

Remark 4.3.2. *Note that, as in Lemma 4.3.1, the estimate*

$$\left|\langle\Psi, P^{Wick}\Phi\rangle\right| \leq \frac{\varepsilon^2}{4}\,||\Psi||_{\mathcal{F}_+^3}\ \ ||\Phi||_{\mathcal{F}_+^3} \tag{4.3.4}$$

holds true for any $\Psi, \Phi \in \mathcal{S}$ *and* $\varepsilon \in (0, 1]$.

We can show that h^{Wick} is associated to a self-adjoint operator by considering its restriction to each sector $L_s^2(\mathbb{R}^n)$, however we will prefer the following point of view.

Proposition 4.3.3. *There exists a unique self-adjoint operator* H_ε *such that*

$$\langle\Psi, h^{Wick}\Phi\rangle = \langle\Psi, H_\varepsilon\Phi\rangle \ \text{ for any } \ \Psi \in \mathcal{F}_+^3, \Phi \in \mathcal{D}(H_\varepsilon) \cap \mathcal{F}_+^3\,.$$

Moreover, $e^{-it/\varepsilon H_\varepsilon}$ *preserves* $\mathcal{F}_+^3$.

Proof. We first use the KLMN theorem ([102, Theorem X17]) and Lemma 4.3.1 to show that the quadratic form $h^{Wick} + N^3 + 1$ is associated to a unique (positive) self-adjoint operator L with

$$\mathcal{Q}(L) = \mathcal{Q}(\mathrm{d}\Gamma(-\Delta) + N^3) = \mathcal{F}_+^3\,.$$

Observe that we also have

$$||[\mathrm{d}\Gamma(-\Delta) + N^3]^{1/2}\Psi|| \leq ||L^{1/2}\Psi|| \text{ for any } \Psi \in \mathcal{F}_+^3\,. \tag{4.3.5}$$

Next, by the Nelson commutator theorem (Theorem 4.B.2) we can prove that the quadratic form h^{Wick} is uniquely associated to a self-adjoint operator denoted by H_ε with $\mathcal{D}(L) \subset \mathcal{D}(H_\varepsilon) \cap \mathcal{F}_+^3$ and deduce the invariance of $\mathcal{F}_+^3$. Indeed, we easily check using Lemma 4.3.1 and (4.3.5) that

$$\left|\langle\Psi, h^{Wick}\Phi\rangle\right| \leq \frac{5}{4}\,||L^{1/2}\Psi||\ \ ||L^{1/2}\Phi|| \text{ for any } \Psi, \Phi \in \mathcal{F}_+^3. \tag{4.3.6}$$

Furthermore, we have for $\Psi, \Phi \in \mathcal{F}_+^3$ and $\lambda > 0$

$$\begin{aligned}\langle L(\lambda L+1)^{-1}\Psi, h^{Wick}(\lambda L+1)^{-1}\Phi\rangle \\ - \langle (\lambda L+1)^{-1}\Psi, h^{Wick}L(\lambda L+1)^{-1}\Phi\rangle = 0\,. \quad (4.3.7)\end{aligned}$$

The statements (4.3.6)-(4.3.7) with the help of Lemma 4.B.3, allow to use Theorem 4.B.2. □

Remark 4.3.4. *The same argument as in Proposition 4.3.3 shows that the quadratic form on $\mathcal{F}_+^3$ given by*

$$G := \varepsilon^{-1}\mathrm{d}\Gamma(-\Delta) + \varepsilon^{-2}P^{Wick} + \varepsilon^{-1}N + 1\,,$$

is associated to a unique (positive) self-adjoint operator which we denote by the same symbol G.

4.4 The cubic NLS equation

The energy functional h given by (4.3.2) has the associated vector field

$$\begin{aligned} X : H^1(\mathbb{R}) &\longrightarrow H^{-1}(\mathbb{R}) \\ z &\longmapsto X(z) = -\Delta z + \partial_{\bar z}P(z)\,, \end{aligned}$$

which leads to the nonlinear classical field equation

$$\begin{aligned} i\partial_t\varphi &= X(\varphi) \\ &= -\Delta\varphi + |\varphi|^2\varphi \end{aligned} \quad (4.4.1)$$

with initial data $\varphi_{|t=0} = \varphi_0 \in H^1(\mathbb{R})$. It is well-known that the above cubic defocusing NLS equation is globally well-posed on $H^s(\mathbb{R})$ for $s \geq 0$. In particular, the equation (4.4.1) admits a unique global solution on $C^0(\mathbb{R}, H^m(\mathbb{R})) \cap C^1(\mathbb{R}, H^{m-2}(\mathbb{R}))$ for any initial data $\varphi \in H^m(\mathbb{R})$ when $m = 1$ and $m = 2$ (see [92] for $m = 1$ and [106] for $m = 2$). Moreover, we have energy and mass conservations i.e.,

$$h(\varphi_t) = h(\varphi_0) \quad \text{and} \quad ||\varphi_t||_{L^2(\mathbb{R})} = ||\varphi_0||_{L^2(\mathbb{R})}\,,$$

for any initial data $\varphi_0 \in H^1(\mathbb{R})$ and φ_t solution of (4.4.1). It is not difficult to prove the following estimates

$$\begin{aligned} ||\varphi||^2_{L^\infty(\mathbb{R})} &\leq 2||\varphi||_{L^2(\mathbb{R})}\,||\partial_x\varphi||_{L^2(\mathbb{R})} \leq 2\,||\varphi||_{L^2(\mathbb{R})}\,h(\varphi)^{1/2}\,, \\ ||\varphi||^p_{L^p(\mathbb{R})} &\leq 2^{\frac{p-2}{2}}\,||\varphi||^{\frac{p+2}{2}}_{L^2(\mathbb{R})}\,||\partial_x\varphi||^{\frac{p-2}{2}}_{L^2(\mathbb{R})} \leq 2^{\frac{p-2}{2}}\,||\varphi||^{\frac{p+2}{2}}_{L^2(\mathbb{R})}\,h(\varphi)^{\frac{p-2}{4}}\,, \end{aligned} \quad (4.4.2)$$

for $p \geq 2$ and any $\varphi \in H^1(\mathbb{R})$. Furthermore, using Gronwall's inequality we show for any $\varphi_0 \in H^2(\mathbb{R})$ the existence of $c > 0$ depending only on φ_0 such that

$$||\varphi_t||_{H^2(\mathbb{R})} \leq e^{c\,|t|}\;\;||\varphi_0||_{H^2(\mathbb{R})}\,, \quad (4.4.3)$$

where φ_t is a solution of the NLS equation (4.4.1) with initial condition φ_0.

4.5 Time-dependent quadratic dynamics

In this section we construct a time-dependent quadratic approximation for the Schrödinger dynamics. We prove existence of a unique unitary propagator for this approximation using the abstract results for non-autonomous linear Schrödinger equation stated in the Appendix 4.C. This step will be useful for the study of propagation of coherent states in the semiclassical limit in section 4.6.

The polynomial P has the following Taylor expansion for any $z_0 \in H^1(\mathbb{R})$

$$P(z+z_0) = \sum_{j=0}^{4} \frac{D^{(j)}P}{j!}(z_0)[z] \,.$$

Let φ_t be a solution of the NLS equation (4.4.1) with an initial data $\varphi_0 \in H^1(\mathbb{R})$. Consider the time-dependent quadratic polynomial on $\mathcal{S}(\mathbb{R})$ given by

$$\begin{aligned} P_2(t)[z] &:= \frac{D^{(2)}P}{2}(\varphi_t)[z] \\ &= \mathrm{Re} \int_{\mathbb{R}} \overline{z(x)}^2 \, \varphi_t(x)^2 \, dx + 2 \int_{\mathbb{R}} |z(x)|^2 \, |\varphi_t(x)|^2 \, dx \,. \end{aligned}$$

Let $\{A_2(t)\}_{t\in\mathbb{R}}$ be the ε-independent family of quadratic forms on $\mathcal{S}$ defined by

$$\varepsilon A_2(t) := \mathrm{d}\Gamma(-\Delta) + P_2(t)^{Wick} \,. \qquad (4.5.1)$$

Lemma 4.5.1. *For $\varphi_0 \in H^1(\mathbb{R})$ let*

$\vartheta_1 := 16^2(\|\varphi_0\|_{L^2(\mathbb{R})}+1)^3(h(\varphi_0)+1)$ *and* $\vartheta_2 := 16^2(\|\varphi_0\|_{L^2(\mathbb{R})}+1)^{\frac{3}{2}}\sqrt{h(\varphi_0)+1}.$

The quadratic forms on $\mathcal{S}$ defined by

$$S_2(t) := A_2(t) + \vartheta_1 \varepsilon^{-1} N + \vartheta_2 1 \,, \qquad t \in \mathbb{R} \,,$$

are associated to unique self-adjoint operators, still denoted by $S_2(t)$, satisfying

- $S_2(t) \geq 1$,
- $\mathcal{D}(S_2(t)^{1/2}) = \mathcal{F}^1_+$ *for any* $t \in \mathbb{R}$.

Proof. The case $\varphi_0 = 0$ is trivial. By definition of Wick quantization we have for $\Psi, \Phi \in \mathcal{S}$,

$$\begin{aligned}
&\langle \Phi, P_2(t)^{Wick}\Psi\rangle = \\
&2\sum_{n=1}^{\infty} \varepsilon n \int_{\mathbb{R}^n} |\varphi_t(x_1)|^2\, \overline{\Phi^{(n)}(x_1,\cdots,x_n)}\Psi^{(n)}(x_1,\cdots,x_n)\, dx_1\cdots dx_n \\
&+\sum_{n=0}^{\infty} \varepsilon\sqrt{(n+1)(n+2)} \\
&\quad\times \int_{\mathbb{R}^n} \overline{\Phi^{(n)}(x_1,\cdots,x_n)} \left(\int_{\mathbb{R}} \overline{\varphi_t(x)}^2\, \Psi^{(n+2)}(x,x,x_1,\cdots,x_n)dx\right) dx_1\cdots dx_n \\
&+\sum_{n=0}^{\infty} \varepsilon\sqrt{(n+1)(n+2)} \\
&\quad\times \int_{\mathbb{R}^n} \Psi^{(n)}(x_1,\cdots,x_n) \left(\int_{\mathbb{R}} \varphi_t(x)^2\, \overline{\Phi^{(n+2)}(x,x,x_1,\cdots,x_n)}dx\right) dx_1\cdots dx_n.
\end{aligned} \tag{4.5.2}$$

Therefore, using Cauchy-Schwarz inequality, we show

$$\begin{aligned}
&|\langle \Phi, P_2(t)^{Wick}\Psi\rangle| \\
&\le 2||\varphi_t||^2_{L^\infty(\mathbb{R})}||N^{1/2}\Phi|| \times ||N^{1/2}\Psi|| \\
&\quad + ||\varphi_t||^2_{L^4(\mathbb{R})}\, ||(N+\varepsilon)^{1/2}\Phi|| \\
&\qquad \times \left[\sum_{n=0}^{\infty} \varepsilon(n+2)||\Psi^{(n+2)}(x,x,x_1,\cdots,x_n)||^2_{L^2(\mathbb{R}^{n+1})}\right]^{1/2} \\
&\quad + ||\varphi_t||^2_{L^4(\mathbb{R})}\, ||(N+\varepsilon)^{1/2}\Psi|| \\
&\qquad \times \left[\sum_{n=0}^{\infty} \varepsilon(n+2)||\Phi^{(n+2)}(x,x,x_1,\cdots,x_n)||^2_{L^2(\mathbb{R}^{n+1})}\right]^{1/2} .
\end{aligned}$$

Now we prove, by Lemma 4.A.1, the crude estimate

$$\begin{aligned}
|\langle \Phi, P_2(t)^{Wick}\Psi\rangle| \;\le\;& \max(||\varphi_t||^2_{L^4(\mathbb{R})}, ||\varphi_t||^2_{L^\infty(\mathbb{R})})\,\Big[2||N^{1/2}\Phi|| \times ||N^{1/2}\Psi|| \\
&+\; ||(N+\varepsilon)^{1/2}\Phi|| \times ||(\alpha \mathrm{d}\Gamma(-\Delta) + \alpha^{-1}N)^{1/2}\Psi|| \\
&+\; ||(N+\varepsilon)^{1/2}\Psi|| \times ||(\alpha \mathrm{d}\Gamma(-\Delta) + \alpha^{-1}N)^{1/2}\Phi||\Big] .
\end{aligned}$$

This yields for any $\alpha > 0$

$$\begin{aligned}
|\langle \Phi, P_2(t)^{Wick}\Psi\rangle| \;\le\;& \alpha\, \max(||\varphi_t||^2_{L^4(\mathbb{R})}, ||\varphi_t||^2_{L^\infty(\mathbb{R})}) \\
&\times|| \left[\mathrm{d}\Gamma(-\Delta) + (\alpha^{-1}+3)\alpha^{-1}N + \alpha^{-1}\varepsilon 1\right]^{1/2} \Phi|| \\
&\times|| \left[\mathrm{d}\Gamma(-\Delta) + (\alpha^{-1}+3)\alpha^{-1}N + \alpha^{-1}\varepsilon 1\right]^{1/2} \Psi|| .
\end{aligned} \tag{4.5.3}$$

Remark now that (4.4.2) yields

$$\max(||\varphi_t||^2_{L^4(\mathbb{R})}, ||\varphi_t||^2_{L^\infty(\mathbb{R})}) \le 2\,(||\varphi_0||_{L^2(\mathbb{R})} + 1)^{3/2}\sqrt{h(\varphi_0) + 1}\,.$$

Hence, for $\alpha^{-1} = 3(||\varphi_0||_{L^2(\mathbb{R})} + 1)^{3/2}\sqrt{h(\varphi_0)+1} > 0$, we obtain

$$\begin{aligned}
\varepsilon^{-1}|\langle \Phi, P_2(t)^{Wick}\Psi\rangle| \;\le\;& \tfrac{2}{3}\, ||[\varepsilon^{-1}\mathrm{d}\Gamma(-\Delta) + \vartheta_1\varepsilon^{-1}N + \vartheta_2 1]^{1/2}\Phi|| \\
&\times||[\varepsilon^{-1}\mathrm{d}\Gamma(-\Delta) + \vartheta_1\varepsilon^{-1}N + \vartheta_2 1]^{1/2}\Psi|| .
\end{aligned} \tag{4.5.4}$$

Applying now the KLMN theorem (see [102, Theorem X.17]) with the help of inequality (4.5.4) we show that

$$S_2(t) = A_2(t) + \vartheta_1 \varepsilon^{-1} N + \vartheta_2 1 \ \text{ with } \vartheta_1 > (\alpha^{-1}+3)\alpha^{-1}, \text{ and } \vartheta_2 > \alpha^{-1}+1\,,$$

are associated to unique self-adjoint operators $S_2(t)$ satisfying $S_2(t) \geq 1$. Furthermore, we have that the form domains of those operators are time-independent, i.e.,

$$\mathcal{Q}(S_2(t)) = \mathcal{F}^1_+$$

for any $t \in \mathbb{R}$. □

Remark 4.5.2. *The choice of ϑ_1, ϑ_2 in the previous lemma takes into account the use of KLMN's theorem in the proof of Lemma 4.6.3.*

We consider the non-autonomous Schrödinger equation

$$\begin{cases} i\partial_t u = A_2(t)u\,, & t \in \mathbb{R}, \\ u(t=s) = u_s\,. \end{cases} \tag{4.5.5}$$

Here $\mathbb{R} \ni t \mapsto A_2(t)$ is considered as a norm continuous $\mathcal{L}(\mathcal{F}^1_+, \mathcal{F}^1_-)$-valued map (see Lemma 4.5.3). We show in Proposition 4.5.5 the existence of a unique solution for any initial data $u_s \in \mathcal{F}^1_+$ using Corollary 4.C.4. Moreover, the Cauchy problem's features allow to encode the solutions on a *unitary propagator* mapping $(t,s) \mapsto U_2(t,s)$ such that

$$U_2(t,s)u_s = u_t\,,$$

satisfying Definition 4.C.1 with $\mathcal{H} = \mathcal{F}$, $\mathcal{H}_\pm = \mathcal{F}^1_\pm$ and $I = \mathbb{R}$.

In the following two lemmas we check the assumptions in Corollary 4.C.4.

Lemma 4.5.3. *For any $\varphi_0 \in H^1(\mathbb{R})$ and $t \in \mathbb{R}$ the quadratic form $A_2(t)$ defines a symmetric operator on $\mathcal{L}(\mathcal{F}^1_+, \mathcal{F}^1_-)$ and the mapping $t \in \mathbb{R} \mapsto A_2(t) \in \mathcal{L}(\mathcal{F}^1_+, \mathcal{F}^1_-)$ is norm continuous.*

Proof. Using (4.5.4) we show for any $\Psi, \Phi \in \mathcal{S}$

$$\begin{aligned} |\langle \Phi, A_2(t)\Psi\rangle| &\leq |\langle \Phi, \varepsilon^{-1} \mathrm{d}\Gamma(-\Delta)\Psi\rangle| + |\langle \Phi, \varepsilon^{-1} P_2(t)^{Wick}\Psi\rangle| \\ &\leq ||S_1^{1/2}\Phi||\, ||S_1^{1/2}\Psi|| + \tfrac{2}{3}\vartheta_1 ||S_1^{1/2}\Phi||\, ||S_1^{1/2}\Psi|| \\ &\leq \tfrac{5}{3}\vartheta_1\, ||\Psi||_{\mathcal{F}^1_+}\, ||\Phi||_{\mathcal{F}^1_+}\,, \end{aligned} \tag{4.5.6}$$

where ϑ_1, ϑ_2 are the parameters introduced in Lemma 4.5.1. Hence, this allows to consider $A_2(t)$ as a bounded operator in $\mathcal{L}(\mathcal{F}^1_+, \mathcal{F}^1_-)$. Since $A_2(t)$ is a symmetric quadratic form it follows that it is also symmetric as an operator in $\mathcal{L}(\mathcal{F}^1_+, \mathcal{F}^1_-)$.

Now, using a similar estimate as (4.5.3) we prove norm continuity. Indeed, we have

$$\begin{aligned}|\langle\Phi,[A_2(t)-A_2(s)]\Psi\rangle| &= \varepsilon^{-1}|\langle\Phi,[P_2(t)-P_2(s)]^{Wick}\Psi\rangle| \\ &\le 4\ \max\Big(||\varphi_t^2-\varphi_s^2||_{L^2(\mathbb{R})},\big|\big||\varphi_t|^2-|\varphi_s|^2\big|\big|_{L^\infty(\mathbb{R})}\Big)\ ||\Psi||_{\mathcal{F}^1_+}\ ||\Phi||_{\mathcal{F}^1_+}\,.\end{aligned}$$

Note that it is not difficult to prove that

$$\max\Big(||\varphi_t^2-\varphi_s^2||_{L^2(\mathbb{R})},\big|\big||\varphi_t|^2-|\varphi_s|^2\big|\big|_{L^\infty(\mathbb{R})}\Big)\longrightarrow 0 \qquad \text{when } t\to s\,.$$

This follows by (4.4.2) and the fact that $\varphi_t\in C^0(\mathbb{R},H^1(\mathbb{R}))$. □

Lemma 4.5.4. *For any $\varphi_0\in H^2(\mathbb{R})$ there exists $c>0$ (depending only on φ_0) such that the two statements below hold true.*
(i) For any $\Psi\in\mathcal{F}^1_+$, we have

$$|\partial_t\langle\Psi,S_2(t)\Psi\rangle|\le e^{c(|t|+1)}||S_2(t)^{1/2}\Psi||_{\mathcal{F}}\,.$$

(ii) For any $\Psi,\Phi\in\mathcal{D}(S_2(t)^{3/2})$, we have

$$|\langle\Psi,A_2(t)S_2(t)\Phi\rangle-\langle S_2(t)\Psi,A_2(t)\Phi\rangle|\le c\,||S_2(t)^{1/2}\Psi||_{\mathcal{F}}\ ||S_2(t)^{1/2}\Phi||_{\mathcal{F}}\,.$$

Proof. (i) Let $\Psi\in\mathcal{S}$, we have

$$\begin{aligned}\partial_t\langle\Psi,S_2(t)\Psi\rangle &= \varepsilon^{-1}\ \partial_t\langle\Psi,P_2(t)^{Wick}\Psi\rangle \\ &= \varepsilon^{-1}\langle\Psi,[\partial_tP_2(t)]^{Wick}\,\Psi\rangle\,,\end{aligned}$$

where $\partial_tP_2(t)$ is a continuous polynomial on $\mathcal{S}(\mathbb{R})$ given by

$$\partial_tP_2(t)[z]=2\mathrm{Re}\int_{\mathbb{R}}\overline{z(x)}^2\,\varphi_t(x)\partial_t\varphi_t(x)\,dx+4\mathrm{Re}\int_{\mathbb{R}}|z(x)|^2\,\overline{\varphi_t(x)}\partial_t\varphi_t(x)\,dx\,.$$

A simple computation yields

$$\begin{aligned}&\langle\Psi,[\partial_tP_2(t)]^{Wick}\,\Psi\rangle \\ &=4\mathrm{Re}\sum_{n=1}^\infty n\varepsilon\overbrace{\int_{\mathbb{R}^n}\overline{\varphi_t(x_1)}\partial_t\varphi_t(x_1)\,|\Psi^{(n)}(x_1,\cdots,x_n)|^2\,dx_1\cdots dx_n}^{(1)} \\ &\quad+\sum_{n=0}^\infty\varepsilon\sqrt{(n+2)(n+1)}\int_{\mathbb{R}^n}\overline{\Psi^{(n)}(x_1,\cdots,x_n)} \\ &\quad\times\Big(\int_{\mathbb{R}}\overline{\varphi_t(x)}\,\overline{\partial_t\varphi_t(x)}\,\Psi^{(n+2)}(x,x,x_1,\cdots,x_n)\,dx\Big)\,dx_1\cdots dx_n \\ &\quad+hc\,.\end{aligned}$$

From (4.4.2) we get

$$\begin{aligned}|(1)| &\leq \|\varphi_t\,\partial_t\varphi_t\|_{L^1(\mathbb{R})} \int_{\mathbb{R}^{n-1}} \sup_{x_1\in\mathbb{R}} \left|\Psi^{(n)}(x_1,\cdots,x_n)\right|^2 dx_2\cdots dx_n \\ &\leq \|\varphi_t\|_{L^2(\mathbb{R})} \times \|\partial_t\varphi_t\|_{L^2(\mathbb{R})} \,\langle(1-\partial_{x_1}^2)\Psi^{(n)},\Psi^{(n)}\rangle_{L^2(\mathbb{R}^n)}\,.\end{aligned}$$

Now we apply Cauchy-Schwarz inequality,

$$\begin{aligned}&|\langle\Psi,[\partial_t P_2(t)]^{Wick}\,\Psi\rangle| \\ &\quad\leq 4\,\|\varphi_t\|_{L^2(\mathbb{R})}\,\|\partial_t\varphi_t\|_{L^2(\mathbb{R})}\left(\sum_{n=1}^{\infty}\varepsilon n\,\langle(1-\partial_{x_1}^2)\Psi^{(n)},\Psi^{(n)}\rangle_{L^2(\mathbb{R}^n)}\right) \\ &\quad+2\|\varphi_t\|_{L^\infty(\mathbb{R})}\|\partial_t\varphi_t\|_{L^2(\mathbb{R})}\left(\sum_{n=0}^{\infty}\varepsilon(n+2)\|\Psi^{(n+2)}(x,x,.)\|^2_{L^2(\mathbb{R}^{n+1})}\right)^{1/2} \\ &\qquad\times\left(\sum_{n=0}^{\infty}\varepsilon(n+1)\|\Psi^{(n)}\|^2_{L^2(\mathbb{R}^n)}\right)^{1/2}.\end{aligned}$$

In the same spirit as in (4.5.3), we obtain a rough inequality

$$\begin{aligned}&|\langle\Psi,[\partial_t P_2(t)]^{Wick}\,\Psi\rangle| \\ &\leq \max(\|\varphi_t\|_{L^\infty(\mathbb{R})},\|\varphi_t\|_{L^2(\mathbb{R})})\,\|\partial_t\varphi_t\|_{L^2(\mathbb{R})}\,\Big[4\,\|(\mathrm{d}\Gamma(-\Delta)+N)^{1/2}\Psi\|^2 \\ &\qquad+2\ \|(\mathrm{d}\Gamma(-\Delta)+N+1)^{1/2}\Psi\|^2\Big]\,.\end{aligned}$$

Observe that (4.5.4) implies $S_1 \leq 3\,S_2(t)$ for all $t\in\mathbb{R}$. Hence, we have

$$\begin{aligned}&\varepsilon^{-1}|\langle\Psi,[\partial_t P_2(t)]^{Wick}\,\Psi\rangle| \\ &\quad\leq 6\,\max(\|\varphi_t\|_{L^\infty(\mathbb{R})},\|\varphi_t\|_{L^2(\mathbb{R})})\,\|\partial_t\varphi_t\|_{L^2(\mathbb{R})}\,\|\Psi\|^2_{\mathcal{F}^1_+} \\ &\quad\leq 18\,\max(\|\varphi_t\|_{L^\infty(\mathbb{R})},\|\varphi_t\|_{L^2(\mathbb{R})})\,\|\partial_t\varphi_t\|_{L^2(\mathbb{R})}\,\|S_2(t)^{1/2}\Psi\|^2_{\mathcal{F}}\,.\end{aligned}$$

This proves (i) since (4.4.2)-(4.4.3) ensure the existence of $c>0$ (depending only on φ_0) such that

$$\max(\|\varphi_t\|_{L^\infty(\mathbb{R})},\|\varphi_t\|_{L^2(\mathbb{R})})\,\|\partial_t\varphi_t\|_{L^2(\mathbb{R})}\leq e^{c(|t|+1)}\,.$$

(ii) If $\Psi,\Phi\in\mathcal{D}(S_2(t)^{3/2})$ the quantity

$$\mathcal{C} := \langle\Psi,A_2(t)S_2(t)\Phi\rangle - \langle S_2(t)\Psi,A_2(t)\Phi\rangle,$$

is well-defined since $A_2(t)\in\mathcal{L}(\mathcal{F}^1_+,\mathcal{F}^1_-)$ and $S_2(t)\mathcal{D}(S_2(t)^{3/2})\subset\mathcal{D}(S_2(t)^{1/2})=\mathcal{F}^1_+$. Note that $N\in\mathcal{L}(\mathcal{F}^1_+,\mathcal{F}^1_-)$. Hence, we can write

$$\begin{aligned}\mathcal{C} &= \langle\Psi,[S_2(t)-\vartheta_1\varepsilon^{-1}N-\vartheta_2 1]\,S_2(t)\Phi\rangle - \langle S_2(t)\Psi,[S_2(t)-\vartheta_1\varepsilon^{-1}N-\vartheta_2 1]\,\Phi\rangle \\ &= \vartheta_1\left(\langle S_2(t)\Psi,\varepsilon^{-1}N\Phi\rangle - \langle\varepsilon^{-1}N\Psi,S_2(t)\,\Phi\rangle\right)\,.\end{aligned}$$

Observe that, for $\lambda > 0$, $\varepsilon^{-1}N(\lambda\varepsilon^{-1}N+1)^{-1}\mathcal{F}_+^1 \subset \mathcal{F}_+^1$ and that

$$s - \lim_{\lambda\to 0^+} \varepsilon^{-1}N(\lambda\varepsilon^{-1}N+1)^{-1} = \varepsilon^{-1}N \text{ in } \mathcal{L}(\mathcal{F}_+^1, \mathcal{F}_-^1).$$

Therefore, we have

$$\mathcal{C} = \vartheta_1 \lim_{\lambda\to 0^+} \underbrace{\langle S_2(t)\Psi, \varepsilon^{-1}N(\lambda\varepsilon^{-1}N+1)^{-1}\Phi\rangle - \langle \varepsilon^{-1}N(\lambda\varepsilon^{-1}N+1)^{-1}\Psi, S_2(t)\Phi\rangle}_{\mathcal{C}_\lambda}.$$

Let N_λ denote $\varepsilon^{-1}N(\lambda\varepsilon^{-1}N+1)^{-1}$. A simple computation yields

$$\begin{aligned}\varepsilon\mathcal{C}_\lambda &= \langle \Psi, P_2(t)^{Wick} N_\lambda\,\Phi\rangle - \langle N_\lambda\,\Psi, P_2(t)^{Wick}\Phi\rangle \\ &= \langle \Psi, g(t)^{Wick} N_\lambda\Phi\rangle - \langle N_\lambda\Psi, g(t)^{Wick}\Phi\rangle\,,\end{aligned}$$

where $g(t)$ is the polynomial given by

$$g(t)[z] = \mathrm{Re}\int_{\mathbb{R}} \overline{z(x)}^2\ \varphi_t(x)^2\,dx\,.$$

A similar computation as (4.5.2) yields

$$\begin{aligned}&\mathcal{C}_\lambda = \\ &\sum_{n=0}^{\infty}\kappa(n)\int_{\mathbb{R}^n}\overline{\Psi^{(n)}(x_1,\cdots,x_n)}\left(\int_{\mathbb{R}}\overline{\varphi_t(x)}^2\Phi^{(n+2)}(x,x,x_1,\cdots,x_n)dx\right)dx_1\cdots dx_n \\ &-\sum_{n=0}^{\infty}\kappa(n)\int_{\mathbb{R}^n}\Phi^{(n)}(x_1,\cdots,x_n)\left(\int_{\mathbb{R}}\varphi_t(x)^2\overline{\Psi^{(n+2)}(x,x,x_1,\cdots,x_n)}dx\right)dx_1\cdots dx_n\,,\end{aligned}$$

where

$$\kappa(n) = \frac{(n+2)\sqrt{(n+1)(n+2)}}{(\lambda(n+2)+1)} - \frac{n\sqrt{(n+1)(n+2)}}{(\lambda n+1)}\,.$$

Note that $\kappa(n) \leq 2(n+2)$. Hence, using Cauchy-Schwarz inequality, we show

$$\begin{aligned}&|\mathcal{C}_\lambda| \leq \\ &2\,||\varphi_t||^2_{L^4(\mathbb{R})}\left[\sum_{n=0}^{\infty}(n+2)||\Psi^{(n)}||^2_{L^2(\mathbb{R}^n)}\right]^{1/2}\left[\sum_{n=0}^{\infty}(n+2)\,||\Phi^{(n+2)}(x,x,.)||^2_{L^2(\mathbb{R}^{n+1})}\right]^{1/2} \\ &+2\,||\varphi_t||^2_{L^4(\mathbb{R})}\left[\sum_{n=0}^{\infty}(n+2)||\Phi^{(n)}||^2_{L^2(\mathbb{R}^n)}\right]^{1/2}\left[\sum_{n=0}^{\infty}(n+2)\,||\Psi^{(n+2)}(x,x,.)||^2_{L^2(\mathbb{R}^{n+1})}\right]^{1/2}.\end{aligned}$$

Using Lemma 4.A.1, with $\alpha = \frac{1}{\sqrt{2}}$, we get

$$\begin{aligned}
&\sum_{n=0}^{\infty}(n+2)\,||\Psi^{(n+2)}(x,x,.)||^2_{L^2(\mathbb{R}^{n+1})} \\
&\quad\leq \frac{1}{2}\,\sum_{n=0}^{\infty}(n+2)\langle D^2_{x_1}\Psi^{(n+2)},\Psi^{(n+2)}\rangle + (n+2)||\Psi^{(n+2)}||^2_{L^2(\mathbb{R}^{n+2})} \\
&\quad\leq \frac{1}{2}\,\langle\Psi, S_1\Psi\rangle\,,
\end{aligned}$$

together with an analogue estimate where Ψ is replaced by Φ. Now, we conclude that there exists $c > 0$ depending only on φ_0 such that

$$\vartheta_1\,|\mathcal{C}_\lambda| \quad\leq\quad c\,||\Psi||_{\mathcal{F}^1_+}\,||\Phi||_{\mathcal{F}^1_+}\,. \tag{4.5.7}$$

This proves part (ii). □

Proposition 4.5.5. *Let $\varphi_0 \in H^2(\mathbb{R})$ and $A_2(t)$ given by (4.5.1). Then the non-autonomous Cauchy problem*

$$\left\{\begin{array}{l} i\partial_t u = A_2(t)u\,, \quad t\in\mathbb{R}, \\ u(t=s) = u_s\,, \end{array}\right.$$

admits a unique unitary propagator $U_2(t,s)$ in the sense of Definition 4.C.1 with $I = \mathbb{R}$ and $\mathcal{H}_\pm = \mathcal{F}^1_\pm$. Moreover, there exists $c > 0$ depending only on φ_0 such that

$$||U_2(t,0)||_{\mathcal{L}(\mathcal{F}^1_+)} \leq e^{ce^{c|t|}}\,.$$

Proof. The proof immediately follows using Corollary 4.C.4 with the help of Lemma 4.5.3-4.5.4 and the inequality

$$c_1 S_1 \leq S_2(t) \leq c_2 S_1,$$

which holds true using (4.5.6). □

4.6 Propagation of coherent states

In finite dimensional phase-space, coherent state analysis is a well developed powerful tool, see for instance [79]. Here we study, using the ideas of Ginibre and Velo in [91], the asymptotics when $\varepsilon \to 0$ of the time-evolved coherent states

$$e^{-it/\varepsilon H_\varepsilon} W(\frac{\sqrt{2}}{i\varepsilon}\varphi_0)\Psi\,,$$

for Ψ in a dense subspace $\mathcal{G}_+ \subset \mathcal{F}$ defined below. We consider the following Hilbert rigging

$$\mathcal{G}_+ \subset \mathcal{F} \subset \mathcal{G}_- ,$$

defined via the ε-independent self-adjoint operator (see Remark 4.3.4) given by

$$G := \varepsilon^{-1}\mathrm{d}\Gamma(-\Delta) + \varepsilon^{-2}P^{Wick} + \varepsilon^{-1}N + 1 ,$$

as the completion of $\mathcal{D}(G^{\pm 1/2})$ with the respect to the inner product

$$\langle \Psi, \Phi \rangle_{\mathcal{G}_\pm} := \langle G^{\pm 1/2}\Psi, G^{\pm 1/2}\Phi \rangle_{\mathcal{F}}.$$

We have the continuous embedding

$$\mathcal{F}_+^3 \subset \mathcal{G}_+ \subset \mathcal{F}_+^1 .$$

The main result of this section is Theorem 4.6.1 which describes the propagation of coherent states in the semiclassical limit.

Theorem 4.6.1. *For any $\varphi_0 \in H^2(\mathbb{R})$ there exists $c > 0$ depending only on φ_0 such that*

$$\left\| e^{-it/\varepsilon H_\varepsilon} W(\frac{\sqrt{2}}{i\varepsilon}\varphi_0)\Psi - e^{i\omega(t)/\varepsilon} W(\frac{\sqrt{2}}{i\varepsilon}\varphi_t) U_2(t,0)\Psi \right\|_{\mathcal{F}} \leq e^{ce^{c|t|}} \, \varepsilon^{1/8} \, \|\Psi\|_{\mathcal{G}_+} ,$$

holds for any $t \in \mathbb{R}$ and $\Psi \in \mathcal{G}_+$ where φ_t solves the NLS equation (4.4.1) with the initial condition φ_0 and $\omega(t) = \int_0^t P(\varphi_s)\, ds$. Here $U_2(t,s)$ is the unitary propagator given by Proposition 4.5.5.

To prove this theorem we need several preliminary lemmas.

Lemma 4.6.2. *The following three assertions hold true.*

(i) For any $\xi \in L^2(\mathbb{R})$ and $k \in \mathbb{N}$, the Weyl operator $W(\xi)$ preserves $\mathcal{D}(N^{k/2})$. If in addition $\xi \in H^1(\mathbb{R})$ then $W(\xi)$ preserves also $\mathcal{F}_+^\mu$ when $\mu \geq 1$.

(ii) For any $\xi \in H^1(\mathbb{R})$, we have in the sense of quadratic forms on $\mathcal{F}_+^3$,

$$W(\frac{\sqrt{2}}{i\varepsilon}\xi)^* \, h^{Wick} \, W(\frac{\sqrt{2}}{i\varepsilon}\xi) = h(. + \xi)^{Wick} .$$

(iii) Let $(\mathbb{R} \ni t \mapsto \varphi_t) \in C^1(\mathbb{R}, L^2(\mathbb{R}))$, then for any $\Psi \in \mathcal{D}(N^{1/2})$ we have in $\mathcal{F}$

$$\begin{aligned} i\varepsilon\partial_t W(\frac{\sqrt{2}}{i\varepsilon}\varphi_t)\Psi &= W(\frac{\sqrt{2}}{i\varepsilon}\varphi_t) \left[\mathrm{Re}\langle \varphi_t, i\partial_t\varphi_t\rangle + 2\mathrm{Re}\langle z, i\partial_t\varphi_t\rangle^{Wick}\right] \Psi \\ &= \left[-\mathrm{Re}\langle \varphi_t, i\partial_t\varphi_t\rangle + 2\mathrm{Re}\langle z, i\partial_t\varphi_t\rangle^{Wick}\right] W(\frac{\sqrt{2}}{i\varepsilon}\varphi_t)\Psi . \end{aligned}$$

Proof. (i) Let $\mathcal{F}_0$ be the linear space spanned by vectors $\Psi \in \mathcal{F}$ such that $\Psi^{(n)} = 0$ for any n except for a finite number. It is known that for any $\xi \in L^2(\mathbb{R})$ and $\Psi \in \mathcal{F}_0$

$$\tilde{N}\Psi := W(\frac{\sqrt{2}}{i\varepsilon}\xi)^* N\, W(\frac{\sqrt{2}}{i\varepsilon}\xi)\Psi = \left(N + 2\mathrm{Re}\langle z,\xi\rangle^{Wick} + ||\xi||^2 1\right)\Psi\,. \quad (4.6.1)$$

For a proof of the latter identity see [76, Lemma 2.10 (iii)]. Hence, by Cauchy-Schwarz inequality it follows that

$$\begin{aligned}
&||N^{1/2}W(\frac{\sqrt{2}}{i\varepsilon}\xi)\Psi||^2 \\
&\quad = \langle\Psi, \left[N + 2\mathrm{Re}\langle z,\xi\rangle^{Wick} + ||\xi||^2 1\right]\Psi\rangle \\
&\quad = \langle\Psi, (N + ||\xi||^2_{L^2(\mathbb{R})}1)\Psi\rangle \\
&\qquad + \sum_{n=0}^{\infty}\sqrt{\varepsilon(n+1)}\int_{\mathbb{R}^n}\overline{\Psi^{(n)}(y)}\left(\int_{\mathbb{R}}\overline{\xi(x)}\Psi^{(n+1)}(x,y)dx\right)dy + hc \\
&\quad \leq (1 + ||\xi||_{L^2(\mathbb{R})})^2\, ||(N+1)^{1/2}\Psi||^2\,.
\end{aligned}$$

Now, for $k \geq 1$ we show the existence of an ε-independent constant $C_k > 0$ depending only on k and $||\xi||_{L^2(\mathbb{R})}$ such that

$$||N^{k/2}W(\frac{\sqrt{2}}{i\varepsilon}\xi)\Psi||^2 = \langle\Psi, \tilde{N}^k\Psi\rangle \leq C_k\, ||(N+1)^{k/2}\Psi||^2\,. \quad (4.6.2)$$

This is a consequence of the number operator estimate (4.2.2) and the fact that $\tilde{N}^k$ is a Wick polynomial in $\sum_{0\leq r,s\leq k}\mathcal{P}_{r,s}(L^2(\mathbb{R}))$ (see, *e.g.*,[76, Prop. 2.7 (i)]). Thus, we have proved the invariance of $\mathcal{D}(N^{k/2})$ since $\mathcal{F}_0$ is a core of $N^{k/2}$.

Now the invariance of $\mathcal{F}_+^{\mu}$, $\mu \geq 1$, follows by Faris-Lavine Theorem 4.B.1 where we take the operator

$$A = \sqrt{2}\mathrm{Re}\langle z,\xi\rangle^{Wick} \quad \text{and} \quad S = S_\mu = \varepsilon^{-1}\mathrm{d}\Gamma(-\Delta) + \varepsilon^{-\mu}N^{\mu} + 1\,,$$

and remember that

$$W(\xi) = e^{i\sqrt{2}\mathrm{Re}\langle z,\xi\rangle^{Wick}}\,.$$

In fact, assuming $\xi \in H^1(\mathbb{R})$ we have to check assumptions (i)-(ii) of Theorem 4.B.1. For any $\Psi \in \mathcal{F}_+^{\mu}$, we have by Wick quantization

$$\begin{aligned}
2\mathrm{Re}\langle z,\xi\rangle^{Wick}\Psi &= \sum_{n=0}^{\infty}\sqrt{\varepsilon(n+1)}\int_{\mathbb{R}}\overline{\xi(x)}\Psi^{(n+1)}(x,x_1,\cdots,x_n)\,dx \\
&\quad + \sum_{n=1}^{\infty}\sqrt{\frac{\varepsilon}{n}}\sum_{j=1}^{n}\xi(x_j)\,\Psi^{(n-1)}(x_1,\cdots,\hat{x}_j,\cdots,x_n)\,.
\end{aligned}$$

Therefore, it is easy to show

$$\begin{aligned} \|\mathrm{Re}\langle z,\xi\rangle^{Wick}\Psi\| &\leq \sqrt{\varepsilon}\|\xi\|_{L^2(\mathbb{R})}\,\|(\varepsilon^{-1}N+1)^{1/2}\Psi\| \\ &\leq \sqrt{\varepsilon}\|\xi\|_{L^2(\mathbb{R})}\,\|S_1\Psi\|\,, \end{aligned}$$

and hence we obtain that $\mathcal{D}(S_\mu)\subset\mathcal{D}(A)$. Let $\Psi\in\mathcal{D}(S_\mu)$, a standard computation yields

$$\begin{aligned} \sqrt{2}\,(\langle A\Psi,S_\mu\Psi\rangle-\langle S_\mu\Psi,A\Psi\rangle) &= \langle a(-\Delta\xi)\Psi,\Psi\rangle-\langle\Psi,a(-\Delta\xi)\Psi\rangle \\ &+ \langle[(\tfrac{N}{\varepsilon}+1)^\mu-(\tfrac{N}{\varepsilon})^\mu]\,\Psi,a^*(\xi)\Psi\rangle-hc\,. \end{aligned} \tag{4.6.3}$$

Each two terms in the same line of (4.6.3) are similar and it is enough to estimate only one of them. We have by Cauchy-Schwarz inequality

$$\begin{aligned} |\langle a(-\Delta\xi)\Psi,\Psi\rangle| &\leq \left|\sum_{n=0}^{\infty}\sqrt{\varepsilon(n+1)}\int_{\mathbb{R}^n}\overline{\Psi^{(n)}(y)}\left(\int_{\mathbb{R}}\overline{-\Delta\xi(x)}\Psi^{(n+1)}(x,y)dx\right)dy\right| \\ &\leq \|\xi\|_{H^1(\mathbb{R})}\,\|S_1^{1/2}\Psi\|^2\,, \end{aligned}$$

and for $1\leq\theta\leq\mu-1$

$$\begin{aligned} &\left|\langle\varepsilon^{-\theta}N^\theta\Psi,a^*(\xi)\Psi\rangle\right| \\ &\leq \left|\sum_{n=0}^{\infty}\sqrt{\varepsilon(n+1)}\,(n+1)^\theta\int_{\mathbb{R}^n}\Psi^{(n)}(y)\left(\int_{\mathbb{R}}\xi(x)\overline{\Psi^{(n+1)}(x,y)}dx\right)dy\right| \\ &\leq 2^\mu\|\xi\|_{L^2(\mathbb{R})}\,\|S_\mu^{1/2}\Psi\|^2\,. \end{aligned}$$

This shows for any $\Psi\in\mathcal{D}(S_\mu)$,

$$\pm i\langle\Psi,[A,S_\mu]\Psi\rangle\leq C\,\|S_\mu^{1/2}\Psi\|^2.$$

Part (ii) follows by a similar argument as [76, Lemma 2.10 (iii)] and part (iii) is a well-known formula, see [90, Lemma 3.1 (3)]. □

Set

$$\mathcal{W}(t)=W(\frac{\sqrt{2}}{i\varepsilon}\varphi_t)^*\,e^{-i\omega(t)/\varepsilon}\,e^{-it/\varepsilon H_\varepsilon}W(\frac{\sqrt{2}}{i\varepsilon}\varphi_0)\,.$$

Lemma 4.6.3. *For any $\varphi_0\in H^2(\mathbb{R})$ there exists $c>0$ such that the inequality*

$$\|\mathcal{W}(t)\|_{\mathcal{L}(\mathcal{G}_+,\mathcal{F}^1_+)}\leq e^{ce^{c|t|}}$$

holds for $t\in\mathbb{R}$ uniformly in $\varepsilon\in(0,1]$.

Proof. Observe that the subspace $\mathcal{D}_+$ given as the image of $\mathcal{D}(H_\varepsilon)\cap\mathcal{F}^3_+$ by $W(\frac{\sqrt{2}}{i\varepsilon}\varphi_0)^*$ is dense in $\mathcal{F}$. Let $\Psi\in\mathcal{D}_+$ and $\Phi\in\mathcal{G}_+$, then differentiating the quantity $\langle\Phi,\mathcal{W}(t)\Psi\rangle$ with the help of Lemma 4.6.2 and Proposition 4.3.3, we obtain

$$\begin{aligned}&i\varepsilon\partial_t\langle\Phi,\mathcal{W}(t)\Psi\rangle\\&=\langle\Phi,\,[P(\varphi_t)-\mathrm{Re}\langle\varphi_t,i\partial_t\varphi_t\rangle-2\mathrm{Re}\langle z,i\partial_t\varphi_t\rangle^{Wick}]\,\mathcal{W}(t)\Psi\rangle\\&\quad+\underbrace{\langle\Phi,W(\frac{\sqrt{2}}{i\varepsilon}\varphi_t)^*\,e^{-i\omega(t)/\varepsilon}\,e^{-it/\varepsilon H_\varepsilon}H_\varepsilon\,W(\frac{\sqrt{2}}{i\varepsilon}\varphi_0)\Psi\rangle}_{(1)}\,.\end{aligned}\tag{4.6.4}$$

Let $R_\nu:=1_{[0,\nu]}(\varepsilon^{-1}N)$ and remark that $s-\lim_{\nu\to\infty}R_\nu=1$. Furthermore, we have that $R_\nu\mathcal{G}_+\subset\mathcal{F}^3_+$ since it easily holds that

$$||R_\nu\Phi||^2_{\mathcal{F}^3_+}\leq\nu^3\,||\Phi||^2_{\mathcal{G}_+}\,.$$

Therefore, since $W(\frac{\sqrt{2}}{i\varepsilon}\varphi_t)R_\nu\Phi$ and $W(\frac{\sqrt{2}}{i\varepsilon}\varphi_0)\Psi$ belong to $\mathcal{F}^3_+$, we have

$$\begin{aligned}(1)\;&=\;\lim_{\nu\to\infty}\langle R_\nu\Phi,W(\frac{\sqrt{2}}{i\varepsilon}\varphi_t)^*\,e^{-i\omega(t)/\varepsilon}\,e^{-it/\varepsilon H_\varepsilon}H_\varepsilon\,W(\frac{\sqrt{2}}{i\varepsilon}\varphi_0)\Psi\rangle\\&=\;\lim_{\nu\to\infty}\langle R_\nu\Phi,h(.+\varphi_t)^{Wick}\,\mathcal{W}(t)\Psi\rangle\,.\end{aligned}$$

So, we get

$$\begin{aligned}&i\varepsilon\partial_t\langle\Phi,\mathcal{W}(t)\Psi\rangle\\&=(1)+\lim_{\nu\to\infty}\langle R_\nu\Phi,\Big[P(\varphi_t)-\mathrm{Re}\langle\varphi_t,i\partial_t\varphi_t\rangle-2\mathrm{Re}\langle z,i\partial_t\varphi_t\rangle^{Wick}\Big]\,\mathcal{W}(t)\Psi\rangle\\&=\lim_{\nu\to\infty}\langle R_\nu\Phi,(\underbrace{\varepsilon A_2(t)+P_3(t)^{Wick}+P_4^{Wick}}_{=:\varepsilon\Theta(t)})\mathcal{W}(t)\,\Psi\rangle\,,\end{aligned}$$

where we denote

$$\begin{aligned}P_3(t)[z]:=\;&\tfrac{D^{(3)}P}{3!}(\varphi_t)[z]=\;2\mathrm{Re}\int_{\mathbb{R}}\varphi_t(x)\overline{z(x)}|z(x)|^2\,dx\quad\text{and}\\P_4(z)=\;&\tfrac{D^{(4)}P}{4!}(\varphi_t)[z]=\;\frac{1}{2}\int_{\mathbb{R}}|z(x)|^4\,dx\,.\end{aligned}$$

A simple computation yields

$$\begin{aligned}&\langle\Phi,P_3(t)^{Wick}\Psi\rangle\\&=\sum_{n=1}^\infty\sqrt{n^2(n+1)\varepsilon^3}\int_{\mathbb{R}^{n-1}}\Big(\int_{\mathbb{R}}\overline{\varphi_t(x)}\;\overline{\Phi^{(n)}(x,y)}\;\Psi^{(n+1)}(x,x,y)\,dx\Big)\,dy\\&\quad+\sum_{n=1}^\infty\sqrt{n^2(n+1)\varepsilon^3}\int_{\mathbb{R}^{n-1}}\Big(\int_{\mathbb{R}}\varphi_t(x)\;\overline{\Phi^{(n+1)}(x,x,y)}\;\Psi^{(n)}(x,y)\,dx\Big)\,dy\,.\end{aligned}$$

Using Cauchy-Schwarz inequality and Lemma 4.A.1, we obtain

$$\left|\langle \Phi, P_3(t)^{Wick}\Psi\rangle\right| \leq 2\sqrt{2}\frac{||\varphi_t||_{L^\infty(\mathbb{R})}}{\sqrt{\vartheta_2}} \sqrt{\langle \Phi, [\varepsilon^{-1}P^{Wick} + \vartheta_1\varepsilon^{-1}N + \vartheta_2 1]\Phi\rangle}$$
$$\times \sqrt{\langle \Psi, [\varepsilon^{-1}P^{Wick} + \vartheta_1\varepsilon^{-1}N + \vartheta_2 1]\Psi\rangle}\,, \quad (4.6.5)$$

where ϑ_1, ϑ_2 are the parameters in Lemma 4.5.1. Hence, $\Theta(t)$ extends to a bounded operator in $\mathcal{L}(\mathcal{G}_+, \mathcal{G}_-)$ since $A_2(t)$ and P^{Wick} belong to $\mathcal{L}(\mathcal{G}_+, \mathcal{G}_-)$. As an immediate consequence we obtain

$$i\varepsilon\partial_t\langle \Phi, \mathcal{W}(t)\Psi\rangle = \langle \Phi, \varepsilon\Theta(t)\mathcal{W}(t)\Psi\rangle. \quad (4.6.6)$$

Now, we consider the quadratic form $\Lambda(t)$ on $\mathcal{G}_+$ given by

$$\Lambda(t) := \Theta(t) + \vartheta_1\varepsilon^{-1}N + \vartheta_2 1\,.$$

It is easily follows, by (4.4.2) and (4.6.5), that

$$\left|\langle \Phi, P_3(t)^{Wick}\Psi\rangle\right|$$
$$\leq \frac{1}{4}\,||\left(-\varepsilon^{-1}\mathrm{d}\Gamma(-\Delta) + \varepsilon^{-1}P^{Wick} + \vartheta_1\varepsilon^{-1}N + \vartheta_2 1\right)^{1/2}\Phi||$$
$$\times\,||\left(-\varepsilon^{-1}\mathrm{d}\Gamma(-\Delta) + \varepsilon^{-1}P^{Wick} + \vartheta_1\varepsilon^{-1}N + \vartheta_2 1\right)^{1/2}\Psi||\,. \quad (4.6.7)$$

Therefore, using (4.5.4) and (4.6.7) we show that

$$\varepsilon^{-1}\left[\frac{D^{(2)}P}{2}(\varphi_t)[z] + \frac{D^{(3)}P}{3!}(\varphi_t)[z]\right]^{Wick}$$

is form bounded by $\varepsilon^{-1}\mathrm{d}\Gamma(-\Delta) + \varepsilon^{-1}P^{Wick} + \vartheta_1\varepsilon^{-1}N + \vartheta_2 1$ with a form-bound less than 1 uniformly in $\varepsilon \in (0,1]$. Hence, by the KLMN Theorem [102, Thm. X17], the quadratic form $\Lambda(t)$ is associated to a unique self-adjoint operator which we still denote by $\Lambda(t)$, satisfying $\mathcal{Q}(\Lambda(t)) = \mathcal{G}_+$ and $\Lambda(t) \geq 1$. Moreover, it is not difficult to show the existence of $c_1, c_2 > 0$ such that

$$c_1\, S_1 \leq \Lambda(t) \leq c_2\, G \quad (4.6.8)$$

uniformly in $\varepsilon \in (0,1]$ for any $t \in \mathbb{R}$. Now, we consider the non-autonomous Schrödinger equation

$$i\partial_t u_t = \Theta(t)u_t\,, \quad (4.6.9)$$

with initial data $u_0 \in \mathcal{G}_+$. Next, we prove existence and uniqueness of a unitary propagator $\mathcal{V}(t,s)$ of the Cauchy problem (4.6.9). This will be done if we can check assumptions of Corollary 4.C.4 with $\mathcal{G}_\pm = \mathcal{H}_\pm$, $A(t) = \Theta(t)$ and $S(t) = \Lambda(t)$. Thus, we will conclude that

$$||\Lambda(t)^{1/2}\mathcal{V}(t,0)\Psi||_{\mathcal{F}} \leq e^{ce^{c|t|}} \, ||\Lambda(0)^{1/2}\Psi||_{\mathcal{F}} \,. \qquad (4.6.10)$$

Observe that $\mathbb{R} \ni t \mapsto \Theta(t) \in \mathcal{L}(\mathcal{G}_+, \mathcal{G}_-)$ is norm continuous since

$$\begin{aligned}&|\langle \Phi, (\Theta(t) - \Theta(s))\,\Psi\rangle| \\ &\leq ||\Phi||_{\mathcal{G}_+} \, ||A_2(t) - A_2(s)||_{\mathcal{L}(\mathcal{F}^1_+, \mathcal{F}^1_-)} \, ||\Psi||_{\mathcal{G}_+} + |\langle \Phi, \varepsilon^{-1}(P_3(t) - P_3(s))^{Wick} \,\Psi\rangle| \,,\end{aligned}$$

and an estimate similar to (4.6.5) yields

$$|\langle \Phi, \varepsilon^{-1}(P_3(t) - P_3(s))^{Wick} \,\Psi\rangle| \leq 2\sqrt{2}||\varphi_t - \varphi_s||_{L^\infty(\mathbb{R})} \, ||\Phi||_{\mathcal{G}_+} \, ||\Psi||_{\mathcal{G}_+} \,.$$

Let us check assumption (i) of Corollary 4.C.4. We have for $\Psi \in \mathcal{G}_+ \subset \mathcal{F}^1_+$,

$$\partial_t\langle \Psi, \Lambda(t)\Psi\rangle = \partial_t\langle \Psi, S_2(t)\Psi\rangle + \partial_t\langle \Psi, \varepsilon^{-1}P_3(t)^{Wick}\Psi\rangle \,.$$

A simple computation yields

$$\begin{aligned}&\partial_t\langle \Psi, \varepsilon^{-1}P_3(t)^{Wick}\Psi\rangle \\ &= 2\mathrm{Re}\left[\sum_{n=1}^{\infty} \sqrt{n^2(n+1)\varepsilon} \int_{\mathbb{R}^{n-1}} \left(\int_{\mathbb{R}} \partial_t\varphi_t(x)\Psi^{(n)}(x,y)\overline{\Psi^{(n+1)}(x,x,y)}dx\right) dy\right] \,.\end{aligned}$$

So, by Cauchy-Schwarz inequality and Lemma 4.A.1, we get

$$\begin{aligned}&\left|\partial_t\langle \Psi, \varepsilon^{-1}P_3(t)^{Wick}\Psi\rangle\right| \\ &\leq 2||\partial_t\varphi_t||_{L^2(\mathbb{R})} \, \left[\sum_{n=1}^{\infty}(n+1)||\sup_{x\in\mathbb{R}}\left|\Psi^{(n)}(x,.)\right| \, ||^2_{L^2(\mathbb{R}^{n-1})}\right]^{1/2} \\ &\qquad \times \left[\sum_{n=1}^{\infty} n^2\varepsilon||\Psi^{(n+1)}(x,x,.)||^2_{L^2(\mathbb{R}^n)}\right]^{1/2} \\ &\leq 2\sqrt{2} \, ||\partial_t\varphi_t||_{L^2(\mathbb{R})} \, ||\Lambda(t)^{1/2}\Psi||^2 \,.\end{aligned}$$

The latter estimate with Lemma 4.5.4 (i) and (4.4.2)-(4.4.3) give us

$$|\partial_t\langle \Psi, \Lambda(t)\Psi\rangle| \leq e^{c(|t|+1)}||\Lambda(t)^{1/2}\Psi||^2 \,.$$

Now, we check assumption (ii) of Corollary 4.C.4. We follow the same lines of the proof of Lemma 4.5.4 (ii) by replacing $S_2(t)$ by $\Lambda(t)$ and $A_2(t)$ by $\Theta(t)$. So, we arrive at the step where we have to estimate for $\Psi, \Phi \in \mathcal{D}(\Lambda(t)^{3/2})$ and $\lambda > 0$, the quantity

$$\mathcal{C}_\lambda[g(t)] \;:=\; \langle \Psi, \varepsilon^{-1}g(t)^{Wick}N_\lambda\Phi\rangle - \langle N_\lambda\Psi, \varepsilon^{-1}g(t)^{Wick}\Phi\rangle \,,$$

where $N_\lambda := \varepsilon^{-1}N(\lambda\varepsilon^{-1}N+1)^{-1}$ and $g(t)$ is the continuous polynomial on $\mathcal{S}(\mathbb{R})$ given by

$$g(t)[z] = P_2(t)[z] + P_3(t)[z]\,.$$

Note that the part $\mathcal{C}_\lambda[P_2(t)]$ involving only the symbol $P_2(t)$ is already bounded by (4.5.7). Thus, we need only to consider $\mathcal{C}_\lambda[P_3(t)]$. A simple computation yields

$$\begin{aligned}\mathcal{C}_\lambda[P_3(t)] \;&=\; \sum_{n=1}^{\infty}\kappa(n)\int_{\mathbb{R}^{n-1}}\left(\int_{\mathbb{R}}\overline{\varphi_t(x)}\,\Phi^{(n+1)}(x,x,y)\overline{\Psi^{(n)}(x,y)}\;dx\right)dy\\ &\quad-\sum_{n=1}^{\infty}\kappa(n)\int_{\mathbb{R}^{n-1}}\left(\int_{\mathbb{R}}\varphi_t(x)\Phi^{(n)}(x,y)\overline{\Psi^{(n+1)}(x,x,y)}\,dx\right)dy\,,\end{aligned}$$

where

$$\kappa(n) = \frac{(n+1)\sqrt{\varepsilon n^2(n+1)}}{(\lambda(n+1)+1)} - \frac{n\sqrt{\varepsilon n^2(n+1)}}{(\lambda n+1)}$$

satisfying $|\kappa(n)| \le \sqrt{n^2(n+1)}$ uniformly in $\varepsilon \in (0,1]$ and $\lambda > 0$. So, using a similar estimate as (4.6.5), we obtain

$$|\mathcal{C}_\lambda[P_3(t)]| \le \frac{1}{\sqrt{2}}\,||\varphi_t||_{L^\infty(\mathbb{R})}\;||\Lambda(t)^{1/2}\Psi||\,||\Lambda(t)^{1/2}\Phi||\,.$$

This proves assumption (ii) of Corollary 4.C.4. Now, we check that

$$\mathcal{W}(t) = \mathcal{V}(t,0).$$

In fact, for $\Phi \in \mathcal{G}_+$ and $\Psi \in \mathcal{D}_+$ we have

$$\begin{aligned}&i\partial_r\langle\Phi, \mathcal{V}(0,r)\mathcal{W}(r)\Psi\rangle\\ &\quad= -\langle\Theta(r)\mathcal{V}(r,0)\Phi, \mathcal{W}(r)\Psi\rangle + i\lim_{s\to 0}\,\langle\mathcal{V}(r+s,0)\Phi, \frac{\mathcal{W}(r+s)-\mathcal{W}(r)}{s}\Psi\rangle\,,\end{aligned}$$

and since by (4.6.4) we know that $\lim_{s\to 0}\frac{\mathcal{W}(r+s)-\mathcal{W}(r)}{s}\Psi$ exists in $\mathcal{F}$, we conclude using (4.6.6) that

$$\partial_r\langle\Phi, \mathcal{V}(0,r)\mathcal{W}(r)\Psi\rangle = 0\,.$$

This identifies $\mathcal{W}(t)$ as the unitary propagator of the non-autonomous Schrödinger equation (4.6.9). Therefore, by (4.6.8)-(4.6.10) we get

$$\sqrt{c_1}\,||\mathcal{W}(t)\Psi||_{\mathcal{F}^1_+} \le ||\Lambda(t)^{1/2}\mathcal{W}(t)\Psi||_{\mathcal{F}} \le e^{ce^{c|t|}}||\Lambda(0)^{1/2}\Psi||_{\mathcal{F}} \le \sqrt{c_2}\,e^{ce^{c|t|}}||\Psi||_{\mathcal{G}_+}\,,$$

for any $t \in \mathbb{R}$ uniformly in $\varepsilon \in (0,1]$. □

Lemma 4.6.4. *For any $\varphi_0 \in H^2(\mathbb{R})$ and $\Psi \in \mathcal{G}_+$ we have*

$$\|\mathcal{W}(t)\Psi - U_2(t,0)\Psi\|^2_{\mathcal{F}} = 2\langle \Psi, (1-R_\nu)\Psi\rangle - 2\mathrm{Re}\langle \mathcal{W}(t)\Psi, (1-R_\nu)U_2(t,0)\Psi\rangle$$
$$+ 2\,\mathrm{Im} \int_0^t \langle \mathcal{W}(s)\Psi,\ [\Theta(s)R_\nu - R_\nu A_2(s)]\, U_2(s,0)\Psi\rangle\, ds\,,$$

where $R_\nu := \sigma(\frac{\varepsilon^{-1}N}{\nu})$ with σ any bounded Borel function on $\mathbb{R}_+$ with compact support and here

$$\Theta(s) = A_2(s) + \varepsilon^{-1} Q_s(z)^{wick}\,,$$

with $Q_s(z)$ the continuous polynomial on $\mathcal{S}(\mathbb{R})$ given by

$$Q_s(z) \quad = \quad \frac{D^{(3)}P}{3!}(\varphi_s)[z] + \frac{D^{(4)}P}{4!}(\varphi_s)[z]\,.$$

Proof. We have

$$\begin{aligned}
&\|\mathcal{W}(t)\Psi - U_2(t,0)\Psi\|^2_{\mathcal{F}} \\
&= 2\,\|\Psi\|^2_{\mathcal{F}} - 2\mathrm{Re}\langle \mathcal{W}(t)\Psi, U_2(t,0)\Psi\rangle \\
&= 2\langle \Psi, (1-R_\nu)\Psi\rangle - 2\mathrm{Re}\langle \mathcal{W}(t)\Psi, (1-R_\nu)U_2(t,0)\Psi\rangle \\
&\quad + 2\mathrm{Re}\langle \Psi, R_\nu\Psi\rangle - 2\mathrm{Re}\langle \mathcal{W}(t)\Psi, R_\nu U_2(t,0)\Psi\rangle.
\end{aligned} \tag{4.6.11}$$

Hence to prove the lemma it is enough to show that

$$\mathbb{R} \ni s \mapsto \mathrm{Re}\langle \mathcal{W}(s)\Psi, R_\nu U_2(s,0)\Psi\rangle \in C^1(\mathbb{R}) \tag{4.6.12}$$

and compute its derivative. Recall that the propagator $U_2(s,0) \in C^0(\mathbb{R}, \mathcal{L}(\mathcal{F}^1_+))$, by Proposition 4.5.5 and that $\mathcal{W}(s) \in C^0(\mathbb{R}, \mathcal{L}(\mathcal{G}_+))$ since it is the unitary propagator of the Cauchy problem (4.6.9). It is easily seen that

$$s \mapsto R_\nu U_2(s,0)\Psi\,,$$

are in $\in C^0(\mathbb{R}, \mathcal{G}_+)$ since R_ν maps continuously $\mathcal{F}^1_+$ into $\mathcal{G}_+$. We also have that

$$s \mapsto \mathcal{W}(s)\Psi \in C^1(\mathbb{R}, \mathcal{G}_-) \quad \text{and} \quad s \mapsto U_2(s,0)\Psi \in C^1(\mathbb{R}, \mathcal{F}^1_-)\,.$$

This proves the statement (4.6.12). Therefore, we have

$$\begin{aligned}
&2\mathrm{Re}\langle \Psi, R_\nu\Psi\rangle - 2\mathrm{Re}\langle \mathcal{W}(t)\Psi, R_\nu U_2(t,0)\Psi\rangle = \\
&\qquad -\frac{2}{\varepsilon}\mathrm{Im}\int_0^t i\varepsilon\partial_s\, \langle \mathcal{W}(s)\Psi, R_\nu U_2(s,0)\Psi\rangle\, ds\,.
\end{aligned} \tag{4.6.13}$$

The fact that $\mathcal{W}(t)$ is the unitary propagator of (4.6.9) with Proposition 4.5.5 yields

$$\begin{aligned}
&i\varepsilon\partial_s\langle \mathcal{W}(s)\Psi, R_\nu U_2(s,0)\Psi\rangle = \\
&-\langle \varepsilon\Theta(s)\mathcal{W}(s)\Psi, R_\nu U_2(s,0)\Psi\rangle + \langle \mathcal{W}(s)\Psi, R_\nu \varepsilon A_2(s) U_2(s,0)\Psi\rangle\,.
\end{aligned} \tag{4.6.14}$$

Now, collecting (4.6.11), (4.6.13) and (4.6.14) we obtain the claimed identity. □

Proof of Theorem 4.6.1. We are now ready to prove Theorem 4.6.1.
First observe that we have

$$\left\| e^{-it/\varepsilon H_\varepsilon} W(\frac{\sqrt{2}}{i\varepsilon}\varphi_0)\Psi - e^{i\omega(t)/\varepsilon} W(\frac{\sqrt{2}}{i\varepsilon}\varphi_t) U_2(t,0)\Psi \right\|_{\mathcal{F}}^2 = \|\mathcal{W}(t)\Psi - U_2(t,0)\Psi\|_{\mathcal{F}}^2 .$$

Now, using Lemma 4.6.4 one obtains for $t > 0$ (the case $t < 0$ is similar) the estimate

$$\begin{aligned}\|\mathcal{W}(t)\Psi - U_2(t,0)\Psi\|_{\mathcal{F}}^2 \leq & 2\,|\langle\Psi,(1-R_\nu)\Psi\rangle| + 2\,|\langle\mathcal{W}(t)\Psi,(1-R_\nu)U_2(t,0)\Psi\rangle| \\ & + 2\int_0^t |\langle\mathcal{W}(s)\Psi,\ [\Theta(s)R_\nu - R_\nu A_2(s)]\,U_2(s,0)\Psi\rangle|\ ds .\end{aligned}$$

Here we consider σ to be in the class $C^1(\mathbb{R}_+)$, decreasing and satisfying $\sigma(s) = 1$ if $s \leq 1$ and $\sigma(s) = 0$ if $s \geq 2$. We have for ν positive integer,

$$\begin{aligned}\langle\Psi,(1-R_\nu)\Psi\rangle &\leq \frac{1}{\nu}\sum_{n=\nu+1}^{\infty} n\langle\Psi^{(n)},(D_{x_1}^2+1)\Psi^{(n)}\rangle \\ &\leq \tfrac{1}{\nu}\langle\Psi,\varepsilon^{-1}[\mathrm{d}\Gamma(-\Delta)+N]\Psi\rangle \qquad \leq \tfrac{1}{\nu}\,\|\Psi\|_{\mathcal{F}_+^1}^2 .\end{aligned}$$

Hence, we easily check with the help of Proposition 4.5.5 and Lemma 4.6.3 that

$$\begin{aligned}|\langle\mathcal{W}(t)\Psi,(1-R_\nu)U_2(t,0)\Psi\rangle| &\leq \tfrac{1}{\nu}\,||U_2(t,0)\Psi||_{\mathcal{F}_+^1}\,||\mathcal{W}(t)\Psi||_{\mathcal{F}_+^1} \\ &\leq \tfrac{1}{\nu}\,e^{c_1 e^{c_1 t}}||\Psi||_{\mathcal{F}_+^1}\,||\Psi||_{\mathcal{G}_+} \leq \tfrac{1}{\nu}\,e^{c_1 e^{c_1 t}}\,||\Psi||_{\mathcal{G}_+}^2 .\end{aligned}$$

Next, we show that there exists $C > 0$ depending only on φ_0 such that

$$\left\|\varepsilon^{-1}Q_s(z)^{Wick}R_\nu\right\|_{\mathcal{L}(\mathcal{F}_+^1,\mathcal{F}_-^1)} \leq C\,(\nu\,\varepsilon^{1/2} + \nu^2\varepsilon) .$$

The latter bound follows by Cauchy-Schwarz inequality, Lemma 4.A.1 and (4.4.2),

$$\begin{aligned}&|\langle\Phi, \frac{P_3(s)}{\varepsilon}^{Wick} R_\nu\Psi\rangle| \\ &\leq \sqrt{\varepsilon}||\varphi_t||_{L^\infty(\mathbb{R})}\left[\sum_{n=1}^{2\nu}(n+1)||\Phi^{(n)}||_{L^2(\mathbb{R}^n)}^2\right]^{1/2}\left[\sum_{n=1}^{2\nu}n^2||\Psi^{(n+1)}(x,x,.)||_{L^2(\mathbb{R}^n)}^2\right]^{1/2} \\ &\quad + \sqrt{\varepsilon}||\varphi_t||_{L^\infty(\mathbb{R})}\left[\sum_{n=1}^{2\nu}(n+1)||\Psi^{(n)}||_{L^2(\mathbb{R}^n)}^2\right]^{1/2}\left[\sum_{n=1}^{2\nu}n^2||\Phi^{(n+1)}(x,x,.)||_{L^2(\mathbb{R}^n)}^2\right]^{1/2} \\ &\leq 2\nu\sqrt{\varepsilon}||\varphi_t||_{L^\infty(\mathbb{R})}\,||(\varepsilon^{-1}N+1)^{1/2}\Phi||_{\mathcal{F}}\,||\Psi||_{\mathcal{F}_+^1} \\ &\quad + 2\nu\sqrt{\varepsilon}||\varphi_t||_{L^\infty(\mathbb{R})}\,||(\varepsilon^{-1}N+1)^{1/2}\Psi||_{\mathcal{F}}\,||\Phi||_{\mathcal{F}_+^1} ,\end{aligned}$$

and a similar estimate for P^{Wick},

$$|\langle\Phi, P^{Wick}R_\nu\Psi\rangle| \leq \nu^2\varepsilon^2 \,||\Phi||_{\mathcal{F}^1_+}\, ||\Psi||_{\mathcal{F}^1_+}\,.$$

Hence we can check that

$$\begin{aligned}\int_0^t \left|\langle\mathcal{W}(s)\Psi, \varepsilon^{-1}Q_s(z)^{Wick}R_\nu U_2(s,0)\Psi\rangle\right| \, ds \\ \leq C(\nu\varepsilon^{1/2}+\nu^2\varepsilon)\int_0^t ||\mathcal{W}(s)\Psi||_{\mathcal{F}^1_+}\, ||U_2(s,0)\Psi||_{\mathcal{F}^1_+}\, ds\,.\end{aligned}$$

Now, by Lemma 4.6.3 and Proposition 4.5.5 we obtain

$$\begin{aligned}\int_0^t \|\mathcal{W}(s)\Psi\|_{\mathcal{F}^1_+}\; \|U_2(s,0)\Psi\|_{\mathcal{F}^1_+}\; ds &\leq \int_0^t e^{c_1e^{c_1s}}\, \|\Psi\|_{\mathcal{G}_+}\, \|U_2(s,0)\Psi\|_{\mathcal{F}^1_+}\; ds \\ &\leq \int_0^t e^{c_2e^{c_2s}}\, \|\Psi\|_{\mathcal{G}_+}\; \|\Psi\|_{\mathcal{F}^1_+}\; ds \\ &\leq e^{ce^{cs}}\, \|\Psi\|^2_{\mathcal{G}_+}\,.\end{aligned}$$

A simple computation yields

$$\begin{aligned}A_2(s)R_\nu - R_\nu A_2(s) = \frac{1}{2}\left[\sigma(\frac{\varepsilon^{-1}N+2}{\nu}) - \sigma(\frac{\varepsilon^{-1}N}{\nu})\right]\left(\int_{\mathbb{R}} \varphi_t(x)^2\overline{z(x)}^2\, dx\right)^{Wick} \\ + \frac{1}{2}\left[\sigma(\frac{\varepsilon^{-1}N-2}{\nu}) - \sigma(\frac{\varepsilon^{-1}N}{\nu})\right]\left(\int_{\mathbb{R}} \overline{\varphi_t(x)}^2 z(x)^2\, dx\right)^{Wick}\,.\end{aligned}$$

We easily check that

$$\left\|\sigma(\frac{\varepsilon^{-1}N\pm 2}{\nu}) - \sigma(\frac{\varepsilon^{-1}N}{\nu})\right\|_{\mathcal{L}(\mathcal{F}^1_+)} \leq \frac{2}{\nu}||\sigma'||_{L^\infty(\mathbb{R}_+)}\,,$$

since $\varepsilon^{-1}\mathrm{d}\Gamma(-\Delta) + \varepsilon^{-1}N$ commute with $\varepsilon^{-1}N$. Thus, using (4.5.4) there exists $c_0, c > 0$ such that

$$\begin{aligned}\int_0^t |\langle\mathcal{W}(s)\Psi, [A_2(s), R_\nu]U_2(s,0)\Psi\rangle|\; ds \leq \frac{c_0}{\nu}\int_0^t \|\mathcal{W}(s)\Psi\|_{\mathcal{F}^1_+}\; \|U_2(s,0)\Psi\|_{\mathcal{F}^1_+}\; ds \\ \leq \frac{1}{\nu}e^{ce^{ct}}\, \|\Psi\|^2_{\mathcal{G}_+}\,.\end{aligned}$$

Finally, the claimed inequality in Theorem 4.6.1 follows by collecting the previous estimates and letting $\nu = \varepsilon^{-1/4}$. □

We have the following two corollaries.

Corollary 4.6.5. *For any $\varphi_0 \in H^2(\mathbb{R})$ and any $\xi \in L^2(\mathbb{R})$ we have the strong limit*

$$s - \lim_{\varepsilon\to 0} W(\frac{\sqrt{2}}{i\varepsilon}\varphi_0)^*\, e^{it/\varepsilon H_\varepsilon}\, W(\xi)\, e^{-it/\varepsilon H_\varepsilon}\, W(\frac{\sqrt{2}}{i\varepsilon}\varphi_0) = e^{i\sqrt{2}\mathrm{Re}\langle\xi,\varphi_t\rangle}\, 1\,,$$

where φ_t solves the NLS equation (4.4.1) with initial data φ_0.

Proof. It is enough to prove for any $\Psi, \Phi \in \mathcal{G}_+$ the limit:

$$\lim_{\varepsilon\to 0} \langle e^{-it/\varepsilon H_\varepsilon} W(\frac{\sqrt{2}}{i\varepsilon}\varphi_0)\,\Psi,\, W(\xi)\, e^{-it/\varepsilon H_\varepsilon}\, W(\frac{\sqrt{2}}{i\varepsilon}\varphi_0)\Phi\rangle = e^{i\sqrt{2}\mathrm{Re}(\xi,\varphi_t)}\,\langle \Psi, \Phi\rangle\,. \tag{4.6.15}$$

Indeed, using Theorem 4.6.1, we show

$$\begin{aligned}&\langle e^{-it/\varepsilon H_\varepsilon} W(\frac{\sqrt{2}}{i\varepsilon}\varphi_0)\Psi, W(\xi) e^{-it/\varepsilon H_\varepsilon} W(\frac{\sqrt{2}}{i\varepsilon}\varphi_0)\Phi\rangle\\ &\qquad = \langle W(\frac{\sqrt{2}}{i\varepsilon}\varphi_t) U_2(t,0)\Psi, W(\xi)\, W(\frac{\sqrt{2}}{i\varepsilon}\varphi_t) U_2(t,0)\Phi\rangle + O(\varepsilon^{1/8}).\end{aligned}$$

Therefore by Weyl commutation relations we have

$$\begin{aligned}&\langle W(\frac{\sqrt{2}}{i\varepsilon}\varphi_t)\, U_2(t,0)\Psi,\, W(\xi)\, W(\frac{\sqrt{2}}{i\varepsilon}\varphi_t)\, U_2(t,0)\Phi\rangle\\ &\qquad\qquad = \langle U_2(t,0)\Psi,\, W(\xi)\, U_2(t,0)\Phi\rangle e^{i\sqrt{2}\mathrm{Re}(\xi,\varphi_t)}\,,\end{aligned}$$

Thus the limit is proved since $s-\lim_{\varepsilon\to 0} W(\xi) = 1$. □

Recall that $\mathcal{F}_0$ is the subspace of $\mathcal{F}$ spanned by vectors $\Psi \in \mathcal{F}$ such that $\Psi^{(n)} = 0$ for any index $n \in \mathbb{N}$ except for finite number. Note that $\mathcal{F}_0 \cap \mathcal{G}_+$ is dense in $\mathcal{F}$.

Corollary 4.6.6. *For any $\varphi_0 \in H^2(\mathbb{R})$ and any $\Psi, \Phi \in \mathcal{F}_0 \cap \mathcal{G}_+$ and $b \in \mathcal{P}_{p,q}(L^2(\mathbb{R}))$, we have*

$$\lim_{\varepsilon\to 0} \langle W(\frac{\sqrt{2}}{i\varepsilon}\varphi_0)\Psi,\, e^{it/\varepsilon H_\varepsilon}\, b^{Wick}\, e^{-it/\varepsilon H_\varepsilon}\, W(\frac{\sqrt{2}}{i\varepsilon}\varphi_0)\Phi\rangle = b(\varphi_t)\,\langle \Psi,\, \Phi\rangle\,,$$

where φ_t solves the NLS equation (4.4.1) with initial data φ_0.

Proof. Consider a (p,q)-homogenous polynomial $b \in \mathcal{P}_{p,q}(L^2(\mathbb{R}))$. We have

$$\begin{aligned}\mathcal{A} &:= \langle W(\frac{\sqrt{2}}{i\varepsilon}\varphi_0)\Psi,\, e^{it/\varepsilon H_\varepsilon}\, b^{Wick}\, e^{-it/\varepsilon H_\varepsilon}\, W(\frac{\sqrt{2}}{i\varepsilon}\varphi_0)\Phi\rangle\\ &= \langle (N+1)^q W(\frac{\sqrt{2}}{i\varepsilon}\varphi_0)\Psi, e^{it/\varepsilon H_\varepsilon}\, B_\varepsilon\, e^{-it/\varepsilon H_\varepsilon} (N+1)^p W(\frac{\sqrt{2}}{i\varepsilon}\varphi_0)\Phi\rangle\,,\end{aligned}$$

where $B_\varepsilon := (N+1)^{-q} b^{Wick} (N+1)^{-p}$. The number estimate (4.2.2) yields

$$\|B_\varepsilon\| \leq \left\|\tilde{b}\right\|_{\mathcal{L}(L^2_s(\mathbb{R}^p), L^2_s(\mathbb{R}^q))}\,,$$

uniformly in $\varepsilon \in (0,1]$. Let $\tilde{N}_t$ be the positive operator given by

$$\tilde{N}_t = N + 2\mathrm{Re}\langle z, \varphi_t\rangle^{Wick} + ||\varphi_t||^2_{L^2(\mathbb{R})}\,.$$

By (4.6.1), we get

$$\mathcal{A} = \langle W(\frac{\sqrt{2}}{i\varepsilon}\varphi_0)(\tilde{N}_0+1)^q\Psi,\, e^{it/\varepsilon H_\varepsilon}\, B_\varepsilon\, e^{-it/\varepsilon H_\varepsilon}\, W(\frac{\sqrt{2}}{i\varepsilon}\varphi_0)(\tilde{N}_0+1)^p\Phi\rangle\,.$$

Now, observe that

$$\lim_{\varepsilon\to 0}(\tilde{N}_0+1)^p\Phi = (1+||\varphi||^2_{L^2(\mathbb{R})})^p\Phi \quad\text{and}\quad \lim_{\varepsilon\to 0}(\tilde{N}_0+1)^q\Psi = (1+||\varphi||^2_{L^2(\mathbb{R})})^q\Psi\,.$$

So, using Theorem 4.6.1 we obtain

$$\begin{aligned}\mathcal{A} &= (1+||\varphi_0||^2_{L^2(\mathbb{R})})^{p+q}\,\langle W(\frac{\sqrt{2}}{i\varepsilon}\varphi_t)\,U_2(t,0)\Psi,\; B_\varepsilon\, W(\frac{\sqrt{2}}{i\varepsilon}\varphi_t)U_2(t,0)\Phi\rangle + O(\varepsilon^{1/8})\\ &= \langle U_2(t,0)\Psi,\, (\tilde{N}_t+1)^{-q}\, b(.+\varphi_t)^{Wick}\,(\tilde{N}_t+1)^{-p}\,U_2(t,0)\Phi\rangle + O(\varepsilon^{1/8})\,.\end{aligned}$$

We set $\Psi_\varepsilon = (N+1)^q(\tilde{N}_t+1)^{-q}U_2(t,0)\Psi$ and $\Phi_\varepsilon = (N+1)^p(\tilde{N}_t+1)^{-p}U_2(t,0)\Phi$ and remark that we can show for $\varphi_0 \neq 0$ and μ a positive integer the following strong limit

$$s-\lim_{\varepsilon\to 0}(N+1)^\mu(\tilde{N}_t+1)^{-\mu} = \frac{1}{(1+||\varphi_t||^2_{L^2(\mathbb{R})})^\mu}\,. \tag{4.6.16}$$

This holds since we have by explicit computation

$$||(a(\varphi_t)+a^*(\varphi_t))(N+||\varphi_t||^2+1)^{-1}|| \le \frac{||\varphi_t||}{2\sqrt{||\varphi_t||^2+1}} + \frac{||\varphi_t||}{2\sqrt{||\varphi_t||^2+1-\varepsilon}} < 1,$$

for ε sufficiently small and hence we can write

$$\begin{aligned}&(N+1)(\tilde{N}_t+1)^{-1}\\ &= (N+1)(N+||\varphi_t||^2+1)^{-1}[\overbrace{(a(\varphi_t)+a^*(\varphi_t))(N+||\varphi_t||^2+1)^{-1}}^{\mathcal{R}_\varepsilon}+1]^{-1}\,.\end{aligned}$$

This proves (4.6.16) for $\mu = 1$ since $s-\lim_{\varepsilon\to 0}\mathcal{R}_\varepsilon = 0$. Now, we proceed by induction on μ using a commutator argument

$$\begin{aligned}(N+1)^{\mu+1}(\tilde{N}_t+1)^{-(\mu+1)} &= (N+1)^\mu(\tilde{N}_t+1)^{-\mu}(N+1)(\tilde{N}_t+1)^{-1}\\ &+ (N+1)^\mu(\tilde{N}_t+1)^{-\mu}[(\tilde{N}_t+1)^\mu, N](\tilde{N}_t+1)^{-(\mu+1)}\,,\end{aligned}$$

with the observation that the second term of (r.h.s.) converges strongly to 0. Therefore, we obtain

$$\lim_{\varepsilon\to 0}\Psi_\varepsilon = \frac{1}{(1+||\xi||^2_{L^2(\mathbb{R})})^q}U_2(t,0)\Psi \quad\text{and}\quad \lim_{\varepsilon\to 0}\Phi_\varepsilon = \frac{1}{(1+||\xi||^2_{L^2(\mathbb{R})})^p}U_2(t,0)\Phi\,.$$

It is also easy to show by explicit computation that

$$w-\lim_{\varepsilon\to 0}(N+1)^{-q}b^{Wick}_{r,s}(N+1)^{-p} = 0\,,$$

for any $b_{r,s} \in \mathcal{P}_{r,s}(L^2(\mathbb{R}))$ such that $0 < r \leq p$ and $0 < s \leq q$. Hence, letting $\varepsilon \to 0$, we get

$$\begin{aligned}\lim_{\varepsilon\to 0} \mathcal{A} &= (1+||\varphi_0||^2_{L^2(\mathbb{R})})^{p+q} \lim_{\varepsilon\to 0} \langle \Psi_\varepsilon, (N+1)^{-q} b(\varphi_t)\,(N+1)^{-p}\Phi_\varepsilon\rangle \\ &= b(\varphi_t)\,\langle U_2(t,0)\Psi,\, U_2(t,0)\Phi\rangle = b(\varphi_t)\,\langle \Psi,\, \Phi\rangle\,,\end{aligned}$$

since $||\varphi_t||_{L^2(\mathbb{R})} = ||\varphi_0||_{L^2(\mathbb{R})}$ and $s - \lim_{\varepsilon\to 0}(N+1)^{-\mu} = 1$ for $\mu > 0$. □

We identify the propagator $U_2(t,s)$ as a time-dependent Bogoliubov's transform on the Fock representation of the Weyl commutation relations.

Proposition 4.6.7. *Let $\varphi_0 \in H^2(\mathbb{R})$ and consider the propagator $U_2(t,0)$ given in Proposition 4.5.5. For a given $s \in \mathbb{R}$ let $\xi_s \in H^2(\mathbb{R})$, we have*

$$U_2(t,s)\, W(\frac{\xi_s}{i\sqrt{\varepsilon}})\, U_2(s,t) = W(\frac{\beta(t,s)\xi_s}{i\sqrt{\varepsilon}})$$

where $\beta(t,s)$ is the symplectic propagator on $L^2(\mathbb{R})$, solving the equation

$$\begin{cases} i\partial_t \xi_t(x) = [-\Delta + 2|\varphi_t(x)|^2]\, \xi_t(x) + \varphi_t(x)^2\, \overline{\xi_t(x)}\,, \\ \xi_{|t=s} = \xi_s\,, \end{cases} \tag{4.6.17}$$

such that $\beta(t,s)\xi_s = \xi_t$.

Proof. Observe that if $\varphi_0 \in H^2(\mathbb{R})$ then the solution φ_t of the NLS equation (4.4.1) with initial condition φ_0 satisfies $\varphi_t \in C^0(\mathbb{R}, L^\infty(\mathbb{R}))$. Hence, by standard arguments the equation (4.6.17) admits a unique solution $\xi_t \in C^0(\mathbb{R}, H^2(\mathbb{R})) \cap C^1(\mathbb{R}, L^2(\mathbb{R}))$ for any $\xi_s \in H^2(\mathbb{R})$. Moreover, the propagator

$$\beta(t,s)\xi_s = \xi_t,$$

defines a symplectic transform on $L^2(\mathbb{R})$ for any $t, s \in \mathbb{R}$. This follows by differentiating

$$\mathrm{Im}\langle \beta(t,s)\xi, \beta(t,s)\eta\rangle\,,$$

with respect to t for $\xi, \eta \in H^2(\mathbb{R})$. Furthermore, β satisfies the laws

$$\beta(s,s) = 1, \qquad \beta(t,s)\beta(s,r) = \beta(t,r) \qquad \text{for} \qquad t,r,s \in \mathbb{R}.$$

Now, we differentiate with respect to t the quantity

$$U_2(s,t)\, W(\frac{\xi_t}{i\sqrt{\varepsilon}})\, U_2(t,s)$$

in the sense of quadratic forms on $\mathcal{F}_+^1$, with ξ_t solution of (4.6.17). Hence, using Lemma 4.6.2 (ii), we get

$$\begin{aligned}\partial_t &\left[U_2(s,t)\, W(\frac{\sqrt{2}}{i\sqrt{\varepsilon}}\xi_t)\, U_2(t,s) \right] \\ &= U_2(s,t) W(\frac{\sqrt{2}}{i\sqrt{\varepsilon}}\xi_t) \left[W(\frac{\sqrt{2}}{i\sqrt{\varepsilon}}\xi_t)^* i A_2(t) W(\frac{\sqrt{2}}{i\sqrt{\varepsilon}}\xi_t) - iA_2(t) \right. \\ &\qquad \left. - i \left(\mathrm{Re}\langle \xi_t, i\partial_t \xi_t\rangle + \frac{2}{\sqrt{\varepsilon}} \mathrm{Re}\langle z, i\partial_t\xi_t\rangle^{Wick} \right) \right] U_2(t,s)\,. \qquad (4.6.18)\end{aligned}$$

Now, by [76, Lemma 2.10], we obtain

$$W(\frac{\sqrt{2}}{i\sqrt{\varepsilon}}\xi_t)^* A_2(t) W(\frac{\sqrt{2}}{i\sqrt{\varepsilon}}\xi_t) \quad = \quad \varepsilon^{-1} m(t)[z+\sqrt{\varepsilon}\xi_t]^{Wick}\,,$$

where $m(t)[z]$ is the continuous polynomial on $\mathcal{S}(\mathbb{R})$ given by

$$m(t)[z] = \langle z, -\Delta z\rangle + P_2(t)[z]\,.$$

Therefore, the (r.h.s.) of (4.6.18) is null if we show that

$$m(t)[z+\sqrt{\varepsilon}\xi_t] - m(t)[z] - \big(\varepsilon \mathrm{Re}\langle \xi_t, i\partial_t\xi_t\rangle + 2\sqrt{\varepsilon}\mathrm{Re}\langle z, i\partial_t\xi_t\rangle\big) = 0\,.$$

This follows by straightforward computation. □

4.7 Propagation of chaos

Propagation of chaos for a many-boson system with point pair-interaction in one dimension was studied in [73] (see also the related work [74]). Here we prove this conservation hypothesis for such quantum system using the method in [103]. Thus, we are led to study the asymptotics of time-evolved Hermite states

$$e^{-it/\varepsilon_n H_{\varepsilon_n}}\, \varphi_0^{\otimes n} \quad \text{with} \quad \varphi_0 \in H^2(\mathbb{R}),\ ||\varphi_0||_{L^2(\mathbb{R})} = 1\,,$$

when $n \to \infty$ with $n\varepsilon_n = 1$. We denote the coherent states by

$$E(\varphi_0) := W(\frac{\sqrt{2}}{i\varepsilon}\varphi_0)\Omega_0,$$

where $\Omega_0 = (1, 0, \cdots)$ is the vacuum vector in the Fock space $\mathcal{F}$. To pass from coherent states to Hermite states we use the integral representation proved in [103],

$$\varphi_0^{\otimes n} = \frac{\gamma_n}{2\pi} \int_0^{2\pi} e^{-i\theta n}\, E(e^{i\theta}\varphi_0)\, d\theta\,, \quad \text{where} \quad \gamma_n := \frac{e^{1/2\varepsilon_n}\sqrt{n!}}{\varepsilon_n^{-n/2}}. \qquad (4.7.1)$$

Asymptotically, the factor γ_n grows as $(2\pi n)^{1/4}$ when $n \to \infty$. In the following we prove the chaos conservation hypothesis.

Proof of Theorem 4.2.3. It is known that if a sequence of positive trace-class operators ρ_n on $L^2(\mathbb{R})$ converges in the weak operator topology to ρ such that $\lim_{n\to\infty} \mathrm{Tr}[\rho_n] = \mathrm{Tr}[\rho] < \infty$ then ρ_n converges in the trace norm to ρ (see, for instance [80]). This argument reduces the proof to the case

$$b(z) = \prod_{i=1}^{p} \langle z, f_i\rangle \, \langle g_i, z\rangle \,,$$

where $f_i, g_i \in L^2(\mathbb{R})$. For shortness, we set

$$E_\theta = E(e^{i\theta}\varphi_0) \quad \text{and} \quad E_\theta^t = e^{-it/\varepsilon_n H_{\varepsilon_n}} E_\theta \,.$$

Using formula (4.7.1), we get

$$\begin{aligned}\Gamma_n &:= \langle \varphi_0^{\otimes n}, e^{it/\varepsilon_n H_{\varepsilon_n}} \, b^{Wick} \, e^{-it/\varepsilon_n H_{\varepsilon_n}} \varphi_0^{\otimes n}\rangle \\ &= \frac{\gamma_n^2}{(2\pi)^2} \int_{[0,2\pi]^2} e^{-in(\theta-\theta')} \langle E_{\theta'}^t, \, b^{Wick} \, E_\theta^t\rangle \, d\theta d\theta' \,.\end{aligned}$$

It is easily seen that

$$(N+1)^{-p} e^{-it/\varepsilon_n H_{\varepsilon_n}} \varphi_0^{\otimes n} = 2^{-p} e^{-it/\varepsilon_n H_{\varepsilon_n}} \varphi_0^{\otimes n} \,.$$

Therefore, we write

$$\begin{aligned}\Gamma_n = \frac{4^p \gamma_n^2}{(2\pi)^2} \int_{[0,2\pi]^2} & e^{-in(\theta-\theta')} \\ & \langle E_{\theta'}^t, \, (N+1)^{-p} \prod_{i=1}^{p} a^*(f_i) \prod_{j=1}^{p} a(g_j) (N+1)^{-p} \, E_\theta^t\rangle \, d\theta d\theta' \,.\end{aligned}$$

Now, we use the decomposition

$$\begin{aligned}\prod_{i=1}^{p} a^*(f_i) \prod_{j=1}^{p} a(g_j) = & \sum_{I,J \subset \mathcal{N}_p} \prod_{i\in I^c} [a^*(f_i) - \langle \varphi_t^{\theta'}, f_i\rangle] \\ & \times \prod_{j\in J^c} [a(g_j) - \langle g_j, \varphi_t^{\theta}\rangle] e^{-i(\#I\theta' - \#J\theta)} \prod_{i\in I} \overline{\langle f_i, \varphi_t\rangle} \prod_{j\in J} \langle g_j, \varphi_t\rangle \,,\end{aligned}$$

where the sum runs over all subsets I, J of $\mathcal{N}_p := \{1, \cdots, p\}$. Thus, we can write

$$\begin{aligned}&\Gamma_n - b(\varphi_t) = \\ &\sum_{I,J\subset\mathcal{N}_p}^{\#I+\#J<2p} \frac{4^p \gamma_n^2}{(2\pi)^2} \int_{[0,2\pi]^2} e^{-i[(n-\#J)\theta - (n-\#I)\theta']} \langle \tilde{E}_{\theta'}^t, \, B_{I,J}^{Wick} \, \tilde{E}_\theta^t\rangle \, d\theta d\theta' \,,\end{aligned} \tag{4.7.2}$$

where $\tilde{E}^t_\theta := (N+1)^{-p}\, E^t_\theta$ and $B_{I,J}(z)$ are sums of homogenous polynomials such that

$$\langle \tilde{E}^t_{\theta'}, B^{Wick}_{I,J} \tilde{E}^t_\theta \rangle = \prod_{i\in I} \langle \varphi_t, f_i\rangle \prod_{j\in J} \langle g_j, \varphi_t\rangle \times \left\langle \prod_{i\in I^c} [a(f_i) - \langle f_i, \varphi_t^{\theta'}\rangle] \tilde{E}^t_{\theta'}, \prod_{j\in J^c} [a(g_j) - \langle g_j, \varphi_t^{\theta}\rangle] \tilde{E}^t_\theta \right\rangle .$$

We have, for $0 \le \#I, \#J < p$, by Cauchy-Schwarz inequality

$$\left|\langle \tilde{E}^t_{\theta'}, B^{Wick}_{I,J} \tilde{E}^t_\theta \rangle\right| \le \prod_{i\in I, j\in J} ||g_j||_{L^2(\mathbb{R})}\, ||f_i||_{L^2(\mathbb{R})} \times \left\| \prod_{i\in I^c} [a(f_i) - \langle f_i, \varphi_t^{\theta'}\rangle] \tilde{E}^t_{\theta'} \right\|_{\mathcal{F}} \times \left\| \prod_{j\in J^c} [a(g_j) - \langle g_j, \varphi_t^{\theta}\rangle] \tilde{E}^t_\theta \right\|_{\mathcal{F}} .$$

In the following we make use of the positive self-adjoint operator

$$\tilde{N} := N + 2\mathrm{Re}\langle z, \varphi_t\rangle^{Wick} + ||\varphi_t||^2 1 .$$

Observe that we have for any $\theta' \in [0, 2\pi]$ and $r \ge 1$,

$$\begin{aligned} \left\| \prod_{i=1}^{r} [a(f_i) - \langle f_i, \varphi_t^{\theta'}\rangle] \tilde{E}^t_{\theta'} \right\|_{\mathcal{F}} &= \left\| \prod_{i=1}^{r} a(f_i) (\tilde{N}+1)^{-p} \mathcal{W}(t)\Omega_0 \right\|_{\mathcal{F}} \\ &\le \left\| \prod_{i=1}^{r-1} a(f_i) (\tilde{N}+1)^{-p} a(f_r) \mathcal{W}(t)\Omega_0 \right\|_{\mathcal{F}} \\ &+ \left\| \prod_{i=1}^{r-1} a(f_i) [a(f_r), (\tilde{N}+1)^{-p}] \mathcal{W}(t)\Omega_0 \right\|_{\mathcal{F}} . \end{aligned}$$

We easily show that

$$\|a(f_r)\mathcal{W}(t)\Omega_0\|_{\mathcal{F}} \le ||f_r||_{L^2(\mathbb{R})} \sqrt{\varepsilon_n}\, \|\mathcal{W}(t)\|_{\mathcal{L}(\mathcal{G}_+, \mathcal{F}^1_+)} .$$

Furthermore, we have

$$\left\| [a(f_r), (\tilde{N}+1)^p] (\tilde{N}+1)^{-p} \right\|_{\mathcal{L}(\mathcal{F})} \le C\, \varepsilon_n ,$$

using (4.6.2) and the fact that $[a(f_r), (\tilde{N}+1)^p]$ is a Wick polynomial where we gained ε_n in its symbol, see [76, Proposition 2.7 (ii)]. Recall also that we have by the number estimate (4.2.2) and (4.6.2),

$$\left\| \prod_{i=1}^{r-1} a(f_i) (\tilde{N}+1)^{-p} \right\|_{\mathcal{L}(\mathcal{F})} \le C ,$$

uniformly in n and $\theta' \in [0, 2\pi]$. Therefore, we have

$$\left| \sum_{0 \le \#I, \#J < p} \frac{4^p \gamma_n^2}{(2\pi)^2} \int_{[0,2\pi]^2} e^{-i[(n-\#J)\theta - (n-\#I)\theta']} \langle \tilde{E}_{\theta'}^t ,\, B_{I,J}^{Wick} \, \tilde{E}_\theta^t \rangle \, d\theta d\theta' \right| \le C \, \gamma_n^2 \varepsilon_n \overset{n\to\infty}{\longrightarrow} 0 \; . \quad (4.7.3)$$

It still to control the terms $\#I = p, \#J = p - 1$ and $\#I = p - 1, \#J = p$ which are similar. In fact, remark that we have

$$\frac{4^p \gamma_n^2}{(2\pi)^2} \int_{[0,2\pi]^2} e^{-i[(n-p)\theta - (n-p+1)\theta']} \langle \tilde{E}_{\theta'}^t ,\, B_{I,\mathcal{N}_p}^{Wick} \, \tilde{E}_\theta^t \rangle \, d\theta d\theta' = \frac{4^p \gamma_n}{2\pi} \int_0^{2\pi} e^{i(n-p+1)\theta'} \langle \tilde{E}_{\theta'}^t ,\, B_{I,\mathcal{N}_p}^{Wick} \; e^{it/\varepsilon_n H_{\varepsilon_n}} \; \varphi_0^{\otimes(n-p)} \rangle \, d\theta' \, .$$

Now, a similar estimate as (4.7.3) yields that

$$\left| \frac{4^p \gamma_n^2}{(2\pi)^2} \int_{[0,2\pi]^2} e^{-i[(n-p)\theta - (n-p+1)\theta']} \; \langle E_{\theta'}^t ,\, B_{I,\mathcal{N}_p}^{Wick} \, \tilde{E}_\theta^t \rangle \; d\theta d\theta' \right| \le C \; \gamma_n \sqrt{\varepsilon_n} \overset{n\to\infty}{\longrightarrow} 0 \; .$$

Thus, we conclude that $\lim_{n\to\infty} \Gamma_n - b(\varphi_t) = 0$. □

Remark 4.7.1.
1) *Let $\gamma_{k,n}^t$ be the k-particle correlation functions, defined by (4.1.4), associated to the states $e^{-it/\varepsilon_n H_{\varepsilon_n}} \varphi_0^{\otimes n}$. Then Theorem 4.2.3 implies the following convergence in the trace norm*

$$\lim_{n\to\infty} \gamma_{k,n}^t = \varphi_t(x_1) \cdots \varphi_t(x_k) \; \overline{\varphi_t(y_1) \cdots \varphi_t(y_k)} \, .$$

2) *In terms of Wigner measures, introduced in [76, 75], Theorem 4.2.3 says that the sequence $(e^{-it/\varepsilon_n H_{\varepsilon_n}} \varphi_0^{\otimes n})_{n\in\mathbb{N}}$ admits a unique (Borel probability) Wigner measure μ_t given by*

$$\mu_t = \frac{1}{2\pi} \int_0^{2\pi} \delta_{e^{i\theta}\varphi_t} \, d\theta \, ,$$

where $\delta_{e^{i\theta}\varphi_t}$ is the Dirac measure on $L^2(\mathbb{R})$ at the point $e^{i\theta}\varphi_t$.

4.A Elementary estimate

Lemma 4.A.1. *For any $\alpha > 0$ and any $\Psi^{(n)} \in \mathcal{S}_s(\mathbb{R}^n)$, we have*

$$\int_{\mathbb{R}^{n-1}} |\Psi^{(n)}(x_2, x_2, \cdots, x_n)|^2 dx_2 \cdots dx_n \le \frac{\alpha}{\sqrt{2}} \langle D_{x_1}^2 \Psi^{(n)}, \Psi^{(n)} \rangle_{L^2(\mathbb{R}^n)} + \frac{\alpha^{-1}}{2\sqrt{2}} |\Psi^{(n)}|_{L^2(\mathbb{R}^n)}^2 \, . \quad (4.A.1)$$

Proof. Let $x', \xi' \in \mathbb{R}^{n-1}$ and $g \in \mathcal{S}(\mathbb{R}^n)$. Let us denote the Fourier transform of g by

$$\hat{g}(\xi) = \int_{\mathbb{R}^n} e^{-ix\xi} g(x)\, dx.$$

We have

$$g(0, x') = \frac{1}{(2\pi)^{n-1}} \int_{\mathbb{R}^{n-1}} e^{ix'\xi'} \left(\frac{1}{2\pi} \int_{\mathbb{R}} \hat{g}(\xi_1, \xi')\, d\xi_1 \right) d\xi' .$$

Cauchy-Schwarz inequality yields

$$\left| \int_{\mathbb{R}} \hat{g}(\xi_1, \xi')\, d\xi_1 \right|^2 \leq \int_{\mathbb{R}} \left|\hat{g}(\xi_1, \xi')\right|^2 (\alpha^{-1} + \alpha\xi_1^2)\, d\xi_1 \times \int_{\mathbb{R}} \frac{d\xi_1}{\alpha^{-1} + \alpha\xi_1^2} .$$

Therefore, we get

$$\begin{aligned} \int_{\mathbb{R}^{n-1}} \left|g(0, x')\right|^2 dx' &= \frac{1}{4\pi^2(2\pi)^{n-1}} \int_{\mathbb{R}^{n-1}} \left| \int_{\mathbb{R}} \hat{g}(\xi_1, \xi')\, d\xi_1 \right|^2 d\xi' \\ &\leq \frac{1}{2(2\pi)^n} \int_{\mathbb{R}^n} |\hat{g}(\xi_1, \xi')|^2 (\alpha^{-1} + \alpha\xi_1^2)\, d\xi_1 d\xi' . \end{aligned}$$

Set $g(x_1, \cdots, x_n) = \Psi^{(n)}(\frac{x_1+x_2}{\sqrt{2}}, \frac{x_2-x_1}{\sqrt{2}}, x_3, \cdots, x_n)$, we obtain

$$\begin{aligned} &\int_{\mathbb{R}^{n-1}} \left|\Psi^{(n)}(x_2, x_2, \cdots, x_n)\right|^2 dx_2 \cdots dx_n \\ &= \frac{1}{\sqrt{2}} \int_{\mathbb{R}^{n-1}} \left|g^{(n)}(0, x_2, \cdots, x_n)\right|^2 dx_2 \cdots dx_n \\ &\leq \frac{(2\pi)^{-n}}{2\sqrt{2}} \int_{\mathbb{R}^n} |\hat{g}^{(n)}(\xi_1, \xi')|^2 (\alpha^{-1} + \alpha\xi_1^2 + \alpha\xi_2^2)\, d\xi_1 d\xi' \\ &\leq \frac{(2\pi)^{-n}}{2\sqrt{2}} \int_{\mathbb{R}^n} |\hat{\Psi}^{(n)}(\xi_1, \xi')|^2 (\alpha^{-1} + \alpha\xi_1^2 + \alpha\xi_2^2)\, d\xi_1 d\xi' . \end{aligned}$$

Thus, by Plancherel's identity we obtain

$$\begin{aligned} &\int_{\mathbb{R}^{n-1}} |\Psi^{(n)}(x_2, x_2, \cdots, x_n)|^2 dx_2 \cdots dx_n \\ &\qquad \leq \frac{\alpha}{2\sqrt{2}} \langle (D_{x_1}^2 + D_{x_2}^2)\Psi^{(n)}, \Psi^{(n)} \rangle_{L^2(\mathbb{R}^n)} + \frac{\alpha^{-1}}{2\sqrt{2}} |\Psi^{(n)}|_{L^2(\mathbb{R}^n)}^2 . \end{aligned}$$

Thanks to the symmetry of $\Psi^{(n)}$, it is easy to see that

$$\langle (D_{x_1}^2 + D_{x_2}^2)\Psi^{(n)}, \Psi^{(n)} \rangle = 2\langle D_{x_1}^2 \Psi^{(n)}, \Psi^{(n)} \rangle .$$

Hence, we arrive at the claimed estimate (4.A.1). □

4.B Commutator theorems

Here we first recall an abstract regularity argument from Faris-Lavine work [85, Theorem 2].

Theorem 4.B.1. *Let A be a self-adjoint operator and let S be a positive self-adjoint operator satisfying*

- $\mathcal{D}(S) \subset \mathcal{D}(A)$,
- $\pm i\,[\langle A\Psi, S\Psi\rangle - \langle S\Psi, A\Psi\rangle] \leq c||S^{1/2}\Psi||^2$ *for all* $\Psi \in \mathcal{D}(S)$.

Then $\mathcal{Q}(S)$ is invariant by e^{-itA} for any $t \in \mathbb{R}$ and the inequality

$$||S^{1/2}e^{-itA}\Psi|| \leq e^{c|t|}\,||S^{1/2}\Psi||$$

holds true.

Next we recall the Nelson commutator theorem (see, *e.g.*, [102, Theorem X.36'],[101]) with a useful regularity property added as a consequence of Faris-Lavine's Theorem 4.B.1.

Theorem 4.B.2. *Let S be a self-adjoint operator on a Hilbert space $\mathcal{H}$ such that $S \geq 1$. Consider a quadratic form $a(.,.)$ with $\mathcal{Q}(a) = \mathcal{D}(S^{1/2})$ and satisfying:*

(i) $|a(\Psi,\Phi)| \leq c_1||S^{1/2}\Psi||\,||S^{1/2}\Phi||$ *for any* $\Psi, \Phi \in \mathcal{D}(S^{1/2})$;

(ii) $|a(\Psi, S\Phi) - a(S\Psi,\Phi)| \leq c_2||S^{1/2}\Psi||\,||S^{1/2}\Phi||$ *for any* $\Psi, \Phi \in \mathcal{D}(S^{3/2})$.

Then the linear operator $A : \mathcal{D}(A) \to \mathcal{H}$, $\mathcal{D}(A) = \{\Phi \in \mathcal{D}(S^{1/2}) : \mathcal{H} \ni \Psi \mapsto a(\Psi,\Phi)$ continuous $\}$ associated to the quadratic form $a(.,.)$ through the relation

$$\langle \Psi, A\Phi\rangle_{\mathcal{H}} = a(\Psi,\Phi) \text{ for all } \Psi \in \mathcal{D}(S^{1/2}), \Phi \in \mathcal{D}(A)$$

is densely defined and satisfies:

1. $\mathcal{D}(S) \subset \mathcal{D}(A)$ *and* $||A\Psi|| \leq c||S\Psi||$ *for any* $\Psi \in \mathcal{D}(S)$;
2. *A is essentially self-adjoint on any core of S;*
3. $e^{-it\tilde{A}}$ *preserves* $\mathcal{D}(S^{1/2})$ *with the inequality*

$$||S^{1/2}e^{-it\tilde{A}}\Psi|| \leq e^{c_2|t|}\,||S^{1/2}\Psi||$$

where $\tilde{A}$ denotes the self-adjoint extension of A.

Proof. The point (3) follows from Theorem 4.B.1 since its assumptions:

- $\mathcal{D}(S) \subset \mathcal{D}(A)$,

- $\pm i\,[\langle A\Psi, S\Psi\rangle - \langle S\Psi, A\Psi\rangle] \le c_2 ||S^{1/2}\Psi||^2$, for any $\Psi \in \mathcal{D}(S)$,

hold true using items 1), 2) and hypothesis (ii). □

We naturally associate to a self-adjoint operator $S \ge 1$ acting on a Hilbert space $\mathcal{H}$, a Hilbert rigging $\mathcal{H}_{\pm 1}$ where $\mathcal{H}_{+1}$ is defined as $\mathcal{D}(S^{1/2})$ endowed with the inner product

$$\langle \psi, \phi\rangle_{\mathcal{H}_{+1}} := \langle S^{1/2}\psi, S^{1/2}\phi\rangle_{\mathcal{H}},$$

and $\mathcal{H}_{-1}$ is the completion of $\mathcal{D}(S^{-1/2})$ with respect to the inner product

$$\langle \psi, \phi\rangle_{\mathcal{H}_{-1}} := \langle S^{-1/2}\psi, S^{-1/2}\phi\rangle_{\mathcal{H}}.$$

Assumption (ii) of Theorem 4.B.2 can be reformulated in some other slightly different ways.

Lemma 4.B.3. *Consider a self-adjoint operator S satisfying $S \ge 1$ with the associated Hilbert rigging $\mathcal{H}_{\pm 1}$ defined above. Let A be a symmetric bounded operator in $\mathcal{L}(\mathcal{H}_{+1}, \mathcal{H}_{-1})$, then the three following statements are equivalent,*

(1) *There exists $c > 0$ such that for any $\Psi, \Phi \in \mathcal{D}(S^{3/2})$,*

$$|\langle S\Psi, A\Phi\rangle - \langle A\Psi, S\Phi\rangle| \le c\, ||\Psi||_{\mathcal{H}_{+1}}\, ||\Phi||_{\mathcal{H}_{+1}},$$

(2) *There exists $c > 0$ such that for any $\Psi, \Phi \in \mathcal{D}(S^{1/2})$ and $\lambda > 0$,*

$$|\langle (\lambda S+1)^{-1}S\Psi, A(\lambda S+1)^{-1}\Phi\rangle - \langle A(\lambda S+1)^{-1}\Psi, (\lambda S+1)^{-1}S\Phi\rangle| \le c\, ||\Psi||_{\mathcal{H}_{+1}}\, ||\Phi||_{\mathcal{H}_{+1}},$$

(3) *There exists $c > 0$ such that for any $\Psi, \Phi \in \mathcal{D}(S^{1/2})$ and $\lambda > 0$,*

$$|\langle (\lambda S+1)^{-1}S\Psi, A\Phi\rangle - \langle A\Psi, (\lambda S+1)^{-1}S\Phi\rangle| \le c\, ||\Psi||_{\mathcal{H}_{+1}}\, ||\Phi||_{\mathcal{H}_{+1}}.$$

Proof. • (1)⇔(2):
Observe that if $\lambda > 0$ then $(\lambda S+1)^{-1}\mathcal{D}(S^{1/2}) \subset \mathcal{D}(S^{3/2})$. Assume (1) and let us prove (2) for $\Psi, \Phi \in \mathcal{D}(S^{1/2})$. Using (1) with $\tilde{\Psi} = (\lambda S+1)^{-1}\Psi \in \mathcal{D}(S^{3/2})$ and $\tilde{\Phi} = (\lambda S+1)^{-1}\Phi \in \mathcal{D}(S^{3/2})$, we obtain

$$\left|\langle S\tilde{\Psi}, A\tilde{\Phi}\rangle - \langle A\tilde{\Psi}, S\tilde{\Phi}\rangle\right| \le c\,\left\|(\lambda S+1)^{-1}\Psi\right\|_{\mathcal{H}_{+1}} \times \left\|(\lambda S+1)^{-1}\Phi\right\|_{\mathcal{H}_{+1}} \tag{4.B.1}$$

It is easy to see that the right hand side of (4.B.1) is bounded by $c||\Psi||_{\mathcal{H}_{+1}}||\Phi||_{\mathcal{H}_{+1}}$. Thus, we obtain (2). Now, to prove (2)⇒(1), we observe that $(\lambda S+1)\mathcal{D}(S^{3/2}) \subset \mathcal{D}(S^{1/2})$ and use (2) with $\Psi_\lambda = (\lambda S+1)\Psi \in \mathcal{D}(S^{1/2})$, $\Phi_\lambda = (\lambda S+1)\Phi \in \mathcal{D}(S^{1/2})$ such that $\Psi, \Phi \in \mathcal{D}(S^{3/2})$. Therefore, we get for $\lambda > 0$

$$|\langle S\Psi, A\Phi\rangle - \langle A\Psi, S\Phi\rangle| \le c\,\|\Psi_\lambda\|_{\mathcal{H}_{+1}} \times \|\Phi_\lambda\|_{\mathcal{H}_{+1}}. \tag{4.B.2}$$

Letting $\lambda \to 0$ in the right hand side of (4.B.2), we obtain (2).

• (2)$\Leftrightarrow$(3):

Let $\Psi, \Phi \in \mathcal{D}(S^{1/2})$ and $\lambda > 0$, we have as identity in $\mathcal{L}(\mathcal{H}_{+1}, \mathcal{H}_{-1})$

$$A(\lambda S + 1)(\lambda S + 1)^{-1} = A\lambda S(\lambda S + 1)^{-1} + A(\lambda S + 1)^{-1},$$

since $\lambda S(\lambda S + 1)^{-1} \in \mathcal{L}(\mathcal{H}_{+1})$ and $(\lambda S + 1)^{-1} \in \mathcal{L}(\mathcal{H}_{+1})$. Therefore, since $(\lambda S + 1)^{-1} S\Psi \in \mathcal{H}_{+1}$ and $(\lambda S + 1)^{-1} S\Phi \in \mathcal{H}_{+1}$, the following computation is justified

$$\begin{aligned}
&\langle (\lambda S + 1)^{-1} S\Psi, A\Phi\rangle - \langle A\Psi, (\lambda S + 1)^{-1} S\Phi\rangle \\
&= \langle (\lambda S + 1)^{-1} S\Psi, A(\lambda S + 1)(\lambda S + 1)^{-1}\Phi\rangle \\
&\quad - \langle A(\lambda S + 1)(\lambda S + 1)^{-1}\Psi, (\lambda S + 1)^{-1} S\Phi\rangle \\
&= \langle (\lambda S + 1)^{-1} S\Psi, A(\lambda S + 1)^{-1}\Phi\rangle - \langle A(\lambda S + 1)^{-1}\Psi, (\lambda S + 1)^{-1} S\Phi\rangle .
\end{aligned}$$

So, this shows the equivalence of the statements (2) and (3). □

4.C Non-autonomous Schrödinger equation

Consider the Hilbert rigging

$$\mathcal{H}_+ \subset \mathcal{H} \subset \mathcal{H}_- .$$

This means that $\mathcal{H}$ is a Hilbert space with an inner product $(.,.)_\mathcal{H}$ and $\mathcal{H}_+$ is a dense subspace of $\mathcal{H}$ which is itself a Hilbert space with respect to another inner product $(.,.)_{\mathcal{H}_+}$ such that

$$||u||_\mathcal{H} := \sqrt{(u,u)_\mathcal{H}} \leq ||u||_{\mathcal{H}_+} := \sqrt{(u,u)_{\mathcal{H}_+}} \qquad \forall u \in \mathcal{H}_+ .$$

The Hilbert space $\mathcal{H}_-$ is defined as the completion of $\mathcal{H}$ with respect to the norm

$$||u||_{\mathcal{H}_-} := \sup_{f \in \mathcal{H}_+, ||f||_{\mathcal{H}_+} = 1} |(f,u)_\mathcal{H}| . \tag{4.C.1}$$

This extends by continuity the inner product $(.,.)_\mathcal{H}$ to a sesquilinear form on $\mathcal{H}_- \times \mathcal{H}_+$ satisfying

$$|(\xi,u)_\mathcal{H}| \leq ||u||_{\mathcal{H}_+} \, ||\xi||_{\mathcal{H}_-} \quad \forall u \in \mathcal{H}_+, \forall \xi \in \mathcal{H}_- .$$

Furthermore, we have

$$||u||_{\mathcal{H}_+} = \sup_{\xi \in \mathcal{H}_-, ||\xi||_{\mathcal{H}_-} = 1} |(\xi,u)_\mathcal{H}| . \tag{4.C.2}$$

Let I be a closed interval of $\mathbb{R}$ and let $\big(A(t)\big)_{t\in I}$ denote a family of self-adjoint operators on $\mathcal{H}$ such that $\mathcal{D}(A(t)) \cap \mathcal{H}_+$ is dense in $\mathcal{H}_+$ and $A(t)$

are continuously extendable to bounded operators in $\mathcal{L}(\mathcal{H}_+, \mathcal{H}_-)$. We aim to solve the following abstract non-autonomous Schrödinger equation

$$\begin{cases} i\partial_t u = A(t)u\,, & t \in I \\ u(t=0) = u_0\,, \end{cases} \tag{4.C.3}$$

where $u_0 \in \mathcal{H}_+$ is given and $t \mapsto u(t) \in \mathcal{H}_+$ is the unknown. This is a particular case of the more general topic of solving non-autonomous Cauchy problems where $-iA(t)$ are infinitesimal generators of C_0-semigroups (see [104],[97]). We provide here a useful result (Theorem 4.C.2) which follows from the work of Kato [96].

Definition 4.C.1. We say that the map

$$I \times I \ni (t,s) \mapsto U(t,s)$$

is a unitary propagator of the problem (4.C.3) iff:
(a) $U(t,s)$ is unitary on $\mathcal{H}$,
(b) $U(t,t) = 1$ and $U(t,s)U(s,r) = U(t,r)$ for all $t,s,r \in I$,
(c) The map $t \in I \mapsto U(t,s)$ belongs to $C^0(I, \mathcal{L}(\mathcal{H}_+)) \cap C^1(I, \mathcal{L}(\mathcal{H}_+, \mathcal{H}_-))$ and satisfies

$$i\partial_t U(t,s)\psi = A(t)U(t,s)\psi, \quad \forall \psi \in \mathcal{H}_+, \forall t,s \in I.$$

Here $C^k(I, \mathfrak{B})$ denotes the space of k-continuously differentiable $\mathfrak{B}$-valued functions where $\mathfrak{B}$ is endowed with the strong operator topology.

Theorem 4.C.2. *Let I be a compact interval and let $\mathcal{H}_+ \subset \mathcal{H} \subset \mathcal{H}_-$ be a Hilbert rigging with $\big(A(t)\big)_{t\in I}$ a family of self-adjoint operators on $\mathcal{H}$ as above satisfying:*
(i) $I \ni t \mapsto A(t) \in \mathcal{L}(\mathcal{H}_+, \mathcal{H}_-)$ is norm continuous.
(ii) $\mathbb{R} \ni \tau \mapsto e^{i\tau A(t)} \in \mathcal{L}(\mathcal{H}_+)$ is strongly continuous.
(iii) There exists a family of Hilbertian norms $\big(||.||_t\big)_{t\in I}$ on $\mathcal{H}_+$ equivalent to $||.||_{\mathcal{H}_+}$ such that:

$$\exists c > 0, \forall \psi \in \mathcal{H}_+ : \quad ||\psi||_t \leq e^{c|t-s|}\, ||\psi||_s \quad \text{and} \quad ||e^{i\tau A(t)}\psi||_t \leq e^{c|\tau|} ||\psi||_t\,.$$

Then the non-autonomous Cauchy problem (4.C.3) admits a unique unitary propagator $U(t,s)$.
Moreover, the following estimate holds

$$\forall \psi \in \mathcal{H}_+, \quad ||U(t,s)\psi||_t \leq e^{2c|t-s|}\, ||\psi||_s\,.$$

Proof. We follow the same strategy as in [96] and split the proof into three steps. We assume, for reading convenience, that the interval I is of the form $[0,T], T > 0$ however the proof works exactly in the same way for any compact interval. Remark also that there is no restriction if we assume that $||.||_{\mathcal{H}_+} = ||.||_0$.

Propagator approximation:

Let $(t_0, \cdots, t_n)$ be a regular partition of the interval I with

$$t_j = \frac{jT}{n}, \quad j = 0, \cdots, n.$$

Consider the sequence of operator-valued step functions defined by

$$A_n(t) := A(T) 1_{\{T\}}(t) + \sum_{j=0}^{n-1} A(t_j)\, 1_{[t_j, t_{j+1}[}(t)\,,$$

for any $n \in \mathbb{N}^*$ and $t \in I$. Assumption (i) ensures that

$$\lim_{n\to\infty} ||A_n(t) - A(t)||_{\mathcal{L}(\mathcal{H}_+, \mathcal{H}_-)} = 0\,,$$

uniformly in $t \in I$. We now construct an approximating unitary propagator $U_n(t,s)$ as follows:

$$\begin{cases} \text{if } t_j \le t, s \le t_{j+1} \text{ then } U_n(t,s) = e^{-i(t-s)A(t_j)} \\ \text{if } t_j < s \le t_{j+1} < \cdots < t_l \le t < t_{l+1} \text{ then } U_n(t,s) = e^{-i(t-t_l)A(t_l)} \cdots e^{-i(t_{j+1}-s)A(t_j)} \\ \text{if } t_j < t \le t_{j+1} < \cdots < t_l \le s < t_{l+1} \text{ then } U_n(t,s) = e^{-i(t-t_{j+1})A(t_j)} \cdots e^{-i(t_l-s)A(t_l)}\,, \end{cases} \tag{4.C.4}$$

for any $j = 0, \cdots, n-1$ and $l = 1, \cdots, n$ with $j < l$.

By definition, the operators $U_n(t,s)$ are unitary on $\mathcal{H}$ for $t, s \in I$ and satisfy

$$U_n(t,t) = 1, \qquad U_n(t,s)^* = U_n(s,t)\,. \tag{4.C.5}$$

Moreover, one can first check that

$$U_n(t,s)U_n(s,r) = U_n(t,r) \text{ for } r \le s \le t, \text{ with } t, s, r \in I$$

and then extend it for any $(t,s,r) \in I^3$ with the help of (4.C.5). Therefore, $U_n(t,s)$ satisfy the properties (a)-(b) of Definition 4.C.1. Again by (4.C.4) and assumptions (i)-(ii) we have

$$i\partial_t U_n(t,s)\psi \;=\; A_n(t)U_n(t,s)\psi \text{ and } -i\partial_s U_n(t,s)\psi \;=\; U_n(t,s)A_n(s)\psi, \tag{4.C.6}$$

for any $\psi \in \mathcal{H}_+$ and any $t, s \neq t_j$, $j = 0, \cdots, n$. In fact, we have for $\psi \in \mathcal{H}_+$ as identity in $\mathcal{H}_-$

$$e^{-i\tau A(s)}\psi = \psi - iA(s) \int_0^\tau e^{-irA(s)}\psi\, dr\,, \tag{4.C.7}$$

since this holds first for $\psi \in \mathcal{D}(A(s)) \cap \mathcal{H}_+$ and then extends by density of $\mathcal{D}(A(s)) \cap \mathcal{H}_+$ in $\mathcal{H}_+$ using the uniform boundedness principal. By (4.C.7) we have

$$||\frac{e^{-i\tau A(s)}\psi - \psi}{\tau} + iA(s)\psi||_{\mathcal{H}_-} \leq \frac{1}{\tau}||A(s)||_{\mathcal{L}(\mathcal{H}_+,\mathcal{H}_-)} \left|\int_0^\tau ||e^{-irA(s)}\psi - \psi||_{\mathcal{H}_+}\, dr\right|$$

and hence using assumption (ii), we show the differentiability of $\tau \mapsto e^{-i\tau A(s)}\psi$ for $\psi \in \mathcal{H}_+$.

Convergence of the approximation:
Assumption (iii) implies that

$$||e^{-is_nA(t_n)} \cdots e^{-is_1A(t_1)}\psi||_T \leq e^{cT}e^{c(s_1+\cdots+s_n)}||\psi||_0\,,$$

and

$$||e^{-is_1A(t_1)} \cdots e^{-is_nA(t_n)}\psi||_0 \leq e^{cT}e^{c(s_1+\cdots+s_n)}||\psi||_T\,,$$

for any $s_j \geq 0$, $j = 1, \cdots, n$. Hence, using the equivalence of the norms $||.||_0 = ||.||_{\mathcal{H}_+}$ and $||.||_T$ one shows the existence of $M > 0$ ($M = e^{2cT}$) such that

$$||U_n(t,s)||_{\mathcal{L}(\mathcal{H}_+)} \leq M\ e^{c|t-s|} \text{ and by duality } ||U_n(t,s)||_{\mathcal{L}(\mathcal{H}_-)} \leq M\ e^{c|t-s|}\,. \tag{4.C.8}$$

Furthermore, the same argument above yields

$$||U_n(t,s)\psi||_t \leq e^{2c(|t-s|+T/n)}||\psi||_s. \tag{4.C.9}$$

Using (4.C.6) we obtain for any $\psi \in \mathcal{H}_+$

$$\partial_r\left[U_n(t,r)U_m(r,s)\psi\right] = i\, U_n(t,r)[A_n(r) - A_m(r)]U_m(r,s)\psi\,, \tag{4.C.10}$$

for $r \neq \frac{jT}{n}, r \neq \frac{jT}{m}$ with $j = 1, \cdots, \max(n,m)$. Integrating (4.C.10) we get the identity

$$U_m(t,s)\psi - U_n(t,s)\psi = i\int_s^t U_n(t,r)\left[A_n(r) - A_m(r)\right]U_m(r,s)\psi\, dr\,.$$

Now (4.C.8) yields

$$\begin{aligned}||U_m(t,s) - U_n(t,s)||_{\mathcal{L}(\mathcal{H}_+,\mathcal{H}_-)} \\ \leq M^2|t-s|e^{2c|t-s|}\sup_{r\in I}||A_m(r) - A_n(r)||_{\mathcal{L}(\mathcal{H}_+,\mathcal{H}_-)}\,.\end{aligned} \tag{4.C.11}$$

Therefore, for any $t, s \in I$, the sequence $U_n(t,s)$ converges in norm to a bounded linear operator $U(t,s) \in \mathcal{L}(\mathcal{H}_+,\mathcal{H}_-)$. Since $U_n(t,s)$ are norm bounded operators on $\mathcal{H}_-$ uniformly in n, it follows by (4.C.8) that they converge strongly to an operator in $\mathcal{L}(\mathcal{H}_-)$ continuously extending $U(t,s)$. Moreover, this strong convergence yields

$$\lim_{n\to\infty}(\phi, U_n(t,s)\psi)_{\mathcal{H}} = (\phi, U(t,s)\psi)_{\mathcal{H}} \quad \forall\psi\in\mathcal{H}_+, \forall\phi\in\mathcal{H}_+ .$$

Thus, using (4.C.8), we obtain

$$|(\phi, U(t,s)\psi)_{\mathcal{H}}| \le Me^{c|t-s|}||\phi||_{\mathcal{H}_-}\ ||\psi||_{\mathcal{H}_+} .$$

Hence, it is easy to see by (4.C.2) that

$$||U(t,s)||_{\mathcal{L}(\mathcal{H}_+)} \le Me^{c|t-s|} .$$

A similar argument yields

$$||U(t,s)||_{\mathcal{L}(\mathcal{H})} \le 1 . \tag{4.C.12}$$

Now, since $U_n(t,s)$ satisfy part (b) of Definition 4.C.1, we easily conclude that

$$U(t,t) = 1, \quad U(t,r)U(r,s) = U(t,s), \quad t,s,r\in I, \tag{4.C.13}$$

by strong convergence in $\mathcal{L}(\mathcal{H}_-)$. Furthermore, combining (4.C.12) and (4.C.13) we show the unitarity of $U(t,s)$ on $\mathcal{H}$. Thus, we have proved that $U(t,s)$ satisfy (a)-(b) of Definition 4.C.1.

For any $\psi\in\mathcal{H}_+$, the continuity of the map $I\ni t\mapsto U_n(t,s)\psi\in\mathcal{H}_-$ follows from the definition of $U_n(t,s)$. Now, we prove

$$\lim_{t\to s}(\phi, U(t,s)\psi)_{\mathcal{H}} = (\phi,\psi)_{\mathcal{H}} \quad \forall\psi\in\mathcal{H}_+, \forall\phi\in\mathcal{H}_- ,$$

by applying an $\epsilon/3$ argument when writing

$$\begin{aligned}
&|(\phi, U(t,s)\psi)_{\mathcal{H}} - (\phi,\psi)_{\mathcal{H}}| \\
&\qquad \le ||\phi-\phi_\kappa||_{\mathcal{H}_-}||U(t,s)\psi||_{\mathcal{H}_+} + |(\phi_\kappa, [U(t,s)-U_n(t,s)]\psi)_{\mathcal{H}}| \\
&\qquad\qquad + |(\phi_\kappa, [U_n(t,s)-1]\psi)_{\mathcal{H}}| + ||\phi-\phi_\kappa||_{\mathcal{H}_-}\|\psi\|_{\mathcal{H}_+} ,
\end{aligned}$$

where $\phi_\kappa\to\phi$ in $\mathcal{H}_-$ and $\phi_\kappa\in\mathcal{H}_+$. Therefore, by the duality $(\mathcal{H}_+)'\simeq\mathcal{H}_-$, we get the weak limit

$$w-\lim_{t\to s} U(t,s) = 1 ,$$

in $\mathcal{L}(\mathcal{H}_+)$. Now, observe that when $t\to s$ we can show by (4.C.8) that

$$\limsup_{t\to s}\ ||U(t,s)\psi||_{\mathcal{H}_+} \le ||\psi||_{\mathcal{H}_+} .$$

So, we conclude that

$$\limsup_{t\to s} \ ||U(t,s)\psi-\psi||^2_{\mathcal{H}_+} \leq \limsup_{t\to s} \Big(||\psi||^2_{\mathcal{H}_+} + ||U(t,s)\psi||^2_{\mathcal{H}_+} - 2\mathrm{Re}(\psi, U(t,s)\psi)_{\mathcal{H}_+} \Big) = 0 \,.$$

This gives the continuity of $I \ni t \mapsto U(t,s)\psi \in \mathcal{H}_+$ since we have in $\mathcal{H}_+$

$$s-\lim_{t\to r} U(t,s) = s-\lim_{t\to r} U(t,r)U(r,s) = U(r,s).$$

By differentiating $e^{-i(t-r)A(s)}U_m(r,s)\psi$ with $\psi \in \mathcal{H}_+$ and then integrating w.r.t. r, we get

$$U_m(t,s)\psi - e^{-i(t-s)A(s)}\psi = i\int_s^t e^{-i(t-r)A(s)}[A(s)-A_m(r)]U_m(r,s)\psi \, dr \,.$$

Letting $m \to \infty$ in the latter identity and estimating as in (4.C.11), one obtains

$$||U(t,s)\psi - e^{-i(t-s)A(s)}\psi||_{\mathcal{H}_-} \leq M^2 e^{2c|t-s|}\left|\int_s^t ||A(s)-A(r)||_{\mathcal{L}(\mathcal{H}_+,\mathcal{H}_-)}\, dr\right| \, ||\psi||_{\mathcal{H}_+}.$$

Using the fact that

$$\lim_{t\to s} \frac{1}{|t-s|}\int_s^t ||A(s)-A(r)||_{\mathcal{L}(\mathcal{H}_+,\mathcal{H}_-)} dr = 0 \text{ and } \lim_{t\to s} \frac{e^{-i(t-s)A(s)}\psi-\psi}{t-s} = -iA(s)\psi$$

it holds that

$$\lim_{t\to s}\left\|\frac{U(t,s)\psi-\psi}{t-s}+iA(s)\psi\right\|_{\mathcal{H}_-} = 0.$$

Thus, we obtain with the help of (4.C.13)

$$i\partial_s U(s,r)\psi = \lim_{t\to s}\frac{U(t,s)U(s,r)\psi - U(s,r)\psi}{t-s} = A(s)U(s,r)\psi,$$

for any $\psi \in \mathcal{H}_+$ and any $r,s \in I$. Hence we have proved the existence of a unitary propagator $U(t,s)$ for the non-autonomous Cauchy problem (4.C.3).

Uniqueness:

Suppose that $V(t,s)$ is a unitary propagator for (4.C.3). By differentiating $U_n(t,r)V(r,s)\psi$, $\psi \in \mathcal{H}_+$ with respect to r we get

$$V(t,s)\psi - U_n(t,s)\psi = i\int_s^t U_n(t,r)[A_n(r)-A(r)]V(r,s)\psi.$$

Using a similar estimate as (4.C.11) we obtain

$$\|V(t,s)\psi - U_n(t,s)\psi\|_{\mathcal{H}_+}$$
$$\leq M e^{c|t-s|} \sup_{r\in[s,t]} \|V(r,s)\|_{\mathcal{L}(\mathcal{H}_+)} \left| \int_s^t ||A(r) - A_n(r)||_{\mathcal{L}(\mathcal{H}_+,\mathcal{H}_+)} dr \right| \, ||\psi||_{\mathcal{H}_+}$$

and since the r.h.s. vanishes when $n \to \infty$ we conclude that $V(t,s) = U(t,s)$. Finally, the uniform boundedness principle, equivalence of norms $||.||_t, ||.||_{\mathcal{H}_+}$ and the inequality (4.C.9) give us the claimed estimate,

$$\forall \psi \in \mathcal{H}_+, \quad ||U(t,s)\psi||_t \leq \liminf_{n\to\infty} \, ||U_n(t,s)\psi||_t \leq e^{2c|t-s|} ||\psi||_s \, .$$

□

Remark 4.C.3. *It also follows that* $(t,s) \mapsto U(t,s) \in \mathcal{L}(\mathcal{H}_+)$ *is jointly strongly continuous.*

In the following we provide a more effective formulation of the above result (Theorem 4.C.2) which appears as a time-dependent version of the Nelson commutator theorem (see, *e.g.*, [101], [102] and Theorem 4.B.2).

We associate to each family of self-adjoint operators $\{S(t)_{t\in I}, S\}$ on $\mathcal{H}$ such that $S \geq 1$, $S(t) \geq 1$ and $\mathcal{D}(S(t)^{1/2}) = \mathcal{D}(S^{1/2})$ for any $t \in I$, a Hilbert rigging $\mathcal{H}_{\pm 1}$ defined as the completion of $\mathcal{D}(S^{\pm 1/2})$ with respect to the inner product

$$\langle \psi, \phi \rangle_{\mathcal{H}_{\pm 1}} = \langle S^{\pm 1/2}\psi, S^{\pm 1/2}\phi \rangle_{\mathcal{H}}. \tag{4.C.14}$$

Corollary 4.C.4. *Let* $I \subset \mathbb{R}$ *be a closed interval and let* $\{S(t)_{t\in I}, S\}$ *be a family of self-adjoint operators on a Hilbert space* $\mathcal{H}$ *such that:*

- $S \geq 1$ *and* $S(t) \geq 1$, $\forall t \in I$,
- $\mathcal{D}(S(t)^{1/2}) = \mathcal{D}(S^{1/2})$, $\forall t \in I$, *and consider the associated Hilbert rigging* $\mathcal{H}_{\pm 1}$ *given by (4.C.14).*

Let $\{A(t)\}_{t\in I}$ *be a family of symmetric bounded operators in* $\mathcal{L}(\mathcal{H}_{+1}, \mathcal{H}_{-1})$ *satisfying:*

- $t \in I \mapsto A(t) \in \mathcal{L}(\mathcal{H}_{+1}, \mathcal{H}_{-1})$ *is norm continuous.*

Assume that there exists a continuous function $f : I \to \mathbb{R}_+$ *such that for any* $t \in I$*, we have:*
(i) for any $\psi \in \mathcal{D}(S(t)^{1/2})$,

$$|\partial_t \langle \psi, S(t)\psi \rangle| \leq f(t) \, ||S(t)^{1/2}\psi||^2 \, ;$$

(ii) for any $\Phi, \Psi \in \mathcal{D}(S(t)^{3/2})$,

$$|\langle S(t)\Psi, A(t)\Phi\rangle - \langle A(t)\Psi, S(t)\Phi\rangle| \leq f(t)\, ||S(t)^{1/2}\Psi||\; ||S(t)^{1/2}\Phi||.$$

Then the non-autonomous Cauchy problem (4.C.3) admits a unique unitary propagator $U(t,s)$*. Moreover, we have*

$$||S(t)^{1/2}U(t,s)\psi|| \leq e^{2\,|\int_s^t f(\tau)d\tau|}\;\; ||S(s)^{1/2}\psi||\,.$$

In addition, if we have $c_1, c_2 > 0$ *such that* $c_1 S \leq S(t) \leq c_2 S$ *for* $t \in I$*, then there exists* $c > 0$ *such that*

$$||U(t,s)||_{\mathcal{L}(\mathcal{H}_{+1})} \leq c\; e^{2|\int_s^t f(\tau)\mathrm{d}\tau|}\,, \quad \forall t \in I\,. \tag{4.C.15}$$

Proof. First observe that the operator $A(t)$ satisfies the hypothesis of Nelson's commutator theorem (Theorem 4.B.2) for any $t \in I$. Hence, we conclude that $A(t)$ is essentially self-adjoint on $\mathcal{D}(S(t)^{3/2})$ which is dense in $\mathcal{H}_{+1}$. We keep the same notation for its closure. Moreover, the unitary group $e^{i\tau A(t)}$ preserves $\mathcal{H}_{+1}$ and we have the estimate

$$||S(t)^{1/2}e^{i\tau A(t)}\psi||_{\mathcal{H}} \leq e^{f(t)|\tau|}\;||\psi||_{\mathcal{H}}\,. \tag{4.C.16}$$

Now, observe that $t \mapsto e^{-itA(s)}\psi \in \mathcal{H}_{+1}$ is weakly continuous for any $\psi \in \mathcal{H}_+$. This holds using a $\eta/3$-argument with the help of the estimate

$$\begin{aligned}&\left|\langle f, (e^{-itA(s)} - 1)\psi\rangle\right| \\ &\qquad\leq (1 + e^{c(|t|+1)})\,||f - f_\kappa||_{\mathcal{H}_{-1}}\,||\psi||_{\mathcal{H}_{+1}} + \left|\langle (e^{itA(s)} - 1)f_\kappa, \psi\rangle\right|\end{aligned}$$

where $f_\kappa \in \mathcal{H}$ is a sequence convergent to f in $\mathcal{H}_{-1}$ and t is near 0. Since strong and weak continuity of the group of bounded operators $e^{-itA(s)}$ in $\mathcal{L}(\mathcal{H}_{+1})$ are equivalent, we conclude that assumption (ii) of Theorem 4.C.2 holds true.

By assumption (ii), we also have

$$\left|\frac{d}{dt}||S(t)^{1/2}\psi||^2\right| \leq f(t)||S(t)^{1/2}\psi||^2\,.$$

Hence, by Gronwall's inequality we have

$$||S(t)^{1/2}\psi||^2 \leq e^{|\int_s^t f(\tau)d\tau|}||S(s)^{1/2}\psi||^2, \quad \forall t, s \in I. \tag{4.C.17}$$

Now, we use Theorem 4.C.2 with the Hilbert rigging

$$\mathcal{H}_+ = \mathcal{H}_{+1} \subset \mathcal{H} \subset \mathcal{H}_- = \mathcal{H}_{-1}$$

and the family of equivalent norms on $\mathcal{H}_+$ given by

$$||\psi||_t := ||S(t)^{1/2}\psi||_{\mathcal{H}}.$$

Indeed, assumptions (i)-(iii) of Theorem 4.C.2 are satisfied in any compact subinterval of I with the help of (4.C.17)-(4.C.16). Therefore, we obtain existence and uniqueness of a unitary propagator $U(t,s)$ of the Cauchy problem (4.C.3) in the whole interval I with the following estimate

$$||U(t,s)\psi||_t \leq e^{2|t-s| \max_{\tau\in\Delta(t,s)} f(\tau)} \; ||\psi||_s ,$$

for any $t, s \in I$ and where $\Delta(t,s)$ stands for the interval of extremities t, s.

Using the multiplication law of the propagator, we obtain for any partition $(t_0, \cdots, t_n)$ of the interval $\Delta(t,s)$ the inequality

$$||U(t,s)\psi||_t \leq \prod_{j=0}^{n-1} e^{2\,\frac{|t-s|}{n} \max_{\tau\in\Delta_j} f(\tau)} \; ||\psi||_s ,$$

where Δ_j are the subintervals $[t_j, t_{j+1}]$. Since f is continuous, by letting $n \to \infty$, we get

$$||U(t,s)\psi||_t \leq e^{2\,|\int_s^t f(\tau)d\tau|} \; ||\psi||_s .$$

Finally, the assumption $c_1 S \leq S(t) \leq c_2 S$ for $t \in I$, allows to involve the norm $||.||_{\mathcal{H}_{+1}}$. Thus we have

$$\begin{aligned} &||U(t,s)\psi||_{\mathcal{H}_{+1}} \\ &\leq \frac{1}{\sqrt{c_1}}||U(t,s)\psi||_t \leq \frac{1}{\sqrt{c_1}} e^{2\,|\int_s^t f(\tau)d\tau|} \; ||\psi||_s \leq \sqrt{\frac{c_2}{c_1}} \; e^{2\,|\int_s^t f(\tau)d\tau|} \; ||\psi||_{\mathcal{H}_{+1}} . \end{aligned}$$

□

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Résumé

La dérivation d'équations cinétiques consiste à obtenir, à partir d'un modèle microscopique décrivant un système physique donné, des équations d'évolution contenant les informations perti- nentes d'un point de vue macroscopique sur ce système. Dans cette thèse on s'intéresse, dans des cas particuliers, à la dérivation d'équations cinétiques par des méthodes utilisant le formalisme de la théorie quantique des champs (QFT) et le calcul semi-classique en dimension finie et infinie. Après une introduction générale, on traite dans la seconde partie de la dérivation de l'équation de Boltzmann linéaire pour une particule dans un champ aléatoire Gaussien, dans la limite de faible densité (ou de faible couplage). On considère des données initiales plus générales que dans les travaux de Erdös et Yau sur le même sujet mais on renouvelle l'aléa pour obtenir le caractère Markovien de l'évolution. On démontre dans la troisième partie une formule décrivant l'évolution, pour un Hamiltonien quantique quadratique dépendant du temps, d'une observable quantifiée à l'aide de la quantification de Wick. Cette formule est valable en dimension finie ou infinie. Enfin la quatrième partie est un travail conjoint avec Zied Ammari. On y considère des bosons interagissant via un potentiel delta, dans la limite de champ moyen, en dimension un. On dérive de ce modèle l'équation de Schrödinger non-linéaire cubique défocalisante.

Abstract

The derivation of a kinetic equation is the justification from a microscopic model describing a given physical system of an evolution equation containing the relevant information at a macroscopic scale on this system. In this PhD thesis we study, on some particular cases, the derivation of kinetic equations with the framework of quantum field theory (QFT) and semiclassical calculus. After a general introduction, the second part is dedicated to the derivation of the linear Boltzmann equation for a particle in a Gaussian random field, within the low density (or weak interaction) limit. More general initial data are considered than in the work of Erdös and Yau on the same subject, but a renewal of the random field is used to get the Markovian properties of the evolution. In the third part a proof is given of a formula describing the evolution of a Wick quantized observable for a dynamic defined by a quadratic quantum time-dependent Hamiltonian. This formula holds both in finite and infinite dimension. The fourth part is a joint work with Zied Ammari devoted to the derivation of the defocusing cubic nonlinear Schrödinger equation in dimension one, for bosons interacting via a delta potential, within the mean field limit.