Coherent state quantization for conjugated variables

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QUANTIFICATION DE VARIABLES CONJUGUÉES PAR ÉTATS COHÉRENTS

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Présentation

La convergence entre la mécanique classique et la mécanique quantique pose un problème naturel d'interprétation qui a soulevé de longs débats tout au long du siècle dernier. La formulation mathématique établie par Dirac et von Neumann a fait ses preuves en montrant une capacité predictive d'une extreme précision. Cependant, dans le sens et dans la définition des quantités physiques classiques du formalisme quantique demeurent quelques inconsistances, même dans les modèles les plus simples.

Ce travail se concentre sur la méthode de quantification. La façon de procéder dite *canonique* consiste à prendre une paire de variables classiques conjuguées, l'impulsion et la position comme l'exemple le plus commun, et à identifier leur crochet de Poisson, c'est à dire la structure symplectique de l'espace des phases, au commutateur des observables quantiques correspondantes. Ceci donne à ces observables une structure algébrique et implique les inégalités de Heisenberg. Mais la définition de ces quantités doit être faite avec soin. En suivant le formalisme, les observables sont des opérateurs auto-adjoints qui agissent sur un espace d'Hilbert particulier. Les valeurs de ces observables s'expriment comme des résolutions spectrales de ces opérateurs et doivent être en concordance avec les limites du système physique. Notamment, un Hamiltonien avec un sens physique est toujours borné par dessous, et la configuration spatiale peut imposer la définition d'un opérateur de position borné ou semi-borné. Ces restrictions, qui affectent la définition de l'opérateur auto adjoint conjugué, ont ouvert un large débat autour de sa définition. Cette situation est présentée dans un théorème dû à W. Pauli qui explique qu'on ne peut pas définir un opérateur auto-adjoint avec un spectre semi-borné s'il est conjugué à une autre observable avec un spectre sans bornes. Ce théorème est valable si on prête une attention particulière aux domaines des opérateurs, mais soulève la question de la nécessité de définir autrement des quantités physiquement significatives. De cette façon la voie reste ouverte à une méthode alternative de quantification, du moment que le lien canonique entre la mécanique classique et quantique demeure problématique.

Le point de vue adopté dans ce travail assume que les valeurs d'une observable quantique ne sont pas nécessairement décrites par la résolution spectrale sur l'ensemble orthogonal de ses vecteurs propres mais, plus généralement, comme des valeurs moyennes sur une représentation diagonale de l'opérateur associé dans un ensemble non orthogonal d'états dans l'espace de Hilbert. Cette idée est déjà présente dans la mesure d'observables dans des mélanges statistiques d'états, pris en tant que mesures POVM (Positive Operator Valued Measurements) en opposition à la traditionnelle mesure à valeurs projecteurs (PV) de von Neumann. L'ensemble d'états dans lequel l'opérateur auto-adjoint est exprimé peut etre aussi grand qu'on le souhaite, à condition que la somme, ou l'intégrale, sur la totalité de l'ensemble respecte la normalisation qui impose l'interprétation probabiliste de Born, cet à dire, l'ensemble d'états doit être une résolution de l'identité dans l'espace où il habite. En d'autres mots, les systèmes surcomplets sont, en principe, aussi bons que n'importe quel autre système complet de vecteurs pour décrire un opérateur. La question revient naturellement sur quel type de famille utiliser et de quelle manière trouver celles qui ont un sens physique. Les états cohérents pour l'oscillateur harmonique constituent une de ces familles. Leur importance et leur clair sens physique à l'échelle quantique et classique donne un aperçu des usages possibles de sa généralisation. Un effort notable à été fait pour systématiser la définition des états de ce type dans une grande quantité de configurations utilisant plusieurs de ses propriétés et des symétries des systèmes physiques où ils apparaissent. Dans ce travail, nous nous concentreront seulement sur la résolution de l'identité.

La quantification par états cohérents se fonde sur le principe que l'ensemble des états cohérents peut etre indexé par un paramètre discret associé à un famille de vecteurs orthogonaux (les vecteurs propres du Hamiltonien pour l'oscillateur harmonique) et une variable complexe continue (la localisation dans l'espace des phases dans le même exemple). La liberté de choisir la variété dans laquelle le paramètre continu prend des valeurs et le choix de l'ensemble orthogonal des états donne la liberté d'ajuster la méthode à plusieurs cas particuliers. C'est en effet cette paire de paramètres qui rend les états cohérents des bons candidats à traduire les opérateurs indexés par un ensemble discret de valeurs vers des fonctions à variable réelle qui pourrait correspondre à ces contreparties classiques. Par contre, une observable classique, c'est à dire, une fonction réelle, peut trouver par ce moyen un opérateur auto-adjoint bien défini utilisable dans la mécanique quantique. Ceci est important dans les cas où l'auto adjonction est compromise, comme dans les paires conjuguées impliquées dans le théorème de Pauli. Des exemples importants du point de vue théorique et physique ont été choisis dans le but d'explorer les possibilités de cette méthode.

Ce travail se compose de deux parties principales. La première partie est subdivisée en trois chapitres : le premier chapitre contient des outils de base de la mécanique quantique et propose une révision de la théorie sur laquelle repose la définition d'observable quantique, en particulier en ce qui concerne les paires conjuguées. Ensuite, dans le deuxième chapitre, la définition d'état cohérent est revisitée. Enfin, dans le troisième chapitre, j'expose la méthode de quantification par états cohérents.

Dans la deuxième partie, subdivisée en quatre chapitres, quatre cas particuliers sont abordés à partir de l'application de la méthode proposée pour lesquels nous explorons, entre autre, la limite classique. Dans le quatrième chapitre, se trouve un tout premier exemple qui illustre la définition d'un opérateur de phase conjugué à l'action. Cette application donne une alternative à l'opérateur de phase de Pegg-Barnet [32] qui converge analytiquement vers la limite classique. L'opérateur de phase est construit dans un sous-espace fini de Hilbert de l'espace de Hilbert des séries de Fourier. L'étude de la limite pour la dimension infinie des valeurs moyennes de certaines observables mène à une convergence plus simple vers les relations canoniques de commutation. Ceci ouvre la possibilité de définir des phases relatives dans des systèmes à plusieurs niveaux utilisés en calcul quantique.

Le cinquième chapitre présente une construction d'opérateurs de phase relative pour le groupe $SU(N)$ qui pourrait avoir des applications intéressantes.

Dans le sixième chapitre, nous analysons la quantification du mouvement dans le puits infini de potentiel, où l'opérateur d'impulsion problématique est bien défini. Une famille nouvelle d'états cohérents vectoriels à deux composants permet une quantification consistante de l'espace des phases classique pour une particule dans ce potentiel. J'y explore les observables basiques telles que la position, l'énergie, et une version quantique de l'impulsion problématique. Nous prenons en considération, en outre, leurs valeurs moyennes dans des états cohérents et leur dispersion quantique.

Dans le septième chapitre, en guise de dernier exemple, un opérateur de temps pour une particule libre est proposé. Ce modèle d'horloge quantique utilise des états cohérents sur des demi-plans de Poincaré. Ces états cohérents sont du type $SU(1,1)$. Nous analysons les propriétés fonctionnelles des opérateurs $\widehat{q}$ et $\widehat{p}$, versions quantiques des coordonnés classiques, l'opérateur d'énergie $H = \widehat{p^2}/2$, l'opérateur de temps intrinsèque $\widehat{T}$ défini comme la quantification de la fonction $\dfrac{q}{p}$, avec $p \neq 0$, et finalement les commutateurs $[\widehat{q}, \widehat{p}]$ et $[\widehat{T}, \widehat{H}]$.

Les travaux sur l'opérateur de phase et sur le puits infini ont abouti à la publication de deux articles [41] [19] et à la participation à deux conférences et trois séminaires.

Introduction

The convergence between classical and quantum mechanics is a natural problem of interpretation that has raised long debates throughout the last century. The mathematical formalism established by Dirac and von Neumann has a very accurate predictive power but the meaning and the mathematical form of classical physical quantities in the quantum formalism have had some inconsistencies even in the simplest of scholar models.

In this work we focus on the quantization method. The so-called *canonical* way to proceed is to take some conjugated pair of classical variables, position and momentum as the trivial example, and to identify their Poisson bracket, that is the symplectic structure of the phase space, to the commutator of their corresponding quantum observables. This gives an algebraic structure to these observables and implies the well known Heisenberg inequalities. But more care has to be taken in the definition of these quantities. Following the formalism, observables are self-adjoint operators that act in a particular Hilbert space. The values of these observables come as spectral resolutions of these operators and have to be in accord to the limits of the physical system. Namely, a physical relevant Hamiltonian is always lower-bounded, and the spatial configuration may need the definition of bounded or semi-bounded position operators. These restrictions affect the definition of the conjugated self-adjoint operator and opened the discussion on how to define them. The situation is stated in a theorem by Pauli [43] and implies for the case of the Hamiltonian that no self-adjoint operator with semi-bounded spectrum can be defined if it is conjugated to another observable with an unbounded spectrum. The validity of this theorem depends on a careful attention on the domain of the operators but rises question on the need of an alternative way of defining physical relevant quantities, and since it affects the canonical link between classical and quantum mechanics, it opens the way to a new quantization protocol.

The point of view adopted in this work implies the assumption that the values of a quantum observable are not necessarily described by its spectral resolution on the orthogonal set of its eigenvectors but, more generally by a mean value over a diagonal representation of the associated operator on a set of nonorthogonal states in the Hilbert space. This idea is already present in the measurement of observables in statistical mixtures as a Positive Operator Valued Measure (POVM) versus the traditional von Neumann Projection

Valued (PV) Measures. The set of states on which the self-adjoint operator is expressed can be as large as we want whenever the sum, or integration, over the whole set respects the probability normalization that requires the Born probabilistic interpretation, that is the set must be a resolution of the identity in the space where it lives. In other words, overcomplete systems are in principle as good as any complete set of vectors to describe an operator. The point is of course what kind of family to use and how to find the ones with physical relevance. Coherent states for the harmonic oscillator are one of such families. Their relevance and clear meaning in quantum and classical realms give a good glimpse of their possibilities and the possible uses of their generalization. A great effort has been done to systematize the definition of such states in a wide set of configurations using different properties of the states and the symmetries of the physical systems in which they appear, but here we will focus just on the resolution of the identity.

Coherent state quantization uses the fact that the set of coherent states can be labeled by a discrete parameter associated to a set of orthogonal vectors (the eigenvectors of the Hamiltonian in harmonic oscillator) and a continuous complex variable (localization on the phase space in the same example). The freedom of choice on the manyfold on which the continuous parameter takes values and the set of orthogonal states give the freedom to adjust the method to different particular cases. This pair of parameters are what makes them good candidates for translating operators labeled by a discrete set of values into real valued functions that could correspond to their classical counterparts. In the opposite sense, a classical observable, that is, a real valued function, can be mapped by this way onto well defined self-adjoint operators suitable for their use in quantum mechanics. This is important in cases where self-adjointness is compromised as the conjugated pairs implicated in Pauli theorem. In order to explore the possibilities of this method we have worked on a collection of physical and theoretical relevant particular cases.

This work is divided in two main parts. The first one is separated in three chapters that give the basic tools of construction of quantum mechanics and a survey of the theory that lies behind the definition of quantum observables, in particular in what concerns to conjugated pairs. Next, in the second chapter, the definition of coherent states is revisited. In a third chapter the coherent state quantization procedure is exposed.

The second part treats three particular cases where the method is applied and where we explore the classical limit. The first one is the definition of a phase operator conjugated to the action. This application gives an alternative to the Pegg-Barnet phase operator [32] that converges analytically to the classical limit. Phase operator is constructed in finite Hilbert subspaces of the Hilbert space of Fourier series. The study of infinite dimensional limits of mean values of some observables lead towards a simpler convergence to the canonical commutation relations.

This opened the possibility to define relative phases in multilevel systems used in quantum computation. The fifth chapter presents a way of constructing relative phase operators in $SU(N)$ that could lead to interesting applications.

In the sixth chapter we treat the quantization of the motion in an infinite well potential. A new family of 2-component vector-valued coherent states allow a consistent quantization of the classical phase space for a particle trapped in this potential. We explore the basic quantum observables that are derived from such a quantization scheme, namely the position, energy, and a quantum version of the problematic momentum. We also consider their mean values in coherent states ("lower symbols") and their quantum dispersions.

As a last example, time operator for a free particle is exposed in chapter seven. We develop a quantum clock model using vector coherent states on Poincaré half-planes. These coherent states are of the Perelomov SU(1,1) type. We analyze the functional properties of the operators $\widehat{q}$, $\widehat{p}$, quantized versions of the classical canonical coordinates, the energy operator $H = \widehat{p^2}/2$, the intrinsic time operator $\widehat{T}$ defined as the quantization of $\dfrac{q}{p}$, with $p \neq 0$, and the commutators $[\widehat{q}, \widehat{p}]$ and $[\widehat{T}, \widehat{H}]$.

The work on phase operator and on the infinite well lead to the publication of two articles [41] [19] and to the participation in two conferences and three seminars.

Contents

Part I

The tools

1

Mathematical formulation of quantum mechanics

From its beginnings quantum mechanics, with its new set of odd causalities, needed a whole new mathematical formulation to give a clear physical interpretation to these phenomena and to work as an operative theory[1]. Although the interpretation has found certain limits, the mathematical structure was soon developed with proven accuracy. The first formulation started with the wave equation stated by Schrödinger

$$\hat{H}\psi = i\hbar\frac{d}{dt}\psi\,, \tag{1.1}$$

where $\hat{H}$ stands for a second order differential operator identifiable with the classical Hamiltonian, and the wave functions ψ that satisfy this relation are particular states of the system. Since the set of solutions was known to be discrete in certain cases, this revealed to give a suitable description of the observed discrete energy spectra in bounded systems. The dynamics give time dependent wave functions. In a parallel way, Heisenberg conceived the dynamics of the system as a matrix eigenvalue problem, and expressed the motion equation for operators as

$$[\hat{A}(t), \hat{H}] = i\hbar\frac{d}{dt}\hat{A}\,. \tag{1.2}$$

This gave a direct correspondence with the Hamiltonian classical formalism of Poisson brackets and, naturally, a canonical way of translating physical observables into quantum operators. Now, the time dependence is in the operators and the value of the physical quantity comes from its spectrum.

This relation can be generalized to other variables, for example, for position and momentum we can link the Poisson bracket

$$\{q,p\} \stackrel{\text{def}}{=} \frac{d}{dp}p\frac{d}{dq}q - \frac{d}{dq}p\frac{d}{dp}q = 1\,, \tag{1.3}$$

[1] In contrast from classical mechanics, geometric intuition and differential equations are not enough for an understanding of quantum mechanics. Basic notions of functional analysis and measure theory are essential to the construction. A rapid survey to the concepts used through this work is given in the appendix A

with the commutator

$$[\hat{q}, \hat{p}] = i\hbar\,, \tag{1.4}$$

where the Planck constant $\hbar$ scales the non-commutativity to its phenomenological extent. This equation gives a new consequence to the symplectic structure of phase space and also reveals clearly the complex nature of quantum mechanics.

Schrödinger himself, and Dirac [33] in a more formal way, proved the equivalence of both approaches, but the complete formulation of quantum mechanics using the tools of functional analysis came with the work of von Neumann [28]. In these, now assumed, mathematical foundations, observables are self-adjoint operators acting in a Hilbert space $\mathcal{H}$ and wave functions $\psi(x,t)$ are vectors in it. Schrödinger and Heisenberg equations are proved to be equivalent and linked by a unitary transformation by the Stone-von Neumann theorem.

The physical meaning for the quantum states proposed by Born introduced the now consensual statistical point of view. This *probabilistic interpretation* implies that the integral of the squared norm of a state needs to be a probability measure on the real line

$$\int_{\mathbb{R}} |\psi(x,t)|^2 dx = 1\,, \tag{1.5}$$

at any value of t. By this means, the squared norm gives the probability distribution of the position of localizable object. To keep the probabilistic interpretation valid, the Hilbert space where wave functions live is the one of square integrable functions $L^2(\mathbb{R}, dx)$ with the scalar product

$$\langle\phi|\psi\rangle = \int_{\mathbb{R}} \overline{\psi(x)}\phi(x)dx\,. \tag{1.6}$$

Once the states linked with a distribution, a major restriction comes from the classical correspondence (1.4), as any classical conjugated pair of variables a and b, with non-null Poisson bracket implies a lower bound for the product of variances of their associated quantum observables $\hat{A}$ and $\hat{B}$:

$$\Delta\hat{A}\,\Delta\hat{B} \geq \frac{\hbar}{2}\,. \tag{1.7}$$

This is the well known Heisenberg inequality and result in that joint measures of both observables cannot be done simultaneously with arbitrary precision. Moreover, the spectra of both operators will be linked and their definition will depend on each other.

1.1 Measurement of a quantum observable

As has been said, the possible states that a system can attain are represented as vectors $|\psi\rangle$ (using the Dirac convention) in a Hilbert space. In fact each state is linked to a class of vectors, a ray, since they can be defined up to a phase factor due the fact that the physical relevance is on the squared norm. An observable $\hat{A}$, defined as a self-adjoint operator, has a spectral resolution with real values that can be discrete or continuous. But this operator can also be decomposed into a non-orthogonal set of vectors and this will determine the type of measure needed to perform a measurement.

1.1.1 Projection Valued Measures

Let us start by defining the measure associated to the spectral resolution of $\hat{A}$, that is the Projection Valued measure.

Definition 1.1.1 *Take a measurable space (X, M), where X is some set and M a σ-algebra on it, and $\mathbf{P}$ the set of self-adjoint projections on a Hilbert space $\mathcal{H}$, a Projection Valued (PV) Operator Measure π is a mapping*

$$\pi : M \longrightarrow \mathbf{P} . \tag{1.8}$$

The PV measure has the following property:

$$\pi(A)^2 = \pi(A) \quad \text{for all } A \in M . \tag{1.9}$$

This implies that for two subsets of A and B of X, if

$$A \cap B = \emptyset , \tag{1.10}$$

then $\pi(A)$ and $\pi(B)$ are orthogonal projections. This leads to

$$\pi(A)\pi(B) = \pi(A \cap B) . \tag{1.11}$$

If the measure of the whole set maps to the identity operator then the measure is said to be normalized

$$\pi(X) = I_{\mathcal{H}} . \tag{1.12}$$

We can define the complex measure of some subset A of X, and two elements ϕ and ψ in $\mathcal{H}$ as the mapping $A \longrightarrow \langle \pi(A)\phi|\psi\rangle$. The simplest example is the measure of the set of one single eigenvalue $\lambda_i \in \mathbb{R}$ of a self-adjoint operator, which is just the projector on the corresponding eigenstate

$$\pi(\{\lambda_i\}) = |\psi_i\rangle\langle\psi_i| . \tag{1.13}$$

The values of an observable $\hat{A}$, the measurement of this physical quantity, are reached through the expected value of the operator taken in a particular state

$$\langle\psi|\hat{A}\psi\rangle \equiv \langle\psi|\hat{A}|\psi\rangle , \tag{1.14}$$

and it can be shown that this defines again a probability measure. Note that this definition depends on the nature of the state $|\psi\rangle$. If it can be written as a projector, that is, if

$$|\psi\rangle\langle\psi| = P_\psi = P_\psi^2 \,, \tag{1.15}$$

this implies that, for any $\psi \in \mathcal{H}$, it holds that $|P\psi|^2 = \langle\psi|P|\psi\rangle$. This means that $\hat{A}$ can be written as

$$\hat{A} = \sum_{i=1}^{N} \lambda_i |\psi_i\rangle\langle\psi_i| \,, \qquad \lambda_i \in \mathbb{R} \,, \tag{1.16}$$

in terms of the orthogonal projectors $|\psi_i\rangle\langle\psi_i|$, and where $N = dim(\mathcal{H})$. More generally, we have the spectral resolution

$$\hat{A} = \int_{-\infty}^{\infty} \lambda d\tau(\lambda) \,, \tag{1.17}$$

where $\tau(\lambda)$ is the discrete PV measure

$$d\tau(\lambda) = \sum_{i=1}^{N} \delta(\lambda - \lambda_i) d\lambda |\psi_\lambda\rangle\langle\psi_\lambda| \,. \tag{1.18}$$

Using these expressions for $\hat{A}$, the value 1.14 reads as $\langle\psi|\hat{A}|\psi\rangle = \sum_i \lambda_i |\langle\psi_\lambda|\psi\rangle|^2$, where $|\langle\psi_\lambda|\psi\rangle|^2$ represents the probability to get λ_i in a measurement of the observable when the system is in the state $|\psi\rangle$. The measurement of the quantity A in a state $|\psi\rangle$ will *collapse* to a particular state in the set of the eigenvectors of $\hat{A}$. This measurement has the form

$$\langle\psi|\hat{A}|\psi\rangle = \mathrm{tr}(\hat{A}|\psi\rangle\langle\psi|) \,, \tag{1.19}$$

and corresponds to a fully determined situation where the occurrence of the system in this precise state in fully ensured. Moreover, once the measurement done, ulterior measurements will give the same result. The projective measurements defined by Von Neumann [50] are repeatable operations that follow this "projection postulate". As we will see this formalism can be extended to a larger family of measurements that are useful to examine other parameters in the structure of the quantum state.

1.1.2 Positive Operator Valued Measures

A more general measure definition is a positive operator valued measure (POVM), where the measurement of the observables will be recovered through the mean value of their self adjoint operators. We will consider for generality, quantum systems associated to an infinite dimensional Hilbert space $\mathcal{H}$.

Let us take the set of positive[2] bounded[3] operators $\mathcal{L}_+$ acting on a Hilbert space $\mathcal{H}$. Given a measurable space $(X, \mathcal{A})$ with X a nonempty set, and $\mathcal{A}$ a σ-algebra on it, a POVM is a mapping $F(X) : \mathcal{A} \longrightarrow \mathcal{L}_+$ such that it satisfies some basic properties of a measure for all $X, Y \in \mathcal{A}$:

$$F(Y) \leq F(X) \quad Y \subset X \tag{1.20}$$

$$F(\varnothing) = 0 \tag{1.21}$$

And notably

$$F(X) = \mathbb{I}\,, \tag{1.22}$$

that is, the measure is normalized. This last property, the identity resolution, allows a probability interpretation of the POVM and makes it a good frame of reference of the Hilbert space. Moreover this implies that if $\psi \in \mathcal{H}$, the mapping $\mathcal{A} \ni X \longrightarrow \langle F(X)\psi|\psi\rangle$ is also a measure.

The space X can be discrete or continuous, in the second case it is desirable for it to be locally compact in order to define a measure and therefore an integral on it. A POVM gives a natural generalization of a von Neumann measurement in the sense that it can be seen as projective operator in a larger Hilbert space to which belong states as $|\Psi\rangle \otimes |\Phi\rangle$ where the $|\Phi\rangle$ subsystem has been ignored by taking a partial trace. This is known as the Naimark theorem.

A POVM appears in a quantum measurement if the initial state is some statistical mixture of possible outcomes. This state must be written as the *density matrix* ρ defined by the sum of the projectors weighted by their respective probability

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|\,. \tag{1.23}$$

Naturally, the sum $\sum_i p_i = 1$. In this case, the expected value 1.14 is obtained by

$$\mathrm{tr}(\hat{A}\rho) = \langle\psi|\hat{A}|\psi\rangle\,. \tag{1.24}$$

More generally, an operator or a density matrix can be expressed as the sum over a set of non orthogonal projectors, and the size of the set is not bounded anymore by the dimension of the Hilbert space, whenever the sum over all projectors is a resolution of the identity. In this sense, a POVM can be used as an alternative way to express an observable $\hat{A}$. These measures can appear redundant compared with a PV measure but, as we will see, they can be useful to construct a quantization protocol.

[2]An operator $\hat{B}$ is said to be positive if for every vector $|\psi\rangle$ in the domain of $\hat{B}$, $\langle\psi|\hat{B}|\psi\rangle \geq 0$, this implies that all eigenvalues are also positive.

[3]$\hat{B}$ is bounded if there exist a $k > 0$ such that for all vectors $|\psi\rangle \in \mathcal{H}$, $||\hat{B}|\psi\rangle|| \leq k|||\psi\rangle||$.

1.2 Canonical commutation relations

As said before, quantization has been done historically by making Poisson brackets correspond to quantum commutators. If P and Q are two self-adjoint operators, the relation

$$[Q,P] = QP - PQ = iI\,, \tag{1.25}$$

is known to be the *canonical commutation relation* for quantum mechanics in correspondence with the Poisson bracket for real observables

$$\{q,p\} = (\frac{dp}{dp}\frac{dq}{dq} - \frac{dp}{dq}\frac{dq}{dp}) = 1\,. \tag{1.26}$$

This two operators are said to form a *Heisenberg pair* if their realizations on a Hilbert space satisfy

$$[Q,P]\psi = i\psi\,, \tag{1.27}$$

where $\psi \in \mathcal{C}$, and $\mathcal{C}$ is the dense domain of the commutator. The standard quantum realization of these operators is the *Schrödinger representation* with $\mathcal{H} = L^2(\mathbb{R})$ and where the momentum is associated to the closure of the differential operator $P = -id/dx$ and the position is the multiplication by x: $Q = x$.

The problem is which representation to choose in 1.25. A way of stating this problem is using unitary groups. We define the one parameter unitary operators as $U(t) = e^{itP}$ and $V(s) = e^{isQ}$, then 1.25 gives

$$U(t)V(s) = e^{its}V(s)U(t)\,, \tag{1.28}$$

using the power series expansion of the exponential. If the commutation relation can be written as 1.28, operators U and V are said to be a *Weyl pair*.

1.2.1 Heisenberg pairs vs Weyl pairs

Even when it is clear that the generators of the unitary operators in (1.28) satisfy (1.25), the opposite is not always true [35]. Then both problems are not equivalent. All the self-adjoint operators that don't admit a series expansion leading to the exponential unitary operator definition may not form a Weyl pair. The incompatibility also arises when one or both operators are bounded since

$$[Q^n,P] = inQ^{n-1}\,, \tag{1.29}$$

leads to

$$||nQ||^{n-1} = n||Q^{n-1}|| \leq 2||P||||Q||^n \longrightarrow 2||P||||Q|| \geq n\,, \tag{1.30}$$

which is contradictory. It can be shown that all operators that form a Weyl pair are unitarily equivalent to the standard example and they must have a continuous unbounded spectrum. This leads to the fact that operators with bounded or discrete spectra, will not have Weyl canonical conjugates. Still they can have a Heisenberg conjugate.

1.3 Imprimitivity vs covariance

The link between self-adjoint operators and unitary representation of a group acting in the configuration space of a particular physical system is a very useful notion. Unitary representations and measure can be associated in systems that will extend the implication of canonical commutation relations.

Definition 1.3.1 *Let G be a group acting on a measurable space X, A a Borel set in X. A system of imprimitivity based on (G, X) for infinite dimensional spaces consists in a separable vector space $\mathcal{H}$, a strongly continuous unitary representation U_g of the group G acting on $\mathcal{H}$, and a PV measure π on the Borel sets of X valued in the projections of $\mathcal{H}$. The system of imprimitivity has to satisfy for A a Borel set in X,*

$$U_g \pi(A) U_{g^{-1}} = \pi(g \cdot A) . \tag{1.31}$$

This notion is generalized if the measure is not a PV measure but a POVM. In that case the system is called a *system of covariance.*

1.3.1 Pauli Theorem

The theorem stated by Pauli in 1926 [43] on the definition of self adjoint operators for canonical conjugated pairs has been subject of a long discussion since it restricts the quantization of conjugated observables. For example this affects the definition of a dynamical theory of time in quantum mechanics, once we admit there is a time observable conjugated to the Hamiltonain, but also some widely used models as the motion in an infinite well or in the circle. So it is worth to make a detailed analysis of its formulation.

This theorem can be stated at various levels of detail. In a coarse manner one can establish the following causality

Theorem 1.3.2 *Given two bounded densely defined self-adjoint operators $\hat{A}$ and $\hat{B}$, that satisfy $\hat{A}\hat{B} - \hat{B}\hat{A} = -i$, and if the spectrum of $\hat{A}$ is semi-bounded, then $\hat{B}$ cannot be self-adjoint.*

This theorem implies that $\hat{A}$ and $\hat{B}$ cannot form a system of imprimitivity since the application of the unitary representation associated to $\hat{B}$ would generate arbitrary translations in the PV measure associated to $\hat{A}$, that is, in its spectrum. Nevertheless, if both operators form a system of covariance, the unitary group acts generating translations on the measurable space. In this case it will not produce shifts on the spectrum any more but just reorder the projectors on the POVM so the implications of Pauli are overcome.

1.3.2 Conjugated pairs and coherent states quantization

As will be shown in the following, quantization of canonical pairs, such as coordinates of the phase space, angle and action, or time and energy, overcomes several definition problems once the representation of the operators is done on coherent state families. The method exposed in the next chapter, and the one proposed for different particular problems is a general one that might hopefully be extended to other problematic cases and could lead to the construction of measuring devices.

2

On how blocks are piled up

2.1 Coherent States

The field of coherent states has been very active for almost half a century since their rediscovery in the context of quantum optics. Their first appearance, in a work by Schrödinger [18] on the correspondence principle, showed their closest to classical behaviour which was retaken much later by Glauber [25] in the context of quantum optics.

2.1.1 The canon in two features

The establishment of a *canon* for coherent states is not a consensual matter. For their historic prevalence, coherent states for the harmonic oscillator or their generalization to group-generated Perelomov-Glauber states are taken to occupy this place. Besides the need to fill this category, a much wider set of states are considered as coherent states and at the end of the day two main features can be retained for their definition: continuity and identity resolution [29]. The saturation of an uncertainty relation, which can be accounted for the "coherent" behavior, and the invariance under the action of some non self-adjoint operator are features that will be found only in some cases. But in all of them we deal with sets of vectors $|z\rangle$ in a finite or countable infinite Hilbert space $\mathcal{H}$.

The first property shared by all these particular sets is **continuity** understood in the strong sense. This is that the limit

$$\lim_{z \longrightarrow z'} \| \, |z\rangle - |z'\rangle \| = 0 \,, \tag{2.1}$$

where the norm is $\| \, |\phi\rangle \| = \sqrt{\langle \phi | \phi \rangle}$ and z must be an element of a "label" set $\mathcal{Z}$ where continuity can be defined. Note then that vectors satisfying this are hardly orthogonal since a discrete family is in general excluded, as well as a continuous orthogonal family as the set of delta functions $\delta(z - z')$. This implies also that a basis of eigenvectors of a self-adjoint operator will not in general form a set of coherent states, even if such a basis can be a subset of CS.

The second general feature is **completeness**. As a direct consequence that one can find a positive measure $\mu(dz)$ on $\mathcal{Z}$ such that the unity operator can be expressed as

$$I = \int_{\mathcal{Z}} |z\rangle\langle z|\mu(dz)\,. \tag{2.2}$$

That is, coherent states are a *resolution of the identity*. This expression converges weakly, i.e. in the matrix elements of both sides of 2.2.

In an analog way to linear independence for discrete and orthogonal basis which imply

$$|\psi\rangle = \sum_{n=0}^{\infty} a_n|n\rangle = 0 \Leftrightarrow a_n \equiv 0 \quad \forall n \in \mathbb{N}\,, \tag{2.3}$$

for a vector $|\psi\rangle \in \mathcal{H}$ expressed in coherent states we have

$$|\psi\rangle = \int_{\mathcal{Z}} f(z)|z\rangle\mu(dz) = 0 \Leftrightarrow f(z) \equiv 0 \quad \forall z \in \mathcal{Z}\,, \tag{2.4}$$

at least if we impose on f some smoothness condition, and this means that we can represent the abstract Hilbert space by means of a class of functions $\psi(z) = \langle z|\psi\rangle \in \mathfrak{H}$. Introducing an inner product

$$\langle\phi|\psi\rangle = \int_{\mathcal{Z}} \langle\phi|z\rangle\langle z|\psi\rangle\mu(dz)\,, \tag{2.5}$$

this class of functions defines a Hilbert space isometric to $\mathfrak{H}$.

The fact that the identity can be expressed in this way implies that the whole set of states $|z\rangle$ span the Hilbert space. Some subsets of coherent states may have also the same property, as was noted by Von Neumann [28], and be *complete*, so the set of $|z\rangle$ states is called an *overcomplete* family.

2.1.2 Representing the Hilbert space

Resolution of identity 2.2 allows to represent the Hilbert space $\mathcal{H}$ to some extent in a “continuous” way. Objects in it will have the following form.

- An abstract vector $|\psi\rangle$ can be writen as a function

$$\psi(z) = \langle\psi|z\rangle\,, \tag{2.6}$$

- the inner product of two vectors

$$\langle\phi|\psi\rangle = \int_{\mathcal{Z}} \langle\phi|z\rangle\langle z|\psi\rangle\mu(dz)\,, \tag{2.7}$$

- the vector transformation,

$$\langle\phi|A|\psi\rangle = \int_{\mathcal{Z}} \langle\phi|A|z\rangle\langle z|\psi\rangle\mu(dz)\,, \tag{2.8}$$

- the operator decomposition

$$A = \int_{\mathcal{Z}} |z\rangle\langle z|A|z'\rangle\langle z'|\mu(dz)\mu(dz')\,, \tag{2.9}$$

- and in particular the diagonal representation of operators

$$A = \int_{\mathcal{Z}} f(z)|z\rangle\langle z|\mu(dz) \tag{2.10}$$

We will discuss later the conditions for this equation to be valid.

2.1.3 Harmonic oscillator

To illustrate the features exposed above, let us revisit the coherent states for the harmonic oscillator as they take a particularly simple form and satisfy a set of relevant properties remarkably a closest to classical behavior.

The harmonic oscillator can be constructed from the Weyl-Heisenberg algebra of operators $\hat{a}$, $\hat{a}^\dagger$ and the identity I that satisfy the following relations

$$[\hat{a}, \hat{a}^\dagger] = 1, \qquad [\hat{a}, I] = [\hat{a}^\dagger, I] = 0\,, \tag{2.11}$$

where $[\cdot,\cdot]$ is the usual antisymmetric commutator. Now, taking an orthonormal basis $|n\rangle$ such that the action of $\hat{a}$ and $\hat{a}^\dagger$ in the $|n\rangle$ states is

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle, \qquad \hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle, \tag{2.12}$$

and defining the vector $|0\rangle$ such that $\hat{a}|0\rangle = 0$, the repeated action of $\hat{a}^\dagger$ on $|0\rangle$ produces all the states $|n\rangle$

$$\frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}|0\rangle = |n\rangle\,. \tag{2.13}$$

It is easy to see that the operator $\widehat{N} = \hat{a}^\dagger\hat{a}$ has these states as eigenstates

$$\widehat{N}|n\rangle = n|n\rangle\,, \tag{2.14}$$

and satisfies

$$[\widehat{N}, \hat{a}] = -\hat{a}\,, \qquad [\widehat{N}, \hat{a}^\dagger] = \hat{a}^\dagger\,. \tag{2.15}$$

Operators $\hat{a}$ and $\hat{a}^\dagger$ are not self-adjoint so their eigenvalues are expected to be complex.

For the classical harmonic oscillator the dynamical variables are q and p, that correspond to the quantum operators $\widehat{q}$ and $\widehat{p} = -i\frac{\mathrm{d}}{\mathrm{d}q}$ that verify $[\widehat{q}, \widehat{p}] = i$. The quantum mechanics Hamiltonian is the same as the classical one

$$H = \frac{1}{2m}(p^2 + m^2\omega^2 q^2)\,, \tag{2.16}$$

where for simplicity we will make the constants $\hbar = \omega = m = 1$. The link with the Weyl-Heisenberg algebra operators is done through their realization in the phase space

$$\hat{a} = \frac{1}{\sqrt{2}}(\widehat{q} + i\widehat{p}) \qquad \hat{a}^{\dagger} = \frac{1}{\sqrt{2}}(\widehat{q} - i\widehat{p}) , \tag{2.17}$$

and conversely

$$\widehat{q} = \frac{1}{\sqrt{2}}(\hat{a} + \hat{a}^{\dagger}) \qquad \widehat{p} = -i\frac{1}{\sqrt{2}}(\hat{a} - \hat{a}^{\dagger}) . \tag{2.18}$$

Operator $\widehat{N}$ is

$$\widehat{N} = \frac{1}{2}(\widehat{p} - i\widehat{q})(\widehat{p} + i\widehat{q}) = \frac{1}{2}(\widehat{p}^2 + \widehat{q}^2 + i[\widehat{q}, \widehat{p}]) , \tag{2.19}$$

It is easy to see that Hamiltonian is then

$$\widehat{H} = \widehat{N} + \frac{1}{2} , \tag{2.20}$$

and the solutions of the Schödinger equation are then the eigenstates of $\widehat{H}$, that is, the ones of $\widehat{N}$,

$$\widehat{H}|n\rangle = (n + \frac{1}{2})|n\rangle . \tag{2.21}$$

These states correspond to concentric circles in the classical phase space. Defining the expectation value as $\langle\cdot\rangle = \langle\psi||\psi\rangle$, dispersion is defined as

$$\Delta\widehat{q} = \langle\widehat{q}^2\rangle - \langle\widehat{q}\rangle^2 . \tag{2.22}$$

The state $|0\rangle$ in phase space has minimal dispersion.

Geometric properties

Coherent states have a clear geometric interpretation on the phase space, they are the displaced ground state centered in a point $\alpha \in \mathbb{C}$. As can be seen in figure 4.3, coherent states preserve the minimal dispersion of the state $|0\rangle$ and they will follow the orbit of the classical solution to the harmonic oscillator equations of motion.

In the Hilbert space

Coherent states for the harmonic oscillator read as

$$|\alpha\rangle = \sum_{n\geq 0} e^{-\frac{|\alpha|^2}{2}} \frac{\alpha^n}{\sqrt{n!}}|n\rangle . \tag{2.23}$$

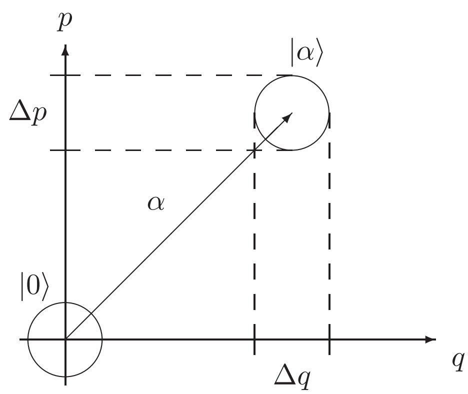


Figure 2.1: Coherent states are a translation of the ground state to a point α on the phase space.

As has been said before this family of coherent states is not an orthogonal one, states overlap as

$$\langle\alpha|\beta\rangle = e^{i\Im\alpha^*\beta}e^{-\frac{1}{2}|\alpha-\beta|^2}\,, \tag{2.24}$$

and the cardinality of the set is higher than the dimension of the Hilbert space spanned by the Fock basis.

The projector set of states $|\alpha\rangle$ resolves the identity

$$\int_{\mathbb{C}} |\alpha\rangle\langle\alpha|\frac{d^2\alpha}{\pi} = 1\,. \tag{2.25}$$

All relations given in section 2.1.2 hold in this case. Between the projections on coherent states there is the one used in general to represent the density matrix of a state, the Glauber-Sudarshan P representation,

$$\widehat{\rho} = \int_{\mathbb{C}} \phi(\alpha,\alpha^*)|\alpha\rangle\langle\alpha|\frac{d^2\alpha}{\pi}\,. \tag{2.26}$$

Here the $\phi(\alpha,\alpha^*)$ is a called a *quasy-probability* distribution. But this integral representation can be generalized to a large class of symmetric operators $\widehat{f}$

$$\widehat{f} = \int_{\mathbb{C}} f(\alpha,\alpha^*)|\alpha\rangle\langle\alpha|\frac{d^2\alpha}{\pi}\,. \tag{2.27}$$

A related notion will be used in the next chapter where we introduce the quantization method through coherent states.

3

Coherent state quantization, or how to climb the tower

3.0.4 Klauder-Berezin-Toeplitz quantization

Let $X = \{x \mid x \in X\}$ be a set equipped with a measure $\mu(dx)$ and $L^2(X,\mu)$ the Hilbert space of square integrable functions $f(x)$ on X:

$$\begin{aligned} \|f\|^2 = & \int_X |f(x)|^2 \, \mu(dx) < \infty \\ \langle f_1|f_2\rangle = & \int_X \overline{f_1(x)} f_2(x) \, \mu(dx) \, . \end{aligned}$$

Let us select, among elements of $L^2(X,\mu)$, an orthonormal set $\mathcal{S}_N = \{\phi_n(x)\}_{n=1}^N$, N being finite or infinite, which spans, by definition, the separable Hilbert subspace $\mathcal{H}_N$. We demand this set to obey the following crucial condition

$$0 < \mathcal{N}(x) \equiv \sum_n |\phi_n(x)|^2 < \infty \text{ almost everywhere} \, . \tag{3.1}$$

Then consider the family of states $\{|x\rangle\}_{x\in X}$ in $\mathcal{H}_N$ through the following linear superpositions:

$$|x\rangle \equiv \frac{1}{\sqrt{\mathcal{N}(x)}} \sum_n \overline{\phi_n(x)} |\phi_n\rangle \, . \tag{3.2}$$

This defines an injective map (which should be continuous w.r.t some minimal topology affected to X for which the latter is locally compact):

$$X \ni x \mapsto |x\rangle \in \mathcal{H}_N \, ,$$

These *coherent* states obey

- **Normalisation**

$$\langle x \, | x \rangle = 1 \, , \tag{3.3}$$

- **Resolution of the unity in $\mathcal{H}_N$**

$$\int_X |x\rangle\langle x| \, \mathcal{N}(x) \, \mu(dx) = \mathbb{I}_{\mathcal{H}_N} \, , \tag{3.4}$$

A *classical* observable is a function $f(x)$ on X having specific properties. Its coherent state or frame quantization consists in associating to $f(x)$ the operator

$$A_f := \int_X f(x)|x\rangle\langle x|\mathcal{N}(x)\,\mu(dx)\,. \tag{3.5}$$

The function $f(x) \equiv \hat{A}_f(x)$ is called upper (or contravariant) symbol of the operator A_f and is nonunique in general. On the other hand, the mean value $\langle x|A_f|x\rangle \equiv \check{A}_f(x)$ is called lower (or covariant) symbol of A_f.

Such a quantization of the set X is in one-to-one correspondence with the choice of the frame

$$\int_X |x\rangle\langle x|\mathcal{N}(x)\,\mu(dx) = \mathbb{I}_{\mathcal{H}_N}\,.$$

To a certain extent, a quantization scheme consists in adopting a certain point of view in dealing with X (compare with Fourier or wavelet analysis in signal processing). Here, the validity of a precise frame choice is asserted by comparing spectral characteristics of quantum observables A_f with data provided by specific protocole in the observation of X.

Coherent state quantization [20, 1, 45, 42, 22, 41, 23] is an alternative way of representing classical observables into a quantum system. The states used in it include Glauber and Perelomov coherent states but lie in a wider definition that admits a large range of state families resolving the identity. Identity resolution is here the crucial condition.

In fact, these coherent states form a frame of reference well suited to represent classical quantities and, in that sense, work as a natural quantization procedure which is in one-to-one correspondence with the choice of the frame. The validity of a precise frame choice is asserted by comparing spectral characteristics of quantum observables $\widehat{f}$ with data from the observational space. Unlike canonical quantization where the whole model rests upon a pair of conjugated variables within the Hamilton formalism [34], here we just need the elements that have been described above.

3.0.5 Quantization of the particle motion on the circle S^1

We will apply in the next chapters the method to various cases, as the motion in the infinite square well potential (Chapter 6). The latter can be viewed as a particular case of the motion on the circle S^1, once we have identified the boundaries of the well with each other and imposed Dirichlet conditions on them. Functions on this domain will behave as pinched waves on a circle so it is useful to expose first the more general case.

Applying our scheme of quantization we can define the coherent states on the circle. The measure space X is the cylinder $S^1 \times \mathbb{R} = \{x \equiv (q,p)\,|\,0 \leq q < 2\pi,\ p,q \in \mathbb{R}\}$, *i.e.* the phase space of a particle moving on the circle, where q and p are canonically conjugate variables. We consistently choose the measure on X as the usual one, invariant (up to a factor) with respect to canonical transformations: $\mu(\mathrm{d}x) = \frac{1}{2\pi}\,\mathrm{d}q\,\mathrm{d}p$. The functions $\phi_n(x)$ forming the orthonormal system needed to construct coherent states are suitably weighted Fourier exponentials:

$$\phi_n(x) = \left(\frac{\epsilon}{\pi}\right)^{1/4} \exp\big(-\frac{\epsilon}{2}(p-n)^2\big)\,\mathrm{e}^{\mathrm{i}nq}\,, \qquad n \in \mathbb{Z}\,, \tag{3.6}$$

where $\epsilon > 0$ can be arbitrarily small. This parameter includes the Planck constant together with the physical quantities characterizing the classical motion (frequency, mass, etc.). Actually, it represents a regularization. Notice that the continuous distribution $x \mapsto |\phi_n(x)|^2$ is the normal law centered at n (for the angular momentum variable p). We establish a one-to-one correspondence between the functions ϕ_n and the states $|n\rangle$ which form an orthonormal basis of some generic separable Hilbert space $\mathcal{H}$ that can be viewed or not as a subspace of $\mathrm{L}^2(X, \mu(\mathrm{d}x))$. coherent states, as vectors in $\mathcal{H}$, read then as

$$|p,q\rangle = \frac{1}{\sqrt{\mathcal{N}(p)}}\,\left(\frac{\epsilon}{\pi}\right)^{1/4} \sum_{n\in\mathbb{Z}} \exp\big(-\frac{\epsilon}{2}(p-n)^2\big)\,\mathrm{e}^{-\mathrm{i}nq}|n\rangle\,, \tag{3.7}$$

where the normalization factor

$$\mathcal{N}(x) \equiv \mathcal{N}(p) = \sqrt{\frac{\epsilon}{\pi}} \sum_{n\in\mathbb{Z}} \exp\big(-\epsilon(p-n)^2\big) < \infty\,, \tag{3.8}$$

is a periodic train of normalized Gaussian functions and is proportional to an elliptic Theta function. Applying the Poisson summation yields the alternative form:

$$\mathcal{N}(p) = \sum_{n\in\mathbb{Z}} \exp(2\pi\mathrm{i}np)\,\exp(-\frac{\pi^2}{\epsilon}n^2)\,. \tag{3.9}$$

From this formula it is easy to prove that $\lim_{\epsilon\to 0}\mathcal{N}(p) = 1$.

The coherent states (3.7) have been previously proposed, however through quite different approaches, by De Bièvre-González (1992-93) [47], Kowalski-Rembieliński-Papaloucas (1996) [30], and González-Del Olmo (1998) [3].

3.0.6 Quantization of classical observables

The quantum operator acting on $\mathcal{H}$, associated to the classical observable $f(x)$, is obtained as in (3.5). For the most basic one, i.e. the classical observable p itself, the procedure yields

$$\widehat{p} = \int_X \mathcal{N}(p)\,p\,|p,q\rangle\langle p,q|\mu(\mathrm{d}x) = \sum_{n\in\mathbb{Z}} n\,|n\rangle\langle n|\,, \tag{3.10}$$

and this is nothing but the angular momentum operator, which reads in angular position representation (Fourier series): $\widehat{p} = -\mathrm{i}\frac{\partial}{\partial q}$.

For an arbitrary function $f(q)$, we have

$$
\begin{aligned}
\widehat{f(q)} &= \int_X \mu(\mathrm{d}x)\mathcal{N}(p)f(q)\,|p,q\rangle\langle p,q| \\
&= \sum_{n,n'\in\mathbb{Z}} \exp\big(-\frac{\epsilon}{4}\,(n-n')^2\big)\, c_{n-n'}(f)|n\rangle\langle n'|\,,
\end{aligned}
\tag{3.11}
$$

where $c_n(f)$ is the n-th Fourier coefficient of f. In particular, we have for the angular position operator $\widehat{q}$:

$$
\widehat{q} = \pi\mathbb{I}_{\mathcal{H}} + \mathrm{i}\sum_{n\neq n'} \frac{\exp\big(-\frac{\epsilon}{4}(n-n')^2\big)}{n-n'}\,|n\rangle\langle n'|\,. \tag{3.12}
$$

The shift operator is the quantized counterpart of the "Fourier fundamental harmonic":

$$
\widehat{\mathrm{e}^{\mathrm{i}q}} = \mathrm{e}^{-\frac{\epsilon}{4}} \sum_n |n+1\rangle\langle n|\,. \tag{3.13}
$$

The commutation rule between (3.10) and (3.13) gives

$$
[\,\widehat{p}, \widehat{\mathrm{e}^{\mathrm{i}q}}\,] = \widehat{\mathrm{e}^{\mathrm{i}q}}\,, \tag{3.14}
$$

and is canonical in the sense that it is in exact correspondence with the classical Poisson bracket

$$
\big\{p, \mathrm{e}^{\mathrm{i}q}\big\} = \mathrm{i}\mathrm{e}^{\mathrm{i}q}\,. \tag{3.15}
$$

Some interesting aspects of other such correspondences are found in [46]. For arbitrary functions of q the commutator

$$
[\,\widehat{p}, \widehat{f(q)}\,] = \sum_{n,n'}(n-n')\exp\big(-\frac{\epsilon}{4}(n-n')^2\big)\, c_{n-n'}(f)\,|n\rangle\langle n'|\,, \tag{3.16}
$$

can arise interpretational difficulties. In particular, when $f(q) = q$, i.e. for the angle operator

$$
[\,\widehat{p}, \widehat{q}\,] = \mathrm{i}\sum_{n\neq n'} \exp\big(-\frac{\epsilon}{4}(n-n')^2\big)\,|n\rangle\langle n'|\,, \tag{3.17}
$$

the comparison with the classical bracket $\{p, q\} = 1$ is not direct. Actually, these difficulties are only apparent if we consider instead the 2π-periodic extension to $\mathbb{R}$ of $f(q)$. The position observable $f(q) = q$, originally defined in the interval $[0, 2\pi)$, acquires then a sawtooth shape and its periodic discontinuities are accountable for the discrepancy. In fact the obstacle is circumvented if we examine, for instance, the behaviour of the corresponding lower symbols at the limit $\epsilon \to 0$. For the angle operator we have

$$\begin{aligned} \langle p_0, q_0 | \, \widehat{q} \, | p_0, q_0 \rangle &= \pi + \frac{1}{2} \left(1 + \frac{\mathcal{N}(p_0 - \frac{1}{2})}{\mathcal{N}(p_0)} \right) \sum_{n \neq 0} \mathrm{i} \, \frac{\exp(-\frac{\epsilon}{2} n^2 + \mathrm{i} n q_0)}{n} \\ &\underset{\epsilon \to 0}{\sim} \pi + \sum_{n \neq 0} \mathrm{i} \, \frac{\exp(\mathrm{i} n q_0)}{n} \, , \end{aligned} \tag{3.18}$$

where we recognize at the limit the Fourier series of $f(q)$. For the commutator, we recover the canonical commutation rule modulo Dirac singularities on the lattice $2\pi\mathbb{Z}$.

$$\begin{aligned} \langle p_0, q_0 | [\, \widehat{p}, \widehat{q} \,] \, | p_0, q_0 \rangle &= \frac{1}{2} \left(1 + \frac{\mathcal{N}(p_0 - \frac{1}{2})}{\mathcal{N}(p_0)} \right) \left(-\mathrm{i} + \sum_{n \in \mathbb{Z}} \mathrm{i} \exp(-\frac{\epsilon}{2} n^2 + \mathrm{i} n q_0) \right) \\ &\underset{\epsilon \to 0}{\sim} -\mathrm{i} + \mathrm{i} \sum_{n} \delta(q_0 - 2\pi n) \, . \end{aligned} \tag{3.19}$$

Part II

Particular cases

4
Phase operator

In classical mechanics the pair of angle and action variables form a conjugated pair. It is natural to seek the corresponding quantum quantities, but as has been signaled before, the proper definition of the corresponding self-adjoint operators is limited by the bounded character of these quantities. An alternative point of view imposes in the definition of the observables and coherent state quantization will prove to be of great utility to overcome these consistence difficulties. In the first section of this chapter we will revise the phase operator problem and the various issues proposed in literature. The second section will show the alternative way using coherent state quantization.

4.1 Introduction

Since the first attempt by Dirac in 1927 [33] various definitions of phase operator have been proposed with more or less satisfying success in terms of consistency [31, 27, 38, 32, 17]. A natural requirement is that phase operator and number operators form a conjugate Heisenberg pair obeying the canonical commutation relation

$$[\hat{N}, \hat{\theta}] = i I_d \,, \tag{4.1}$$

in exact correspondence with the Poisson bracket for the classical action angle variables.

To obtain this quantum-mechanical analog, the polar decomposition of raising and lowering operators

$$\hat{a} = \exp(i\hat{\theta})\hat{N}^{1/2}, \quad \hat{a}^\dagger = \hat{N}^{1/2}\exp(-i\hat{\theta})\,, \tag{4.2}$$

was originally proposed by Dirac, with the corresponding uncertainty relation

$$\Delta\hat{\theta}\,\Delta\hat{N} \geq \frac{1}{2}\,. \tag{4.3}$$

But the relation between operators (4.1) is misleading. The construction of a unitary operator is a delicate procedure and there are three main problems in it. First we have that for a well-defined number state the uncertainty of the phase would be greater than 2π. This inconvenience, also present in the quantization of the pair angular momentum-angle, adds to the well-known contradiction lying in the matrix elements of the commutator

$$-i\delta_{nn'} = \langle n'|[\hat{N},\hat{\theta}]|n\rangle = (n-n')\langle n'|\hat{\theta}|n\rangle \,. \tag{4.4}$$

In the angular momentum case, this contradiction is avoided to a certain extent by introducing a proper periodical variable $\hat{\Phi}(\phi)$ [40]. If $\hat{\Phi}$ is just a sawtooth function, the discontinuities give a commutation relation

$$[\hat{L}_z,\hat{\Phi}] = -i\{1-2\pi\sum_{n=-\infty}^{\infty}\delta(\phi-(2n+1)\pi)\}\,. \tag{4.5}$$

The singularities in (4.5) can be excluded, as proposed by Louisel [26], taking sine and cosine functions of ϕ to recover a valid uncertainty relation. But the problem reveals to be harder in number-phase case because, as showed by Susskind and Glogower (1964)[31], the decomposition (4.2) itself leads to the definition of non unitary operators:

$$\exp(-i\hat{\theta}) = \sum_{n=0}^{\infty}|n\rangle\langle n+1|\,\{+|\psi\rangle\langle 0|\},\ \text{and h.c.}\,, \tag{4.6}$$

and this non-unitarity explains the inconsistency revealed in (4.4). To overcome this handicap, a different polar decomposition was suggested in [31]

$$\hat{a} = (\hat{N}+1)^{\frac{1}{2}}\hat{E}_-,\quad \hat{a}^\dagger = (\hat{N}+1)^{\frac{1}{2}}\hat{E}_+\,, \tag{4.7}$$

where the operators $E_\pm$ are still non unitary because of their action on the extreme state of the semi-bounded number basis [40]. Nevertheless the addition of the restriction

$$\hat{E}_-|0\rangle = 0\,, \tag{4.8}$$

permits to define hermitian operators

$$\begin{aligned}\hat{C} &= \frac{1}{2}(\hat{E}_- + \hat{E}_+) = \hat{C}^\dagger\,,\\ \hat{S} &= \frac{1}{2\pi}(\hat{E}_- - \hat{E}_+) = \hat{S}^\dagger\,.\end{aligned} \tag{4.9}$$

These operators are named “cosine” and “sine” because they reproduce the same algebraic structure as the projections of the classical state in the phase space of the oscillator problem.

Searching for a hermitian phase operator $\hat{\theta}$ which would avoid constraints like (4.8) and fit (4.1) in the classical limit, Popov and Yarunin [38] and later

Pegg and Barnett [32] used an orthonormal set of eigenstates of $\hat{\theta}$ defined on the number state basis as

$$|\theta_m\rangle = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} e^{in\theta_m} |n\rangle \,. \tag{4.10}$$

where, for a given finite N, these authors selected the following equidistant subset of the angle parameter

$$\theta_m = \theta_0 + \frac{2\pi m}{N}, \; m = 0, 1, \ldots, N-1 \,, \tag{4.11}$$

with θ_0 as a reference phase. Orthonormality stems from the well-known properties of the roots of the unity as happens with the base of discrete Fourier transform

$$\sum_{n=0}^{N-1} e^{in(\theta_m - \theta_{m'})} = \sum_{n=0}^{N-1} e^{i2\pi(m-m')\frac{n}{N}} = N\delta_{mm'} \,. \tag{4.12}$$

The phase operator on $\mathbb{C}^N$ is simply constructed through the spectral resolution

$$\hat{\theta} \equiv \sum_{m=0}^{N-1} \theta_m |\theta_m\rangle\langle\theta_m| \,. \tag{4.13}$$

This construction, which amounts to an adequate change of orthornormal basis in $\mathbb{C}^N$, gives for the ground number state $|0\rangle$ a random phase which avoids some of the drawbacks in previous developments. Note that taking the limit $N \longrightarrow \infty$ is questionable within a Hilbertian framework, this process must be understood in terms of mean values restricted to some suitable subspace and the limit has to be taken afterwards. In [32] the pertinence of the states (4.10) is proved by the expected value of the commutator with the number operator. The problem appears when the limit is taken since it leads to an approximate result.

More recently an interesting approach to the construction of a phase operator has been done by Busch, Lahti and their collaborators within the frame of measurement theory [15][16][17]. Phase observables are constructed here using the sum over an infinite number basis from their original definition.

Here we propose a construction based on a coherent state quantization scheme and not on the arbitrary assumption of a discrete phase nor on an infinite dimension Hilbert space. This will produce a suitable commutation relation at the infinite dimensional limit, still at the level of mean values.

4.2 The approach via coherent state quantization

As was suggested in [32] the commutation relation will approximate better the canonical one (4.1) if one enlarges enough the Hilbert space of states.

We show here that there is no need to discretize the angle variable as in [32] to recover a suitable commutation relation. We adopt instead the Hilbert space $L^2(S^1)$ of square integrable functions on the circle as the natural framework for defining an appropriate phase operator in a finite dimensional subspace. Let us first give an outline of the method already exposed in [20, 1, 45, 42, 22].

Let us now take as a set X the unit circle S^1 provided with the measure $\mu(d\theta) = \frac{d\theta}{2\pi}$. The Hilbert space is $L^2(X,\mu) = L^2(S^1, \frac{d\theta}{2\pi})$ and has the inner product:

$$\langle f|g\rangle = \int_0^{2\pi} \overline{f(\theta)} g(\theta) \frac{d\theta}{2\pi} \,. \tag{4.14}$$

In this space we choose as orthonormal set the first N Fourier exponentials with negative frequencies:

$$\phi_n(\theta) = e^{-in\theta}, \text{ with } \mathcal{N}(\theta) = \sum_{n=0}^{N-1} |\phi_n(\theta)|^2 = N \,. \tag{4.15}$$

The phase states are now defined as the corresponding "coherent states":

$$|\theta) = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} e^{in\theta} |\phi_n\rangle \,, \tag{4.16}$$

where the kets $|\phi_n\rangle$ can be directly identified to the number states $|n\rangle$, and the round bracket denotes the continuous labeling of this family. The overlapping of elements of both families is given by

$$\langle n|\theta) = \frac{1}{\sqrt{N}} e^{in\theta} \,. \tag{4.17}$$

We trivially have normalization and resolution of the unity in $\mathcal{H}_N \simeq \mathbb{C}^N$:

$$(\theta|\theta) = 1, \ \int_0^{2\pi} |\theta)(\theta| \, N\mu(d\theta) = I_N \,. \tag{4.18}$$

Unlike (4.10) the states (4.16) are not orthogonal but overlap as:

$$(\theta'|\theta) = \frac{1}{N} \sum_{n=0}^{N-1} e^{in(\theta-\theta')} \,. \tag{4.19}$$

This sum has a closed form found by a variation on the Gauss sum [37], that is, by adding the same series with decreasing n and using the identities for the sum of sines and cosines, we have, after some reorganization,

$$(\theta'|\theta) = \frac{e^{i\frac{N-1}{2}(\theta-\theta')}}{N} \frac{\sin\frac{N}{2}(\theta-\theta')}{\sin\frac{1}{2}(\theta-\theta')} \,. \tag{4.20}$$

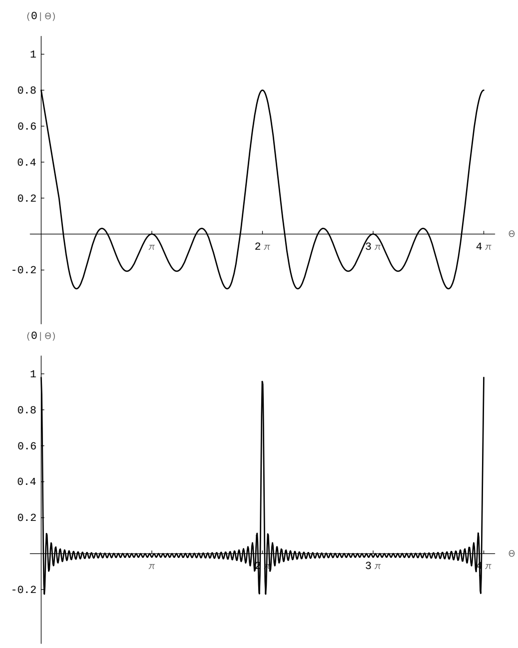


Figure 4.1: Phase coherent states overlap is non null, as can be seen here for $N = 4$ and for $N = 50$ respectively, but at the limit $N \longrightarrow \infty$ it tends to a 2π-periodic comb, that is, to orthogonality.

The overlapping tends to disappear at the limit when $N \longrightarrow \infty$, as one can see in figure 4.1.

Note that for N large enough $|\theta)$ states contain all the Pegg-Barnett phase states and besides they form a continuous family labeled by the points of the circle. The coherent state quantization of a particular function $f(\theta)$ with respect to the continuous set (4.16) yields the operator A_f defined by:

$$f(\theta) \mapsto \int_X f(\theta)|\theta)(\theta|\, N\mu(d\theta) \stackrel{\mathrm{def}}{=} A_f \, . \tag{4.21}$$

An analog procedure has been already used in the frame of positive operator valued measures [15][16] but spanning the phase states over an infinite orthogonal basis with the known drawback on the convergence of the $|\phi\rangle = \sum_n e^{in\theta}|n\rangle$ series out of the Hilbert space and the related questions concerning the operator domain. When expressed in terms of the number states the operator (4.21) takes the form:

$$A_f = \sum_{n,n'=0}^{N-1} c_{n'-n}(f)|n\rangle\langle n'| \, , \tag{4.22}$$

where $c_n(f)$ are the Fourier coefficients of the function $f(\theta)$,

$$c_n(f) = \int_0^{2\pi} f(\theta) e^{-in\theta} \frac{d\theta}{2\pi}\,. \tag{4.23}$$

Therefore, the existence of the quantum version of f is ruled by the existence of its Fourier transform. Note that A_f will be self-adjoint only when $f(\theta)$ is real valued. In particular, a self-adjoint phase operator of the Toeplitz matrix type, is obtained straightforward by choosing $f(\theta) = \theta$:

$$\hat{A}_\theta = -i \sum_{n\neq n' n,n'=0}^{N-1} \frac{1}{n-n'} |n\rangle\langle n'|\,, \tag{4.24}$$

One can see, in figure 4.2, how the eigenvalues of A_θ cover the unit circle for the limit $N \longrightarrow \infty$.

Its lower symbol or expectation value in a coherent state is given by:

$$(\theta|\hat{A}_\theta|\theta) = \frac{i}{N} \sum_{\substack{n\neq n' \\ n,n'=0}}^{N-1} \frac{e^{i(n-n')\theta}}{n'-n}\,. \tag{4.25}$$

Due to the continuous nature of the set of $|\theta)$, all operators produced by this quantization are different of the Pegg-Barnett operators. As a matter of fact, the commutator $[\hat{N}, \hat{A}_\theta]$ expressed in terms of the number basis reads as:

$$[\hat{N}, \hat{A}_\theta] = -i \sum_{\substack{n\neq n' \\ n,n'=0}}^{N-1} |n\rangle\langle n'| = iI_d + (-i)\mathcal{I}_N\,, \tag{4.26}$$

and has all diagonal elements equal to 0. Here $\mathcal{I}_N = \sum_{n,n'=0}^{N-1} |n\rangle\langle n'|$ is the $N \times N$ matrix with all entries $= 1$. The spectrum of this matrix is 0 (degenerate $N-1$ times) and N. The normalized eigenvector corresponding to the eigenvalue N is:

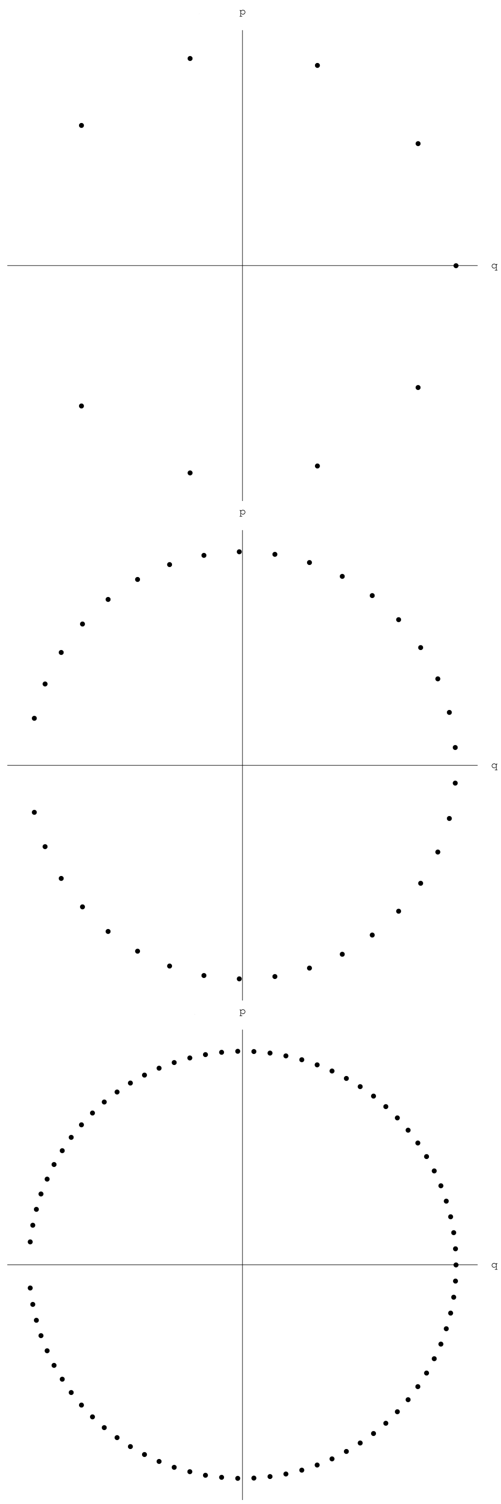
$$|v_N\rangle = |\theta = 0) = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} |n\rangle\,. \tag{4.27}$$

Other eigenvectors span the hyperplane orthogonal to $|v_N\rangle$. We can choose them as the orthonormal set with $N-1$ elements:

$$\left\{ |v_n\rangle \stackrel{\text{def}}{=} \frac{1}{\sqrt{2}}(|n+1\rangle - |n\rangle)\,, n = 0, 1, \ldots, N-2 \right\}. \tag{4.28}$$

The matrix $\mathcal{I}_N$ is just N times the projector $|v_N\rangle\langle v_N|$. Hence the commutation rule reads as:

$$[\hat{N}, \hat{A}_\theta] = -i \sum_{\substack{n\neq n' \\ n,n'=0}}^{N-1} |n\rangle\langle n'| = i\,(I_d - N|v_N\rangle\langle v_N|)\,. \tag{4.29}$$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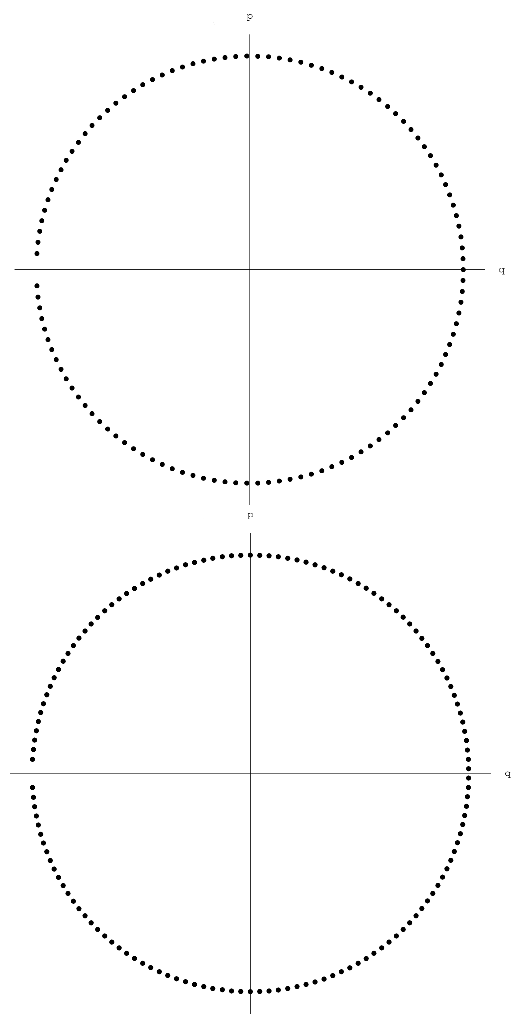


Figure 4.2: Eigenvalues of phase operator distributed over the unit circle in phase space for $N = 9, 36, 81, 121, 144$. Note how for large N the points tend to cover densely the whole $(0, 2\pi]$ interval, and the gap at $\theta = \pi$ closes.

A further analysis of this relation through its lower symbol provides, for the matrix $\mathcal{I}_N$, the function:

$$(\theta|\mathcal{I}_N|\theta) = \frac{1}{N}\sum_{n,n'=0}^{N-1} e^{i(n-n')\theta} = \frac{1}{N}\frac{\sin^2 N\frac{\theta}{2}}{\sin^2\frac{\theta}{2}}\,. \tag{4.30}$$

In the limit at large N this function is the Dirac comb (a well-known result in diffraction theory):

$$\lim_{N\to\infty}\frac{1}{N}\frac{\sin^2 N\frac{\theta}{2}}{\sin^2\frac{\theta}{2}} = \sum_{k\in\mathbb{Z}}\delta(\theta-2k\pi)\,. \tag{4.31}$$

Recombining this with expression (4.29) allows to recover the canonical commutation rule:

$$(\theta|[\hat{N},\hat{A}_\theta]|\theta) \approx_{N\to\infty} i - i\sum_{k\in\mathbb{Z}}\delta(\theta-2k\pi)\,. \tag{4.32}$$

This expression is the expected one for any periodical variable as was seen in (4.5). It means that in the Heisenberg picture for temporal evolution

$$\hbar\frac{d}{dt}\langle\hat{A}_\theta\rangle = -i\langle[\hat{N},\hat{A}_\theta]\rangle = 1 - \sum_{k\in\mathbb{Z}}\delta(\theta-2k\pi)\,. \tag{4.33}$$

A Dirac commutator-Poisson bracket correspondence can be established from here. The Poisson bracket equation of motion for the phase of the harmonic oscillator is:

$$\frac{d\theta}{dt} = \{H,\theta\} = \omega(1-\delta(\theta-2k\pi))\,, \tag{4.34}$$

where $H = \frac{1}{2}(p^2+\omega^2x^2)$ is the Hamiltonian and $\theta = \arctan(p/\omega x)$ is the phase. The identification $[\hat{N},\hat{A}_\theta] = i\hbar\omega\{H,\theta\}$ is straightforward and we recover a sawtooth profile for the phase variable just as happened in (4.5) for the angle variable.

Note that relation (4.32) is found through the expected value over phase coherent states and not in any physical state as in [32]. This shows that states (4.16), as canonical coherent states, hold the closest to classical behavior. Another main feature is that any $|\theta)$ state is equally weighted over the number basis, which confirms a total indeterminacy on the eigenstates of the number operator. The opposite is also true, a number state is equally weighted over all the family (4.16) and in particular this coincides with results in [32].

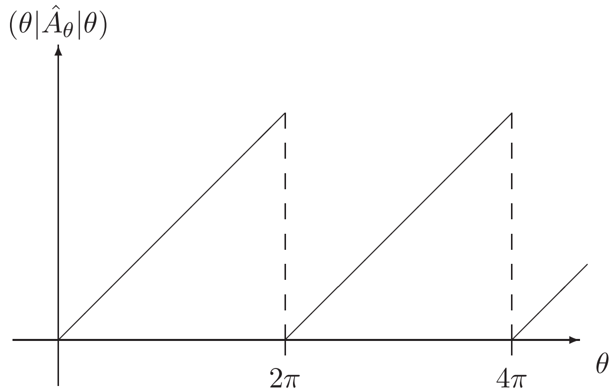


Figure 4.3: Mean value of the phase operator at the $N \to \infty$ limit.

The creation and annihilation operators are obtained using first the quantization (4.21) with $f(\theta) = e^{\pm i\theta}$:

$$\hat{A}_{e^{\pm i\theta}} = \int_0^{2\pi} e^{\pm i\theta} N|\theta)(\theta|\frac{d\theta}{2\pi}\,, \tag{4.35}$$

and then including the number operator as $\hat{A}_{e^{i\theta}}\hat{N}^{\frac{1}{2}} \equiv \hat{a}$ in a similar way to [32] where the authors used instead $e^{i\hat{\theta}_{PB}}\hat{N}^{\frac{1}{2}}$. The commutation relation between both operators is

$$[\hat{a}, \hat{a}^\dagger] = 1 - N|N-1\rangle\langle N-1|\,, \tag{4.36}$$

which converges to the common result only when the expectation value is taken on states where extremal state component vanish as n tends to infinity.

As the phase operator is not built from a spectral decomposition, it is clear that $\hat{A}_{\theta^2} \neq \hat{A}_\theta^2$ and the link with an uncertainty relation is not straightforward as in [32], instead, as is suggested in [16], a different definition for the variance should be used.

The phase operator constructed here has most of the advantages of the Pegg-Barnett operator but allows more freedom within the Hilbertian framework. It is clear that a well-defined phase operator must be parametrised by all points in the circle in order to have a natural convergence to the commutation relation in the classical limit. It remains also clear that as in any measure, like Pegg-Barnett's or this one through coherent sates, the inconveniences due to the non periodicity of the phase pointed in [31] are avoided from the very beginning in the choice of $X \equiv S^1$.

5

SU(N)

Now we will see that coherent state quantization can also permit a good description of the relative phases on a multi-level system. In the two level case, widely used in quantum information since it allows to encode information onto a "quantum bit", the relative phase of any state $\binom{c_1}{c_2}$ is

$$\alpha = \frac{c_1}{c_2} \,. \tag{5.1}$$

The coset space For the harmonic oscillator is the complex plane $\mathbb{C} = \mathrm{H}/U(1)$, where H is the Weyl-Heisenberg group. For the $SU(2)$ group, corresponding to the two level case, a useful compact expression of this space is to project it stereographically into the sphere S^2, in this context called Bloch sphere. A $SU(N)$ Cartan decomposition of the same type can be done in multiple ways, in particular, factorizing the maximal subgroup $S(U(1) \times U(N-1))$, the homogeneous space corresponding to the sphere $S^{2(N-1)}$. This sphere contains all the physical observables of an N level system, and its states, pure and mixed, are represented faithfully by their density matrices up to a general phase.
The measurement of the relative phases requires a generalization of the theory of projective measurements first stated by Von Neumann [50]. Instead of using an orthonormal basis of the observable, the generalization requires the use of a positive operator-valued measure (POVM). This measure, formed by an operator set, must resolve the identity and allows the calculation of a probability, in other words it can be constructed using a total family indexed by the observable to be evaluated. A coherent state density matrix is a natural candidate for constructing a good POVM as it still resolves the identity integrated in a marginal way and thus can be used for measuring the relative phases inside a quantum system. Relative phase measures in quantum information theory are important in the implementation of conditional phase shifts operations [48] which are universal gates for quantum computing.

In this part we will expose first the protocol for coherent state construction using $SU(2)$, then we will apply it to $SU(3)$ via the coset $X = SU(3)/S(U(1) \times U(2))$. With the projector of this coherent state family we will then construct the POVM for the phases on a qutrit. In a final section we will generalize the coherent state construction for $SU(N)$ using a $SU(N)/S(U(N-n)\times U(n))$ coset and then taking a more general coset $SU(N)/S(U_1(n_1)\times U_2(n_2)\times\cdots\times U_j(n_j))$.

5.1 Coherent state construction

The coherent states have been historically constructed using three of their properties; if expanded in the Fock basis they can be generated as the eigenvectors of the annihilation operator, taken as the shift of an extremal state on the phase space [10], or be chosen to minimize the Heisenberg uncertainty relation. In a more general context, the group-theoretical approach [44][54] use the decomposition of the dynamical group of the quantum system G into a maximum stability subgroup H and its coset space G/H. The coherent states are defined then as $\Omega|\phi_0\rangle \equiv |\Omega\rangle$, i.e. the result of applying a group element to an H invariant, referential state $|\phi_0\rangle$ on the Hilbert space of the Hamiltonian as

$$g|\phi_0\rangle = \Omega h|\phi_0\rangle = |\Omega\rangle e^{i\phi(h)}\,, \tag{5.2}$$

where $h\in H$ and $\phi(h)$ is a phase factor depending on the structure of H. Here we present a more general canonical form of construction [21] that will allow us to fit the particular needs of a multi-level system description.

The general procedure consists in doing a Cartan decomposition of an arbitrary element of the group, then finding a homogeneous space X, with a measure $\mu(dX)$ on it, on which the coset is parametrized. Our coherent states will be then constructed as a normalized linear combination of elements of an orthonormal system in this space that will resolve the identity.

Let us expose this procedure for the simplest case, the $SU(2)$ group. As a first step we will decompose any element g of the group via a polar decomposition

$$g=\begin{pmatrix} a & b\\ -\bar{b} & \bar{a}\end{pmatrix} = UT = \begin{pmatrix} |a| & ba/|a|\\ -\bar{b}\bar{a}/|a| & |a|\end{pmatrix}\begin{pmatrix} e^{i\phi/2} & 0\\ 0 & e^{-i\phi/2}\end{pmatrix}, \tag{5.3}$$

where $a,b\in\mathbb{C}$, T is a unitary matrix and $e^{i\phi/2}=a/|a|$. Since the first matrix in the decomposition is parametrized by the homogeneous space $\mathbb{C}=SU(2)/U(1)$, it can be indexed by the variable $\alpha=b/\bar{a}$. We can then reparametrize U as

$$U=\begin{pmatrix} 1/(1+|\alpha|^2)^{1/2} & \alpha/(1+|\alpha|^2)^{1/2}\\ -\bar{\alpha}/(1+|\alpha|^2)^{1/2} & 1/(1+|\alpha|^2)^{1/2}\end{pmatrix}, \tag{5.4}$$

where $\alpha\in\mathbb{C}$.

We need now a measure for building the inner product in the Hilbert space $L^2(\mathbb{C})$:

$$\int_{\mathbb{C}^2}\mu(d\alpha)\bar{f}(\alpha)g(\alpha)\,. \tag{5.5}$$

In $SU(2)$, the invariant measure can be found as follows. Acting with an element of the group over the homogeneous space:

$$x' = gx = \begin{pmatrix} a & b \\ -\bar{b} & \bar{a} \end{pmatrix} \begin{pmatrix} 1/(1+|\alpha|^2)^{1/2} & \alpha/(1+|\alpha|^2)^{1/2} \\ -\bar{\alpha}/(1+|\alpha|^2)^{1/2} & 1/(1+|\alpha|^2)^{1/2} \end{pmatrix} \quad (5.6)$$

$$= \begin{pmatrix} a' & b' \\ -\bar{b}' & \bar{a}' \end{pmatrix}, \quad (5.7)$$

and

$$\alpha' = \frac{b'}{\bar{a}'} = \frac{a\alpha + b}{-\bar{b}\alpha + \bar{a}}. \quad (5.8)$$

Differentiating and reorganizing we find:

$$\frac{d\alpha d\bar{\alpha}}{|1+|\alpha|^2|^2} = \frac{d\alpha' d\bar{\alpha}'}{|1+|\alpha'|^2|^2}, \quad (5.9)$$

which gives the form of the invariant measure.

$$\mu(d\alpha) = \frac{1}{2\pi}\frac{d^2\alpha}{(1+|\alpha|^2)^2}. \quad (5.10)$$

More generally, the power of the denominator can be taken as a parameter ν, in a way to have the measure $\mu(d\alpha)$ parametrized on the homogeneous space as

$$\mu(d\alpha) = \frac{1}{\pi}\frac{d^2\alpha}{(1+|\alpha|^2)^\nu}, \quad (5.11)$$

where π comes from normalizing the function $\mathbf{1}$.

For building the coherent states we take first an orthonormal system $\{|n\rangle\}$ in $L^2(\mathbb{C})$ (or after a stereographical projection, in $L^2(S^2)$), we construct then a new orthogonal system $\Phi_n(\alpha) = C_n\alpha^n$, with $\alpha \in \mathbb{C}$, and finally take the normalized finite linear combination of them:

$$|\alpha\rangle = \frac{1}{\sqrt{\mathcal{N}(\alpha)}}\sum_{n=0}^{\lfloor\nu-1\rfloor} C_n\alpha^n|n\rangle, \quad (5.12)$$

where $\lfloor x \rfloor$ stands for the integer part of a number x and

$$\mathcal{N}(\alpha) = \sum_n |C_n|^2|\alpha|^{2n}. \quad (5.13)$$

To ensure that the states $|\alpha\rangle$ be non trivial and will lie within L^2, we must impose that $\nu > 2$ in the measure. As we will see this choice, quasi-invariant under the action of $SU(2)$, will allow us to manipulate the extent of the sum. Now we can calculate the coefficients C_n, and find the normalized states:

$$|\alpha\rangle = \frac{1}{\sqrt{\mathcal{N}(\alpha)}}\sum_n \binom{\nu+1}{n}^{\frac{1}{2}}\alpha^n|n\rangle, \quad (5.14)$$

where $\mathcal{N}(\alpha) = \sum_n \binom{\nu+1}{n} |\alpha|^{2n}$. We can see that this family of states resolve the identity:

$$\int_{\mathbb{C}} \mathcal{N}(\alpha)|\alpha\rangle\langle\alpha|\mu(d\alpha) = \mathbb{I}\,. \tag{5.15}$$

and so it can be used to represent any state in $L^2(\mathbb{C})$.

We can now follow the same path for the group $SU(3)$ to produce a coherent state family. First we can write any element of the group as

$$g = \begin{pmatrix} c & v\dagger \\ w & m \end{pmatrix}, \tag{5.16}$$

where $c \in \mathbb{C}$, $v\dagger = (v_1, v_2), w = \binom{w_1}{w_2} \in \mathbb{C}^2$, and $m \in M_{2\times 2}(\mathbb{C})$. As before we factorize its maximal compact subgroup $S(U(1) \times U(2))$

$$g = \begin{pmatrix} \frac{1}{(1+\xi\dagger\xi)^{1/2}} & \xi\frac{1}{(1+\xi\xi\dagger)^{1/2}} \\ -\xi\dagger\frac{1}{(1+\xi\dagger\xi)^{1/2}} & \frac{1}{(1+\xi\xi\dagger)^{1/2}} \end{pmatrix} \begin{pmatrix} e^{i\phi} & 0 \\ 0 & u \end{pmatrix}, \tag{5.17}$$

where the first matrix represents the homogeneous space $X = SU(3)/S(U(1)\times U(2)) = \mathbb{C}^2$ parametrized by a complex two element line vector $\xi\dagger = (\alpha \;\; \beta)$, and the second is the maximal subgroup where $u \in U(2)$ and $\det u = e^{-i\phi}$. This factorization is always possible when the matrix m is invertible which covers all the cases but a zero measure space.

We can then construct the measure on the space X normalized under the scalar product (5.5) which must be of the form

$$\mu(d\alpha, d\beta) = \frac{1}{\pi^2}\binom{\nu-1}{\nu-3}\frac{d^2\alpha d^2\beta}{(1+|\alpha|^2+|\beta|^2)^{\nu}}\,, \tag{5.18}$$

where the binomial term, that comes from the normalization of the function $\mathbf{1}$, impose that $\nu \geq 3$. The upper bound of ν will be established latter. We can take now an orthonormal system in $L^2(X, \mu)$ of the form

$$\begin{aligned} \phi_{mn}(\alpha,\beta) &= C_{nm}\bar{\alpha}^n\bar{\beta}^m \\ &= \left[\binom{n+m}{m}\binom{\nu-3}{m+n}\right]^{1/2}\bar{\alpha}^n\bar{\beta}^m, \end{aligned} \tag{5.19}$$

where m, n must satisfy $0 < n+m < \nu-2$ in order to hold the square-integrability. Finally, expanded in this basis, we find the coherent states as

$$\begin{aligned} |\alpha,\beta\rangle &= \frac{1}{\sqrt{\mathcal{N}(\alpha,\beta)}}\sum_{0\leq n+m<\nu-2}\bar{\phi}_{nm}(\alpha,\beta)|\phi_{n,m}\rangle \\ &= \frac{1}{\sqrt{\mathcal{N}(\alpha,\beta)}}\sum_{0\leq n+m<\nu-2}\left[\binom{n+m}{m}\binom{\nu-3}{n+m}\right]^{1/2}\alpha^n\beta^m|n,m\rangle\,. \end{aligned} \tag{5.20}$$

Here we have used the Fock notation $|n,m\rangle = \phi_{nm}$, and the normalization factor is given by:

$$\begin{aligned}\mathcal{N}(\alpha,\beta) &= \sum_{0\leq n+m<\nu-2} |\phi_{mn}(\alpha,\beta)|^2 \\ &= \sum_{0\leq n+m<\nu-2} \binom{n+m}{m}\binom{\nu-3}{n+m}|\alpha|^{2n}|\beta|^{2m} . \end{aligned} \tag{5.21}$$

As in $SU(2)$, resolution of identity is guaranteed through

$$\int_{\mathbb{C}^2} \mathcal{N}(\alpha,\beta)|\alpha,\beta\rangle\langle\alpha,\beta|\mu(d\alpha d\beta) = \mathbb{I} . \tag{5.22}$$

As an example of a particular application of these coherent states we can extend the summation to $\nu = 4$ and obtain the state

$$|\alpha,\beta\rangle = \frac{1}{\sqrt{1+|\alpha|^2+|\beta|^2}} \left(|0,0\rangle + \alpha|1,0\rangle + \beta|0,1\rangle\right) , \tag{5.23}$$

i.e. a three level system, or qutrit, with amplitudes parametrized by X. Note that the identity resolution allows to keep just some terms in larger expansions and still have a total family. We have thus multiple ways of representing a multilevel system.

5.2 Positive Operator Valued Measures and coherent states

As was said before a POVM can be written as projector of an overcomplete system as the coherent states (5.14): $\hat{\Delta} = |\alpha\rangle\langle\alpha|$, which integrated marginally in the homogeneous space X will still satisfy appropriate conditions. If the elements of $X = \mathbb{C}$ are written here as $\alpha = re^{\phi} \in \mathbb{C}$, we will integrate marginally this projector just over the radial part of α:

$$\hat{\Delta}(\phi) = \int_0^\infty \hat{\Delta}(\alpha)\, dr = \int_0^\infty |\alpha\rangle\langle\alpha| dr . \tag{5.24}$$

We expect to be able to measure with it the relative phases in a three level system.

In the case of the qutrit in $SU(3)$ we have many choices for building a POVM for the relative phases. The first option is to take $\nu = 4$ in the coherent state (5.20) to have the sum

$$|\alpha,\beta\rangle = \frac{1}{\sqrt{N}}(|0,0\rangle + \alpha|1,0\rangle + \beta|0,1\rangle) . \tag{5.25}$$

Here can identify the Fock states with the qutrit levels as $|1\rangle = |0,0\rangle$, $|2\rangle = |1,0\rangle$ and $|3\rangle = |0,1\rangle$. Integrating over the radial part of the complex numbers α and β, we obtain the POVM:

$$\begin{aligned}\hat{\Delta}(\theta_1,\theta_2) &= \int_0^\infty \int_0^\infty |\alpha,\beta\rangle\langle\alpha,\beta| dr_1 dr_2 \\ &= \frac{1}{4\pi^2}[\,\mathbb{I} + \frac{\pi}{4}(e^{-i\theta_1}|1\rangle\langle 2| + e^{-i\theta_2}|1\rangle\langle 3| \\ &+ e^{i(\theta_1-\theta_2)}|2\rangle\langle 3| + h.c.)]\,, \end{aligned} \tag{5.26}$$

where $h.c.$ denotes the hermitian conjugate.
Modifying the initial relative phases as $|1\rangle \to e^{-i\theta_1}|1\rangle$ and $|2\rangle \to e^{-i\theta_2}|2\rangle$ we can see that (5.26) gives a measurement of the relative phases in the qutrit with a probability

$$\begin{aligned}P(\theta_1,\theta_2) &= \frac{1}{4\pi^2}[1 + \frac{\pi}{16}(\rho_{12}e^{i2\theta_1-\theta_2} + \rho_{13}e^{i\theta_1+\theta_2} \\ &+ \rho_{23}e^{i2\theta_1-\theta_1)} + h.c.)]\,, \end{aligned} \tag{5.27}$$

where ρ_{ij} are matrix elements of the density matrix for a qutrit. If we work out some phase operator which will not be detailed here (see Appendix II), and we ask it to shift the phases we can see that this POVM is shifted in the phases

$$e^{iE_{12}}\hat{\Delta}(\theta_1,\theta_2)e^{-iE_{12}} = \hat{\Delta}(\theta_1+\phi,\theta_2) \tag{5.28}$$

$$e^{iE_{23}}\hat{\Delta}(\theta_1,\theta_2)e^{-iE_{23}} = \hat{\Delta}(\theta_1,\theta_2+\phi')\,, \tag{5.29}$$

as expected, where E_{12} and E_{23} are the $SU(3)$ generators conjugated to the corresponding relative phases.

Other possible descriptions of the qutrit can be made with higher values of ν. In this case we have to choose three terms from expansion (5.20). For example, with $\nu = 5$ we can keep the terms

$$|\alpha,\beta\rangle = \frac{1}{\sqrt{N}}(|0,0\rangle + \alpha|1,0\rangle + \alpha\beta|1,1\rangle)\,. \tag{5.30}$$

We can also obtain a POVM for this state since this incomplete coherent state sum still resolves the identity. This leads to a measure of the form

$$\begin{aligned}\hat{\Delta}(\theta_1,\theta_2) &= \frac{1}{4\pi^2}[\,\mathbb{I} + \frac{\pi}{16}(e^{-i\theta_1}|0,0\rangle\langle 1,0| + e^{-i\theta_2}|1,0\rangle\langle 1,1| \\ &+ e^{-i(\theta_1+\theta_2)}|0,0\rangle\langle 1,1| + h.c.)]\,. \end{aligned} \tag{5.31}$$

Which gives a probability

$$\begin{aligned}P(\theta_1,\theta_2) &= \frac{1}{4\pi^2}[1 + \frac{\pi}{16}(\rho_{10,00}e^{-i\theta_1} + \rho_{11,10}e^{-i\theta_2} \\ &+ \rho_{11,00}e^{-i(\theta_1+\theta_2)} + h.c.)]\,, \end{aligned} \tag{5.32}$$

of finding the relative phases on the qutrit.

5.3 Coherent states of SU(N)

For a space of N dimensions we have more than one possible Cartan decomposition with coset

$$X = SU(N)/S(U(N-n) \times U(n)) \,. \tag{5.33}$$

We can write a general element of $SU(N)$ taking $m = N - n$ as

$$g = \begin{pmatrix} A & B \\ C & D \end{pmatrix}, \tag{5.34}$$

where A, B, C and D are $m \times m$, $m \times n$, $n \times m$, and $n \times n$ matrices. As done before we can write the Cartan decomposition as

$$g = \begin{pmatrix} (\mathbb{I}_m + ZZ\dagger)^{-\frac{1}{2}} & Z(\mathbb{I}_n + Z\dagger Z)^{-\frac{1}{2}} \\ -Z\dagger(\mathbb{I}_m + ZZ\dagger)^{-\frac{1}{2}} & (\mathbb{I}_n + Z\dagger Z)^{-\frac{1}{2}} \end{pmatrix} \begin{pmatrix} U_A & 0 \\ 0 & U_D \end{pmatrix} . \tag{5.35}$$

We can see that the last matrix has $n^2 + m^2$ parameters, and since Z must have $2mn$ parameters, it can be written as a $m \times n$ complex matrix. Coherent state construction can be done then using the orthonormal system

$$\phi_{\alpha_1\alpha_2\cdots\alpha_{mn}\nu}(\xi_1\xi_2\cdots\xi_{mn}) = C_{\alpha_1\alpha_2\cdots\alpha_{mn}\nu}\bar{\xi}_1^{\alpha_1}\bar{\xi}_2^{\alpha_2}\cdots\bar{\xi}_{mn}^{\alpha_{mn}} \,, \tag{5.36}$$

and a measure of the same type we have used until now

$$\mu(d\xi) = \frac{d^{2mn}\xi}{(1 + ||Z||^2)^\nu} \,, \tag{5.37}$$

where $||Z||^2 = |\xi_1|^2 + |\xi_2|^2 + \cdots + |\xi_{mn}|^2$ and $\xi_j \in \mathbb{C}$. Coefficients can be calculated to be

$$C_{\alpha_1\alpha_2\cdots\alpha_{mn}\nu} = \left[\binom{\nu - mn - 1}{\alpha_1 + \alpha_2 + \cdots + \alpha_{mn}} \binom{\alpha_1 + \alpha_2 + \cdots + \alpha_{mn}}{\alpha_{mn}} \binom{\alpha_1 + \alpha_2 + \cdots + \alpha_{mn-1}}{\alpha_{mn-1}} \cdots \binom{\alpha_1 + \alpha_2}{\alpha_1} \right]^{1/2}, \tag{5.38}$$

Where $0 < \alpha_1 + \alpha_2 + \cdots + \alpha_{mn} < \nu - mn - 1$. The coherent state will take then the form

$$|\xi_1, \xi_2, \cdots, \xi_{mn}\rangle = \frac{1}{\sqrt{\mathcal{N}}} \sum_{\alpha_1,\alpha_2,\cdots\alpha_{mn},\nu} C_{\alpha_1\alpha_2\cdots\alpha_{mn}\nu}\, \xi_1^{\alpha_1}\xi_2^{\alpha_2}\cdots\xi_{mn}^{\alpha_{mn}} |\alpha_1, \alpha_2, \cdots, \alpha_{mn}\rangle \,, \tag{5.39}$$

normalized by

$$\mathcal{N}(\alpha_1, \alpha_2, \cdots, \alpha_{mn}, \nu) = \sum_{\alpha_1,\alpha_2,\cdots\alpha_{mn},\nu} |C_{\alpha_1\alpha_2\cdots\alpha_{mn}\nu}\xi_1^{\alpha_1}\xi_2^{\alpha_2}\cdots\xi_{mn}^{\alpha_{mn}}|^2 \,. \tag{5.40}$$

In quantum information the cases where $SU(N)$ is decomposed as

$$X = SU(N)/S(U_1(2) \times \cdots \times U_n(2) \times \cdots \times U_1(3) \times \cdots \times U_m(3)) , \quad (5.41)$$

are of particular interest as they represent all the possible interactions between qubits and qutrits. The $SU(N)$ group has $N^2 - 1 = 4n^2 + 9m^2 + 12nm - 1 =$ parameters and the homogeneous space X will have then $M = N^2 - 4n - 9m = 4(n^2 - n) + 9(m^2 - m)$ real variables, where n is the number of qubits and m is the number of qutrits. Note that M is always even so we can construct the coherent states generalized from the procedure that we have already followed. More generally, for any multiple partition of $SU(N)$ decomposed then as $SU(N)/S(U_1(n_1) \times U_2(n_2) \times \cdots \times U_j(n_j))$, the homogeneous space will have $M = (\sum_i n_i)^2 - \sum_i n_i^2$ which is always even and we will then be able to parametrize X with $M/2$ complex variables. Namely the decomposition will have the following form

$$\begin{aligned} g &= \begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1j} \\ A_{21} & A_{22} & & \\ \vdots & & \ddots & \\ A_{j1} & \cdots & & A_{jj} \end{pmatrix} \\ &= \begin{pmatrix} (A_{11}A_{11}^\dagger)^{\frac{1}{2}} & A_{12}A_{22}^{-1}(A_{22}A_{22}^\dagger)^{\frac{1}{2}} & \cdots & A_{1j}A_{jj}^{-1}(A_{jj}A_{jj}^\dagger)^{\frac{1}{2}} \\ A_{21}A_{11}^{-1}(A_{11}A_{11}^\dagger)^{\frac{1}{2}} & (A_{22}A_{22}^\dagger)^{\frac{1}{2}} & & \\ \vdots & & \ddots & \\ A_{j1}A_{11}^{-1}(A_{11}A_{11}^\dagger)^{\frac{1}{2}} & \cdots & & (A_{jj}A_{jj}^\dagger)^{\frac{1}{2}} \end{pmatrix} \\ &\times \begin{pmatrix} U_1 & 0 & \cdots & 0 \\ 0 & U_2 & & \\ \vdots & & \ddots & \\ 0 & & & U_j \end{pmatrix} . \end{aligned} \quad (5.42)$$

We have to construct then a measure parametrized by the complex space $\mathbb{C}^{M/2}$ as

$$\mu(d\xi) = \frac{d\xi^{M/2}}{(1 + |\xi|^2)^\nu} , \quad (5.43)$$

and choose the orthonormal vectors $\phi_n(\vec{\xi})$

$$\phi = C_{\alpha_1\alpha_2\cdots\alpha_{M/2}\nu} \bar{\xi}_1^{\alpha_1} \bar{\xi}_2^{\alpha_2} \cdots \bar{\xi}_{M/2}^{\alpha_{M/2}} , \quad (5.44)$$

in the Hilbert space $L^2(\xi)$, with $\xi \in \mathbb{C}$. The general coherent state will be after normalization

$$|\xi_1, \xi_2, \cdots \xi_{M/2}\rangle = \frac{1}{\sqrt{\mathcal{N}}} \sum_{\alpha_1,\alpha_2,\cdots\alpha_{M/2},\nu} C_{\alpha_1\alpha_2\cdots\alpha_{M/2}\nu} \, \xi_1^{\alpha_1} \xi_2^{\alpha_2} \cdots \xi_{M/2}^{\alpha_{M/2}} |\alpha_1, \alpha_2, \cdots \alpha_{M/2}\rangle, \quad (5.45)$$

Where

$$C_{\alpha_1\alpha_2\cdots\alpha_{M/2}\nu} = \left[\binom{\nu - M/2 - 1}{\alpha_1 + \alpha_2 + \cdots + \alpha_{M/2}} \binom{\alpha_1 + \alpha_2 + \cdots + \alpha_{M/2}}{\alpha_{M/2}} \binom{\alpha_1 + \alpha_2 + \cdots + \alpha_{M/2-1}}{\alpha_{M/2-1}} \cdots \binom{\alpha_1 + \alpha_2}{\alpha_1} \right]^{1/2} , \quad (5.46)$$

and normalization is given as before as:

$$\mathcal{N} = \sum_{\alpha_1,\alpha_2,\cdots\alpha_{M/2},\nu} |C_{\alpha_1\alpha_2\cdots\alpha_{M/2}\nu}|^2 |\xi_1|^{2\alpha_1}|\xi_2|^{2\alpha_2}\cdots|\xi_{M/2}|^{2\alpha_{M/2}} \,. \tag{5.47}$$

These coherent states, as before, resolve the identity:

$$\int_X \mathcal{N}|\xi_1,\xi_2,\cdots\xi_{M/2}\rangle\langle\xi_1,\xi_2,\cdots\xi_{M/2}|\mu(d\xi) = \mathbb{I}\,. \tag{5.48}$$

We have then a systematic protocol to produce coherent states for any partition of $SU(N)$.

5.4 Relative phase operator

To construct a phase operator we can again use the projector of a coherent state weighted by an arbitrary phase. This will produce a matrix term by term that we can adjust then to our needs. In the case of $SU(3)$ we can take:

$$\begin{aligned} A_{p,q} &= \int_{\mathbb{C}^2} N(\alpha,\beta)e^{i\,p\,\phi_\alpha}e^{i\,q\,\phi_\beta}|\alpha,\beta\rangle\langle\alpha,\beta|\mu(d\alpha,d\beta) \\ &= \pi^2\sum_{m,n,m',n'} C_\nu C_{m,n}C_{m',n'}B\big(\tfrac{1}{2}(m+n+m'+n')+2,\,\nu-\tfrac{1}{2}(m+n+m'+n')-2\big) \\ &\times\; B\big(\tfrac{1}{2}(m+m')+1,\,\tfrac{1}{2}(n+n')+1\big)\delta_{p,m'-m}\delta_{q,n'-n}|m,n\rangle\langle m',n'|\,, \end{aligned} \tag{5.49}$$

where,

$$C_\nu = \frac{1}{\pi^2}\binom{\nu-1}{\nu-3} \tag{5.50}$$

$$C_{m,n} = \left[\binom{\nu-3}{m+n}\binom{m+n}{m}\right]^{\frac{1}{2}}. \tag{5.51}$$

Here if $\nu = 4$ then $C_\nu = 3/\pi^2$ and p and q take the values given by the following table

For p	=m'-m		For q	=n'-n	
$m\backslash m'$	0	1	$n\backslash n'$	0	1
0	0	1	0	0	1
1	-1	0	1	-1	0

Note that the case where $m = 1, m' = 1$ is allowed when $n = 0, n' = 0$. We have then all the following combinations

p	q	projector	Coefficients
-1	0	$\|1,0\rangle\langle 0,0\|$	$C_\nu C_{1,0}C_{0,0}B(5/2,3/2)B(3/2,1) = 1/8\pi$
-1	1	$\|1,0\rangle\langle 0,1\|$	$C_\nu C_{1,0}C_{0,1}B(3,1)B(3/2,3/2) = 1/24\pi$
0	-1	$\|0,1\rangle\langle 0,0\|$	$C_\nu C_{0,1}C_{0,0}B(5/2,3/2)B(1,3/2) = 1/8\pi$
0	0	$\|0,0\rangle\langle 0,0\|$	$C_\nu C_{0,0}C_{0,0}B(2,2)B(1,1) = 1/2\pi^2$
0	0	$\|0,1\rangle\langle 0,1\|$	$C_\nu C_{0,1}C_{0,1}B(3,1)B(1,2) = 1/2\pi^2$
0	0	$\|1,0\rangle\langle 1,0\|$	$C_\nu C_{1,0}C_{1,0}B(3,1)B(2,1) = 1/2\pi^2$
0	1	$\|0,0\rangle\langle 0,1\|$	$C_\nu C_{0,0}C_{0,1}B(5/2,3/2)B(1,3/2) = 1/8\pi$
1	-1	$\|0,1\rangle\langle 1,0\|$	$C_\nu C_{0,1}C_{1,0}B(3,1)B(3/2,3/2) = 1/24\pi$
1	0	$\|0,0\rangle\langle 1,0\|$	$C_\nu C_{0,0}C_{1,0}B(5/2,3/2)B(3/2,1) = 1/8\pi$

Here all the diagonal terms are given by different ways of writing $A_{0,0}$. If we label the qutrit as $|0\rangle = |0,0\rangle, |1\rangle = |0,1\rangle, |2\rangle = |1,0\rangle$, the operator will be given by:

$$A = \begin{pmatrix} A_{0,0}^{(1)} & A_{0,1} & A_{1,0} \\ A_{0,-1} & A_{0,0}^{(2)} & A_{1,-1} \\ A_{-1,0} & A_{-1,1} & A_{0,0}^{(3)} \end{pmatrix}. \tag{5.52}$$

6

Infinite quantum well

6.1 Introduction

Even though the quantum dynamics in an infinite square well potential represents a rather unphysical limit situation, it is a familiar textbook problem and a simple tractable model for the confinement of a quantum particle. On the other hand this model has a serious drawback when it is analyzed in more detail. Namely, when one proceeds to a canonical standard quantization, the definition of a momentum operator with the usual form $-\mathrm{i}\hbar \mathrm{d}/\mathrm{d}x$ has a doubtful meaning. This subject has been discussed in many places (see [14] for instance), and the attempts of circumventing this anomaly range from self-adjoint extensions [14] to $\mathcal{PT}$ symmetry approaches [36].

First of all, the canonical quantization assumes the existence of a momentum operator (essentially) self-adjoint in $\mathrm{L}^2(\mathbb{R})$ that respects some boundary conditions on the boundaries of the well. As has been shown, these conditions cannot be fullfilled by the usual derivative form of the momentum without the consequence of losing self-adjointness. Moreover there exists an uncountable set of self-adjoint extensions of such a derivative operator which makes truly delicate the question of a precise choice based on physical requirements [14, 51].

When the classical particle is trapped in an infinite well of real interval Δ, the Hilbert space of quantum states is $\mathrm{L}^2(\Delta, \mathrm{d}x)$ and the quantization problem becomes similar, to a certain extent, to the quantization of the motion on the circle S^1. Notwithstanding the fact that boundary conditions are not periodic but impose instead that the wave functions in position representation vanish at the boundary, the momentum operator $\widehat{p}$ for the motion in the infinite well should be the counterpart of the angular momentum operator $\widehat{L}$ for the motion on the circle. Since the energy spectrum for the infinite square well is $\{n^2,\, n \in \mathbb{N}^*\}$, we should expect that the spectrum of $\widehat{p}$ should be $\mathbb{Z}^*$, like the one for $\widehat{L}$ without the null eigenvalue. This similarity between the two problems will be exploited in the present paper. We will adapt the coherent states (CS's) on the circle [47, 30, 3] to the present situation by constructing two-component vector CS's, in the spirit of [7], as infinite superpositions of spinors eigenvectors of $\widehat{p}$.

In the present note, we first describe the CS quantization procedure. We recall the construction of the CS's for the motion on the circle and the resulting quantization. We then revisit the infinite square well problem and propose a family of vector CS's suitable for the quantization of the related classical phase space. Note that various constructions of CS's for the infinite square well have been carried out, like the one in [9] or yet the one resting upon the dynamical $SU(1,1)$ symmetry [2]. Finally, we present the consequences of our choice after examining basic quantum observables, derived from this quantization scheme, as position, energy, and a quantum version of the problematic momentum. In particular we focus on their mean values in CS's ("lower symbols") and quantum dispersions. As will be shown, the classical limit is recovered after choosing appropriate limit values of some parameters present in the expression of our CS's.

6.2 Quantization of the motion in an infinite well potential

6.2.1 The standard quantum context

Any quantum system trapped inside the infinite square well $0 \leqslant q \leqslant L$ must have its wave function equal to zero beyond the boundaries. It is thus natural to impose on the wave functions the conditions

$$\psi(q) = 0, \qquad q \geqslant L \quad \text{and} \quad q \leqslant 0\,. \tag{6.1}$$

Since the motion takes place only inside the interval $[0, L]$, we may as well ignore the rest of the line and replace the constraints (6.1) by the following ones:

$$\psi \in \mathrm{L}^2([0,L], \mathrm{d}q), \qquad \psi(0) = \psi(L) = 0\,. \tag{6.2}$$

Moreover, one may consider the periodized well and instead impose the cyclic boundary conditions $\psi(nL) = 0$, $\forall n \in \mathbb{Z}$.

In either case, stationary states of the trapped particle of mass m are easily found from the eigenvalue problem for the Schrödinger operator with Hamiltonian:

$$H \equiv H_{\mathrm{w}} = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\,. \tag{6.3}$$

This Hamiltonian is self-adjoint [35] on an appropriate dense domain in (6.2). Then

$$\Psi(q,t) = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Ht}\Psi(q,0)\,, \tag{6.4}$$

where $\Psi(q,0) \equiv \psi(q)$ obeys the eigenvalue equation

$$H\psi(q) = E\psi(q)\,, \tag{6.5}$$

together with the boundary conditions (6.2). Normalized eigenstates and corresponding eigenvalues are then given by

$$\psi_n(q) = \sqrt{\frac{2}{L}}\sin\left(n\pi\frac{q}{L}\right)\,, \quad 0 \leqslant q \leqslant L\,, \tag{6.6}$$

$$H\psi_n = E_n\psi_n\,, \qquad n = 1, 2, \ldots,\,, \tag{6.7}$$

with

$$E_n = \frac{\hbar^2\pi^2}{2mL^2}n^2 \;\equiv\; \hbar\omega n^2\,, \qquad \omega = \frac{\hbar\pi^2}{2mL^2} \equiv \frac{2\pi}{T_r}\,, \tag{6.8}$$

where T_r is the "revival" time to be compared with the purely classical round trip time.

6.2.2 The quantum phase space context

The classical phase space of the motion of the particle is the infinite strip $X = [0, L] \times \mathbb{R} = \{x = (q, p) \mid q \in [0, L], p \in \mathbb{R}\}$ equipped with the measure: $\mu(\mathrm{d}x) = \mathrm{d}q\,\mathrm{d}p$. A phase trajectory for a given non-zero classical energy $E_{\mathrm{class}} = \frac{1}{2}mv^2$ is represented in the figure 6.1.

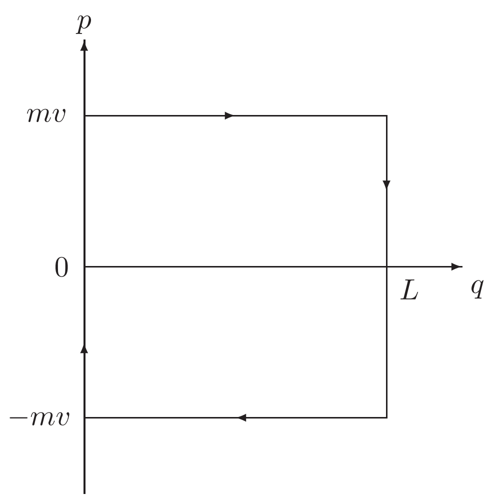


Figure 6.1: Phase trajectory of the particle in the infinite square-well.

Typically, we have two phases in the periodic particle motion with a given energy: one corresponds to positive values of the momentum, $p = mv$ while the other one is for negative values, $p = -mv$. This observation naturally leads us to introduce the Hilbert space of two-component complex-valued functions (or spinors) square-integrable with respect to $\mu(\mathrm{d}x)$:

$$\mathrm{L}^2_{\mathbb{C}^2}(X, \mu(\mathrm{d}x)) \simeq \mathbb{C}^2 \otimes \mathrm{L}^2_{\mathbb{C}}(X, \mu(\mathrm{d}x)) = \left\{ \Phi(x) = \begin{pmatrix} \phi_+(x) \\ \phi_-(x) \end{pmatrix},\ \phi_\pm \in \mathrm{L}^2_{\mathbb{C}}(X, \mu(\mathrm{d}x)) \right\}. \tag{6.9}$$

We now choose our orthonormal system as formed of the following vector-valued functions $\Phi_{n,\epsilon}(x)$, $\kappa = \pm$,

$$\Phi_{n,+}(x) = \begin{pmatrix} \phi_{n,+}(x) \\ 0 \end{pmatrix}, \qquad \Phi_{n,-}(x) = \begin{pmatrix} 0 \\ \phi_{n,-}(x) \end{pmatrix},$$
$$\phi_{n,\kappa}(x) = \sqrt{c}\,\exp\left(-\frac{1}{2\rho^2}(p - \kappa p_n)^2 \right) \sin\left(n\pi \frac{q}{L} \right), \qquad \kappa = \pm\,,\ n = 1, 2, \dots, \tag{6.10}$$

where

$$c = \frac{2}{\rho L \sqrt{\pi}}, \qquad p_n = \sqrt{2mE_n} = \frac{\hbar\pi}{L}\,n\,, \tag{6.11}$$

and the half-width $\rho > 0$ is a parameter that will be used in the following as a regulator which has the dimension of a momentum, say $\rho = \hbar\pi\vartheta/L$ with $\vartheta > 0$

a dimensionless parameter. This parameter can be arbitrarily small (as for the classical limit) and, of course, arbitrarily large (for a very narrow well, for instance).

The functions $\Phi_{n,\kappa}(x)$ are continuous, vanish at the boundaries $q = 0$ and $q = L$ of the phase space, and obey the essential finiteness condition (3.1):

$$\begin{aligned} 0 < \mathcal{N}(x) \equiv \mathcal{N}(q,p) \equiv \mathcal{N}_+(x) + \mathcal{N}_-(x) &= \sum_{\kappa=\pm}\sum_{n=1}^{\infty} \Phi^{\dagger}_{n,\kappa}(x)\Phi_{n,\kappa}(x) \\ &= c\sum_{n=1}^{\infty}\left[\exp\left(-\frac{1}{\rho^2}(p-p_n)^2\right) + \exp\left(-\frac{1}{\rho^2}(p+p_n)^2\right)\right]\sin^2\left(n\pi\frac{q}{L}\right) < \infty\,. \end{aligned} \tag{6.12}$$

The expression of $\mathcal{N}$ simplifies to :

$$\mathcal{N}(q,p) = c\,\mathcal{S}(q,p) = c\,\Re\left\{\frac{1}{2}\sum_{n=-\infty}^{\infty}\left[1-\exp\left(\mathrm{i}2\pi n\frac{q}{L}\right)\right]\exp\left(-\frac{1}{\rho^2}(p-p_n)^2\right)\right\}. \tag{6.13}$$

It then becomes apparent that $\mathcal{N}$ and $\mathcal{S}$ can be expressed in terms of elliptic theta functions. Function $\mathcal{S}$ has no physical dimension whereas $\mathcal{N}$ has the same dimension as c, that is the inverse of an action.

We are now in measure of defining our vector CS's [7]. As in the case of the circle, we set up a one-to-one correspondence between the functions $\Phi_{n,\kappa}$'s and two-component states

$$|n,\kappa\rangle \stackrel{\mathrm{def}}{=} \chi_\kappa \otimes |n\rangle\,, \qquad \chi_+ = \begin{pmatrix}1\\0\end{pmatrix}\,, \quad \chi_- = \begin{pmatrix}0\\1\end{pmatrix}\,, \tag{6.14}$$

forming an orthonormal basis of some separable Hilbert space of the form $\mathcal{K} = \mathbb{C}^2 \otimes \mathcal{H}$. The latter can be viewed also as the subspace of $\mathrm{L}^2_{\mathbb{C}^2}(X,\mu(\mathrm{d}x))$ equal to the closure of the linear span of the set of $\Phi_{n,\kappa}$'s. We choose the following set of 2×2 diagonal real matrices for our construction of vectorial CS's:

$$\mathrm{F}_n(x) = \begin{pmatrix}\phi_{n,+}(q,p) & 0\\ 0 & \phi_{n,-}(q,p)\end{pmatrix} \tag{6.15}$$

$$= \sqrt{c}\begin{pmatrix}\exp\left(-\frac{1}{2\rho^2}(p-p_n)^2\right) & 0\\ 0 & \exp\left(-\frac{1}{2\rho^2}(p+p_n)^2\right)\end{pmatrix}\sin\left(n\pi\frac{q}{L}\right)\,, \tag{6.16}$$

where $n = 1,2,\dots$. Note that $\mathcal{N}(x) = \sum_{n=1}^{\infty}\mathrm{tr}(F_n(x)^2)$.

Vector CS's, $|x,\chi\rangle \in \mathbb{C}^2\otimes\mathcal{H} = \mathcal{K}$, are now defined for each $x \in X$ and $\chi \in \mathbb{C}^2$ by the relation

$$|x,\chi\rangle = \mathcal{N}(x)^{-\frac{1}{2}}\sum_{n=1}^{\infty}\mathrm{F}_n(x)\,\chi\otimes|n\rangle\,. \tag{6.17}$$

In particular, we single out the two orthogonal CS's

$$|x,\kappa\rangle = \frac{1}{\sqrt{\mathcal{N}(x)}}\sum_{n=1}^{\infty}\mathrm{F}_n(x)|n,\kappa\rangle\,, \qquad \kappa = \pm\,. \tag{6.18}$$

By construction, these states also satisfy the infinite square well boundary conditions, namely $|x,\kappa\rangle_{q=0} = |x,\kappa\rangle_{q=L} = 0$. Furthermore they fulfill the normalizations

$$\langle x,\kappa|x,\kappa\rangle = \frac{\mathcal{N}_\kappa(x)}{\mathcal{N}(x)}\,, \qquad \sum_{\kappa=\pm}\langle x,\kappa|x,\kappa\rangle = 1\,, \tag{6.19}$$

and the resolution of the identity in $\mathcal{K}$:

$$\begin{aligned}\int_X |x\rangle\langle x|\mathcal{N}(x)\mu(\mathrm{d}x) &= \sum_{\kappa,\kappa'=\pm}\sum_{n,n'=1}^{\infty}\int_{-\infty}^{\infty}\int_0^L \mathrm{F}_n(q,p)\mathrm{F}_{n'}(q,p)|n,\kappa\rangle\langle n',\kappa'|\mathrm{d}q\mathrm{d}p\\ &= \sum_{\kappa=\pm}\sum_{n=1}^{\infty}|n,\kappa\rangle\langle n,\kappa| = \sigma_0\otimes\mathbb{I}_{\mathcal{H}} = \mathbb{I}_{\mathcal{K}}\,.\end{aligned} \tag{6.20}$$

where σ_0 denotes the 2×2 identity matrix consistently with the Pauli matrix notations σ_μ to be used in the following.

6.2.3 Quantization of classical observables

The quantization of a generic function $f(q,p)$ on the phase space is given by the expression (3.5), that is for our particular CS choice:

$$\begin{aligned}\widehat{f(q,p)} &= \sum_{\kappa=\pm}\int_{-\infty}^{\infty}\int_0^L f(q,p)|x,\kappa\rangle\langle x,\kappa|\mathcal{N}(q,p)\mathrm{d}q\mathrm{d}p\\ &= \sum_{n,n'=1}^{\infty}|n\rangle\langle n'|\otimes\begin{pmatrix}\widehat{f_+(q,p)} & 0\\ 0 & \widehat{f_-(q,p)}\end{pmatrix}\,,\end{aligned} \tag{6.21}$$

where

$$\widehat{f_\pm(q,p)} = \int_{-\infty}^{\infty}\mathrm{d}p\int_0^L \mathrm{d}q\,\phi_{n,\pm}(q,p)f(q,p)\overline{\phi_{n',\pm}}(q,p)\,. \tag{6.22}$$

For the particular case in which f is function of p only, $f(p)$, the operator is given by

$$\begin{aligned}\widehat{f(p)} = \sum_{\kappa=\pm}\int_{-\infty}^{\infty}\int_0^L f(p)|x,\kappa\rangle\langle x,\kappa|\mathcal{N}(q,p)\mathrm{d}q\mathrm{d}p = \frac{1}{\rho\sqrt{\pi}}\sum_{n=1}^{\infty}|n\rangle\langle n|\otimes\\ \otimes\begin{pmatrix}\int_{-\infty}^{\infty}\mathrm{d}p\,f(p)\exp\left(-\frac{1}{\rho^2}(p-p_n)^2\right) & 0\\ 0 & \int_{-\infty}^{\infty}\mathrm{d}p\,f(p)\exp\left(-\frac{1}{\rho^2}(p+p_n)^2\right)\end{pmatrix}\,.\end{aligned} \tag{6.23}$$

Note that this operator is diagonal on the $|n,\kappa\rangle$ basis.

Momentum and Energy

In particular, using $f(p) = p$, one gets the operator

$$\widehat{p} = \sum_{n=1}^{\infty}p_n\,\sigma_3\otimes|n\rangle\langle n|\,, \tag{6.24}$$

where $\sigma_3 = \left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right)$ is a Pauli matrix.

For $f(p) = p^2$, which is proportional to the Hamiltonian, the quantum counterpart reads as

$$\widehat{p^2} = \frac{\rho^2}{2}\mathbb{I}_{\mathcal{K}} + \sum_{n=1}^{\infty} p_n^2\,\sigma_0 \otimes |n\rangle\langle n| = \frac{\rho^2}{2}\mathbb{I}_{\mathcal{K}} + (\widehat{p})^2\,. \tag{6.25}$$

Note that this implies that the operator for the square of momentum does not coincide with the square of the momentum operator. Actually they coincide up to $\mathrm{O}(\hbar^2)$.

Position

For a general function of the position $f(q)$ our quantization procedure yields the following operator:

$$\widehat{f(q)} = \sum_{n,n'=1}^{\infty} \exp\big(-\frac{1}{4\rho^2}(p_n - p_{n'})^2\big)\,[d_{n-n'}(f) - d_{n+n'}(f)]\,\sigma_0 \otimes |n\rangle\langle n'|\,, \tag{6.26}$$

where

$$d_m(f) \equiv \frac{1}{L}\int_0^L f(q)\cos\left(m\pi\frac{q}{L}\right)\mathrm{d}q\,. \tag{6.27}$$

In particular, for $f(q) = q$ we get the "position" operator

$$\begin{aligned}\widehat{q} = \frac{L}{2}\mathbb{I}_{\mathcal{K}} - \frac{2L}{\pi^2}\sum_{n,n'\geq 1, n+n'=2k+1}^{\infty} &\exp\big(-\frac{1}{4\rho^2}(p_n - p_{n'})^2\big)\times \\ \times\left[\frac{1}{(n-n')^2} - \frac{1}{(n+n')^2}\right]&\sigma_0 \otimes |n\rangle\langle n'|\,,\end{aligned} \tag{6.28}$$

with $k \in \mathbb{N}$. Note the appearance of the classical mean value for the position on the diagonal.

Commutation rules

Now, in order to see to what extent these momentum and position operators differ from their classical (canonical) counterparts, let us consider their commutator:

$$[\,\widehat{q}, \widehat{p}\,] = \frac{2\hbar}{\pi}\sum_{\substack{n\neq n' \\ n+n'=2k+1}}^{\infty} C_{n,n'}\,\sigma_3 \otimes |n\rangle\langle n'| \tag{6.29}$$

$$C_{n,n'} = \exp\big(-\frac{1}{4\rho^2}(p_n - p_{n'})^2\big)(n-n')\left[\frac{1}{(n-n')^2} - \frac{1}{(n+n')^2}\right]. \tag{6.30}$$

This is an infinite antisymmetric real matrix. The respective spectra of finite matrix approximations of this operator and of position and momentum operators are compared in figures 6.2 and 6.3 for various values of the regulator $\rho = \hbar\pi\vartheta/L = \vartheta$ in units $\hbar = 1$, $L = \pi$. When ρ takes large values, one can see that the eigenvalues of $[\,\widehat{q}, \widehat{p}\,]$ accumulate around $\pm\mathrm{i}$, i.e. they become almost canonical. Conversely, when $\rho \to 0$ all eigenvalues become null, which corresponds to the classical limit.

Evolution operator

The Hamiltonian of a spinless particle trapped inside the well is simply $H = p^2/2m$. Its quantum counterpart therefore is $\widehat{H} = \widehat{p^2}/2m$. The unitary evolution operator, as usual, is given by

$$U(t) = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\widehat{H}t} = \mathrm{e}^{-i\omega_\vartheta t}\sum_{n=1}^{\infty}\exp\Big(-\frac{\mathrm{i}p_n^2 t}{2m\hbar}\Big)\sigma_0\otimes|n\rangle\langle n|\,. \tag{6.31}$$

Note the appearance of the global time-dependent phase factor with frequency ω_ϑ which can be compared with the revival frequency

$$\omega_\vartheta = \frac{\hbar\pi^2\vartheta^2}{4mL^2} = \frac{\omega\vartheta^2}{2}\,. \tag{6.32}$$

6.3 Quantum behaviour through lower symbols

Lower symbols are computed with normalized CS's. The latter are denoted as follows

$$|x\rangle = |x,+\rangle + |x,-\rangle\,. \tag{6.33}$$

Hence, the lower symbol of a quantum observable A should be computed as

$$\check{A}(x) = \langle x|A|x\rangle \equiv \check{A}_{++}(x) + \check{A}_{+-}(x) + \check{A}_{-+}(x) + \check{A}_{--}(x)\,.$$

This gives the following results for the observables previously considered :

Position

In the same way, the mean value of the position operator in a vector CS $|x\rangle$ is given by:

$$\langle x|\widehat{q}\,|x\rangle = \frac{L}{2} - Q(q,p)\,, \tag{6.34}$$

where we can distinguish the classical mean value for the position corrected by the function

$$\begin{aligned} Q(q,p) = \frac{2L}{\pi^2}\frac{1}{\mathcal{S}}\sum_{\substack{n,n'=1,n\neq n'\\ n+n'=2k+1}}^{\infty} &\exp\Big(-\frac{1}{4\rho^2}(p_n-p_{n'})^2\Big)\left[\frac{1}{(n-n')^2}-\frac{1}{(n+n')^2}\right]\times\\ &\times\Big[\exp\Big(-\frac{1}{2\rho^2}[(p-p_n)^2+(p-p_{n'})^2]\Big)+\\ &+\exp\Big(-\frac{1}{2\rho^2}[(p+p_n)^2+(p+p_{n'})^2]\Big)\Big]\sin\Big(n\pi\frac{q}{L}\Big)\sin\Big(n'\pi\frac{q}{L}\Big)\,. \end{aligned} \tag{6.35}$$

This function depends on the parameter ϑ, that is on the regulator ρ, as we show in figure 6.4 with a numerical approximation using finite matrices. As for $\widehat{p}$, we calculate the dispersion defined as

$$\Delta Q = \sqrt{\check{q^2} - \check{q}^2}\,. \tag{6.36}$$

Its behaviour for different values of ϑ is shown in figure 6.6.

Time evolution of position

The change through time of the position operator is given by the transformation $\widehat{q}(t) := U^{\dagger}(t)\,\widehat{q}\,U(t)$, and differs from $\widehat{q}$ by the insertion of an oscillating term in the series. Its lower symbol is given by

$$\langle x|\widehat{q}(t)|x\rangle = \frac{L}{2} - Q(q,p,t)\,, \tag{6.37}$$

where this time the series have the form

$$Q(q,p,t) = \frac{2L}{\pi^2}\frac{1}{\mathcal{S}} \sum_{\substack{n,n'=1, n\neq n' \\ n+n'=2k+1}}^{\infty} \exp\Big(-\frac{\mathrm{i}}{2m\hbar}(p_n^2 - p_{n'}^2)\,t\Big) \exp\Big(-\frac{1}{4\rho^2}(p_n - p_{n'})^2\Big)\times$$
$$\times\left[\frac{1}{(n-n')^2} - \frac{1}{(n+n')^2}\right]\sin\left(n\pi\frac{q}{L}\right)\sin\left(n'\pi\frac{q}{L}\right)\times$$
$$\times\left[\exp\Big(-\frac{1}{2\rho^2}[(p-p_n)^2 + (p-p_{n'})^2]\Big) + \exp\Big(-\frac{1}{2\rho^2}[(p+p_n)^2 + (p+p_{n'})^2]\Big)\right]. \tag{6.38}$$

Note that the time dependence manifests itself in the form of a Fourier series of with frequencies $(n^2 - n'^2)\,\hbar\pi^2/2mL^2$. This corresponds to the circulation of the wave packet inside the well.

Momentum

The mean value of the momentum operator in a vector CS $|x\rangle$ is given by the affine combination:

$$\langle x|\widehat{p}\,|x\rangle = \frac{\mathcal{M}(x)}{\mathcal{N}(x)}\,,$$
$$\mathcal{M}(x) = c\sum_{n=1}^{\infty} p_n\left[\exp\Big(-\frac{1}{\rho^2}(p-p_n)^2\Big) - \exp\Big(-\frac{1}{\rho^2}(p+p_n)^2\Big)\right]\sin^2\left(n\pi\frac{q}{L}\right). \tag{6.39}$$

This function reproduce the profile of the function p, as can be seen in the figure 6.5. We calculate then the dispersion ΔP, defined as

$$\Delta P = \sqrt{\check{p^2} - \check{p}^2}, \tag{6.40}$$

using the mean values in a CS $|x\rangle$. Its behaviour as a function of x is shown in figure 6.7.

Position-momentum commutator

The mean value of the commutator in a normalized state $\Psi = \binom{\phi_+}{\phi_-}$ is the pure imaginary expression:

$$\langle\Psi|[\,\widehat{q},\widehat{p}\,]|\Psi\rangle = \frac{2\mathrm{i}\hbar}{\pi}\sum_{\substack{n\neq n' \\ n+n'=2k+1}}^{\infty} \exp\Big(-\frac{1}{4\rho^2}(p_n - p_{n'})^2\Big)(n-n')\times$$
$$\times\left[\frac{1}{(n-n')^2} - \frac{1}{(n+n')^2}\right]\Im(\langle\phi_+|n\rangle\langle n'|\phi_+\rangle - \langle\phi_-|n\rangle\langle n'|\phi_-\rangle)\,. \tag{6.41}$$

Given the symmetry and the real-valuedness of states (7.24), the mean value of the commutator when Ψ is one of our CS's vanish, even if the operator does not. This result is due to the symmetric spectrum of the commutator around 0. As is shown in Part c) of figures 6.2, the eigenvalues of the commutator tend to $\pm i\hbar$ as ρ, i.e. ϑ, increases. Still, there are some points with modulus less than $\hbar$. This leads to dispersions $\Delta Q \Delta P$ in CS's $|x\rangle$ that are no longer bounded from below by $\hbar/2$. Actually, the lower bound of this product, for a region in the phase space as large as we wish, decreases as ϑ diminish. Figure 6.8 shows a numerical approximation.

6.4 Discussion

From the mean values of the operators obtained here, we verify that our CS quantization gives well-behaved momentum and position operators. The classical limit is reached once the appropriate limit for the parameter ϑ is found. If we consider the behaviour of the observables as a function of the dimensionless quantity $\vartheta = \rho L/\hbar\pi$, i.e. the regulator ρ, at the limit $\vartheta \to 0$ and when the Gaussian functions for the momentum become very narrow, the lower symbol of the position operator is $\check{q} \sim L/2$. This corresponds to the classical average value position in the well. On the other hand, at the limit $\vartheta \to \infty$, for which the involved Gaussians spread to constant functions, the mean value $\langle x|\hat{q}|x\rangle$ converges numerically to the function q. In other words, our position operator yields a fair quantitative description for the quantum localization within the well. The lower symbol $\langle x|\hat{p}|x\rangle$ behaves as a stair-step function for ρ close to 0 and progressively fits the function p when ρ increases. These behaviours are well illustrated in the figures 6.4 and 6.5. The effect of the parameter ϑ is also noticeable in the dispersions of $\widehat{q}$ and $\widehat{p}$. Here, the variations of the full width at half maximum of the Gaussian function reveal different dispersions for the operators. Clearly, if a classical behaviour is sought, the values of ϑ have to be chosen near 0. This gives localized values for the observables. The numerical explorations shown in figures 6.6 and 6.7 give a good account of this modulation. Consistently with the previous results, the behaviour of the product $\Delta Q \Delta P$ at low values of ϑ shows uncorrelated observables at any point in the phase space, whereas at large values of this parameter the product is constant and almost equal to the canonical quantum lowest limit $\hbar/2$. This is shown in figure 6.8.

It is interesting to note that if we replace the Gaussian distribution, used here for the p variable in the construction of the CS's, by any positive even probability distribution $\mathbb{R} \in p \mapsto \varpi(p)$ such that $\sum_n \varpi(p-n) < \infty$ the results are not so different! The momentum spectrum is still $\mathbb{Z}$ and the energy spectrum has the form $\{n^2 + \text{constant}\}$. In this regard, an interesting approach combining mathematical statistics concepts and group theoretical constructions of CS's has been recently developed by Heller and Wang [11, 12].

The work presented here has possible applications to those particular physical problems where the square well is used as a model for impenetrable barriers [52], in the spirit of what has been done in [5].

The generalization to higher-dimensional infinite potential wells is more or less tractable, depending on the geometry of the barriers. This includes quantum dots and other quantum traps. Nevertheless, we believe that the simplicity and the universality of the method proposed in the present work should reveal itself useful for this purpose.

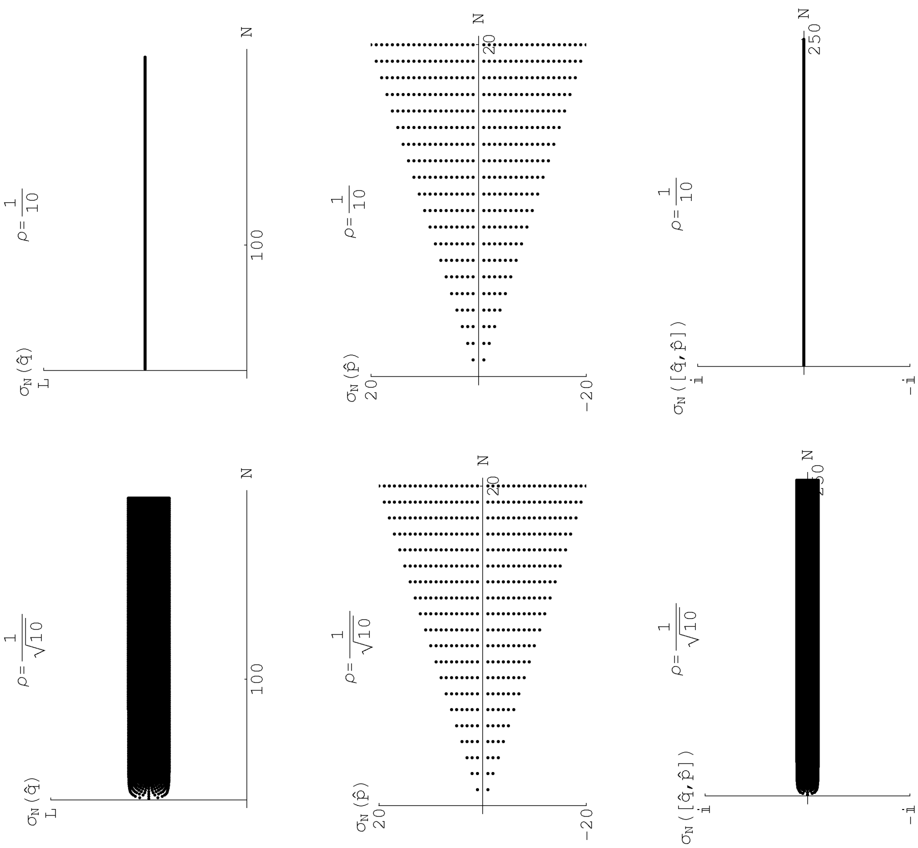


Figure 6.2: Eigenvalues of $\widehat{q}$, $\widehat{p}$ and $[\widehat{q}, \widehat{p}]$ for increasing values of the regulator $\rho = \hbar\pi\vartheta/L$ of the system, and computed for $N \times N$ approximation matrices. Units have been chosen such that $\hbar = 1$, $L = \pi$ so that $\rho = \vartheta$ and $p_n = n$. Note that for $\widehat{q}$ with ρ small, the eigenvalues adjust to the classical mean value $L/2$. The spectrum of $\widehat{p}$ is independent of ρ as is shown in (6.24). For the commutator, the values are purely imaginary.

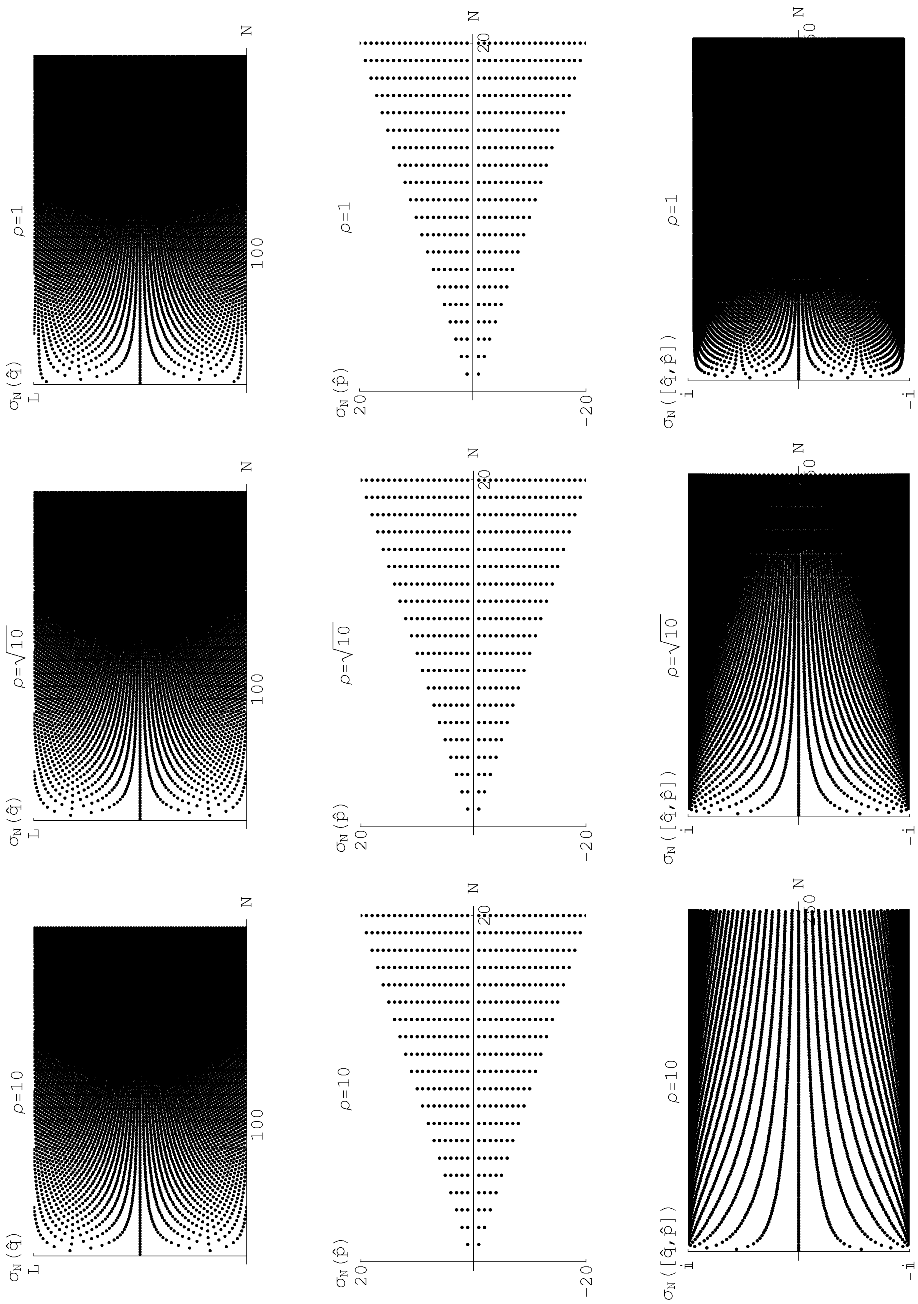
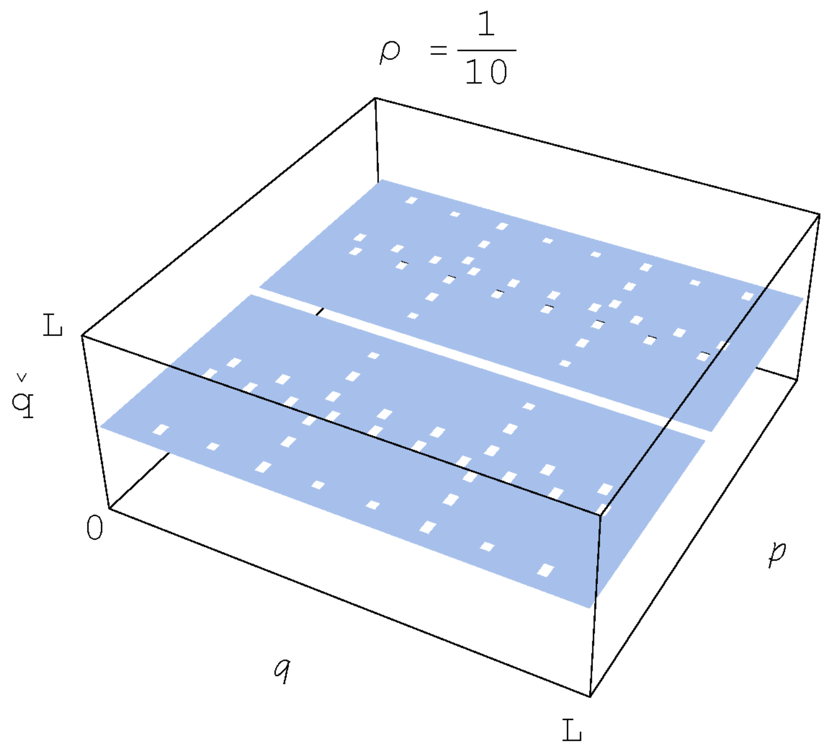
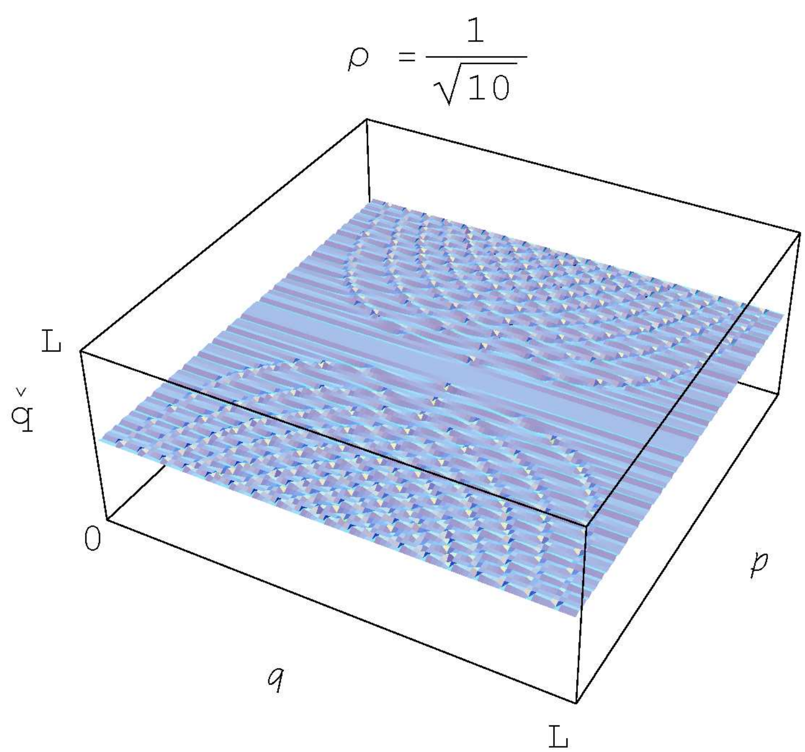
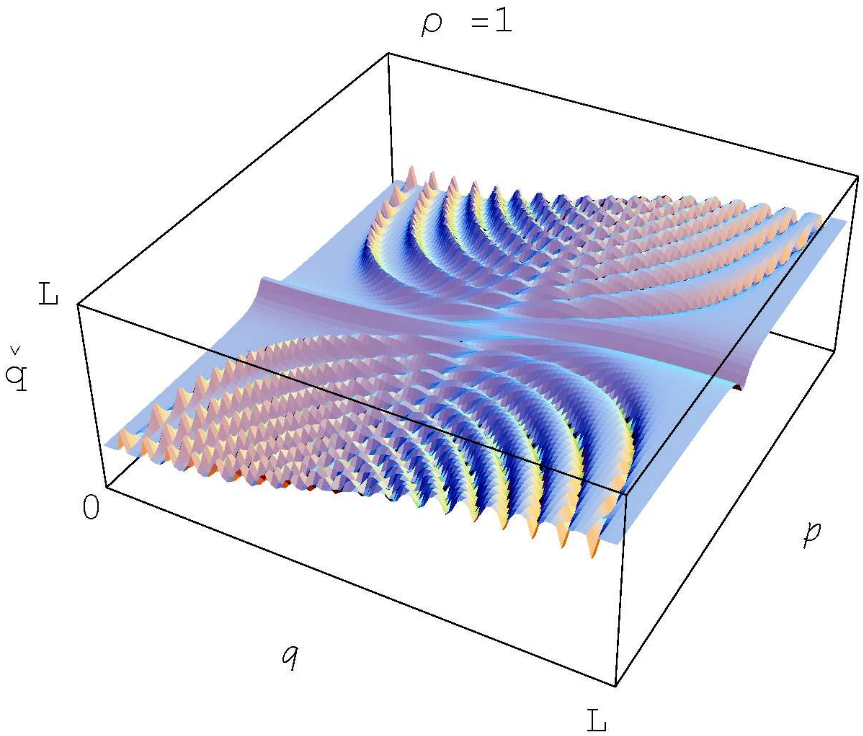
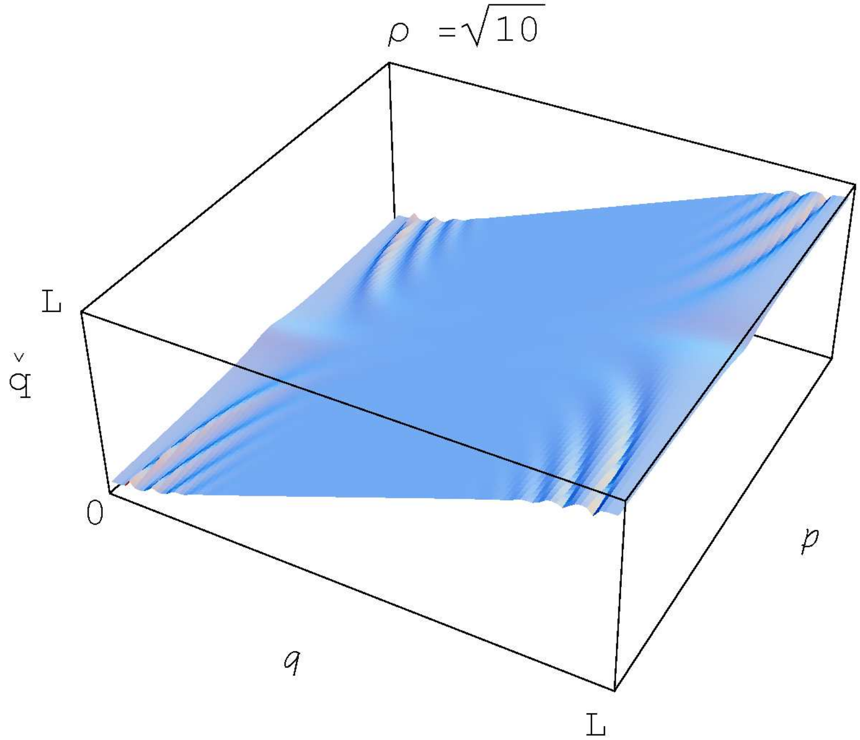


Figure 6.3: Continued from figure 6.2: $N \times N$ approximation matrices eigenvalues of $\widehat{q}$, $\widehat{p}$ and $[\widehat{q}, \widehat{p}]$ for increasingly larger values of $\rho = \hbar\pi\vartheta/L = \vartheta$ in units $\hbar = 1$, $L = \pi$. The spectrum of $\widehat{p}$ is independent of ρ as is shown in (6.24). For the commutator, the eigenvalues are purely imaginary and tend to accumulate around $\mathrm{i}\hbar$ and $-\mathrm{i}\hbar$ as ρ increases.


ρ = 1/10
L
q̌
0
p
q
L


ρ = 1/√10
L
q̌
0
p
q
L


ρ =1
L
q̌
0
p
q
L


ρ =√10
L
q̌
0
p
q
L

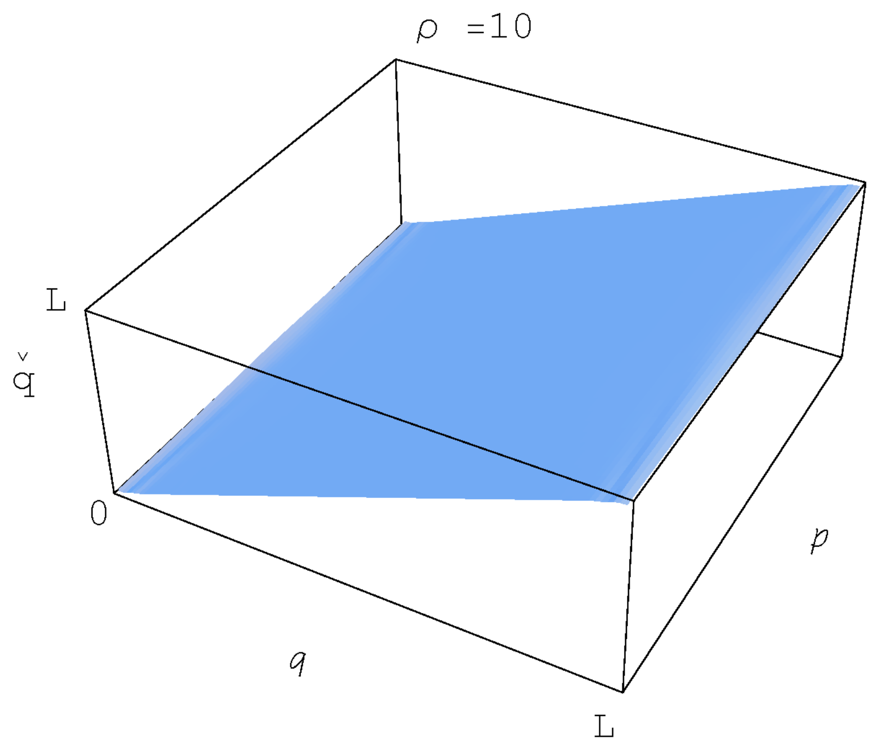
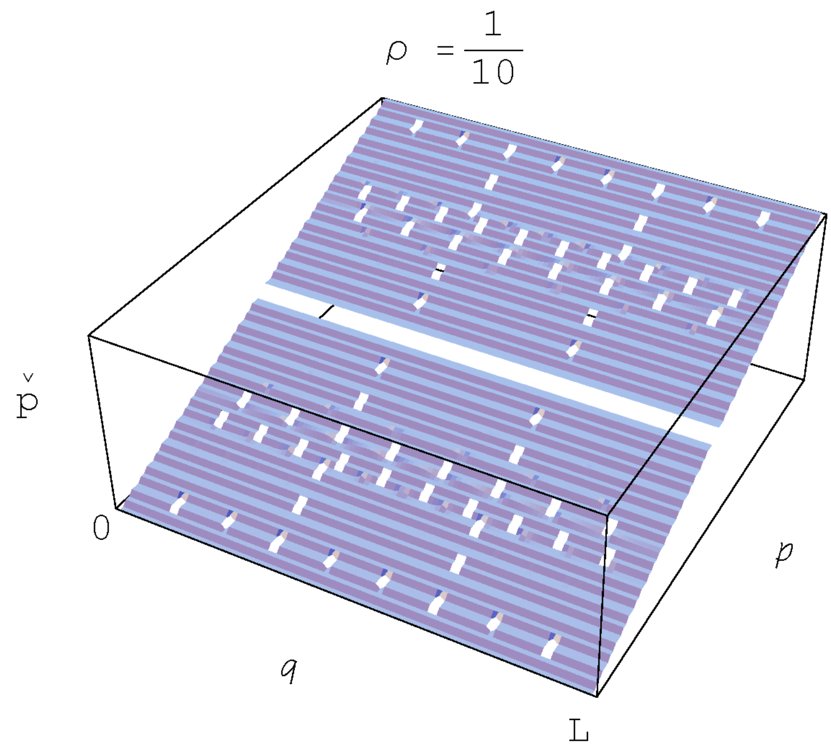
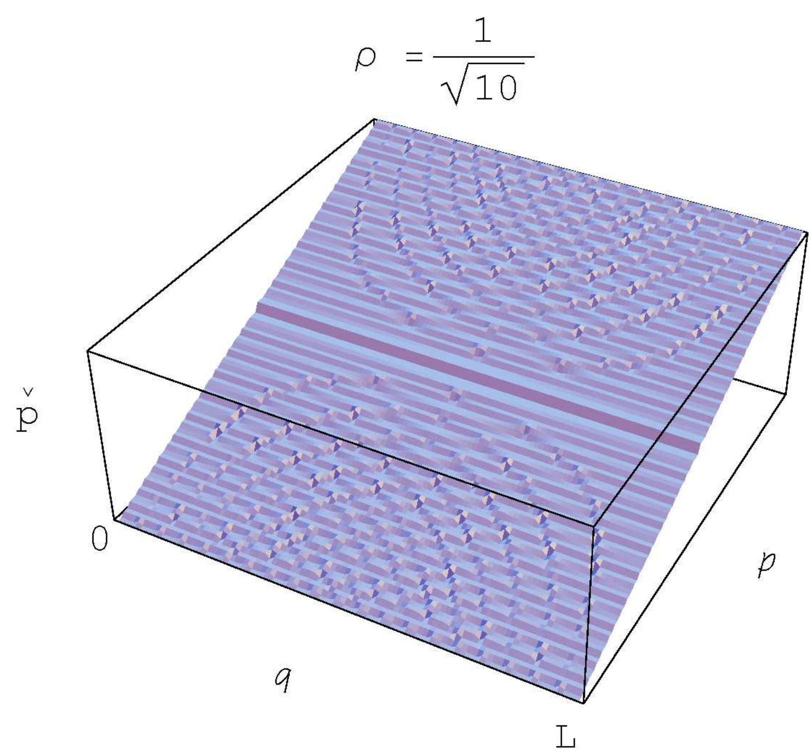
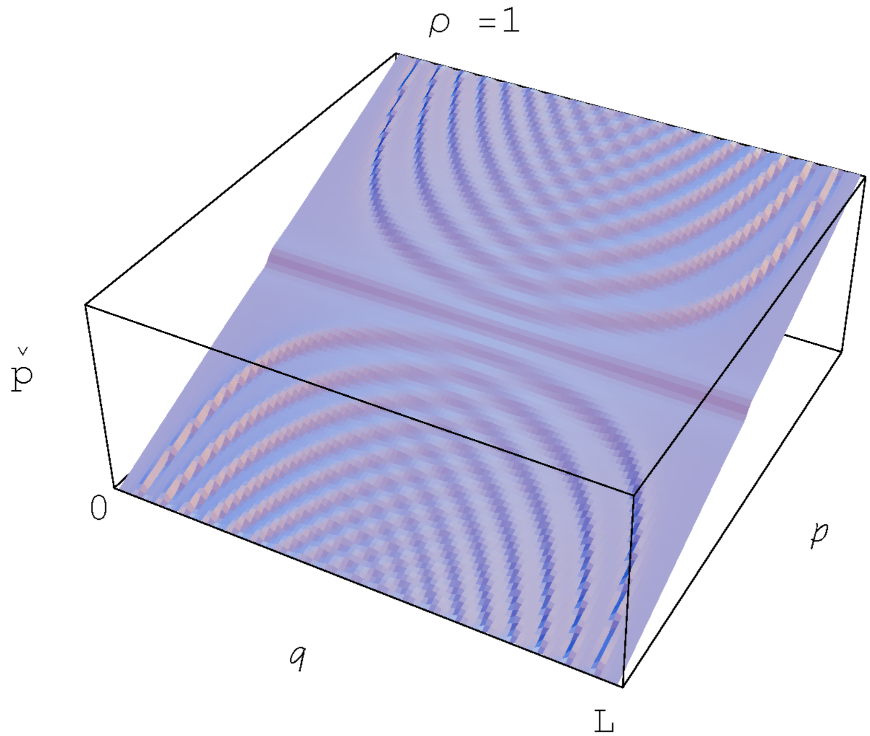
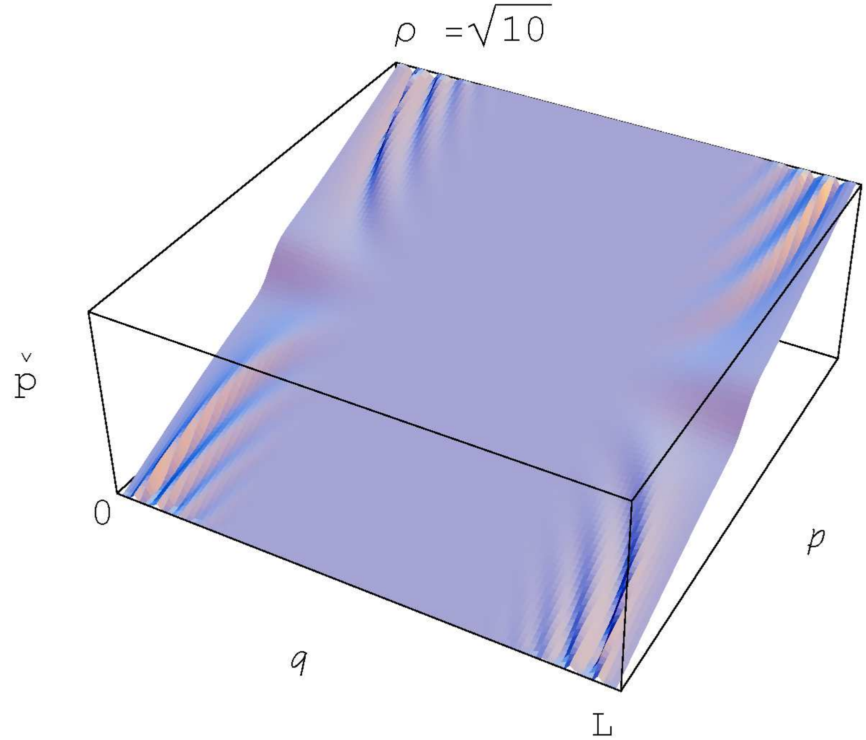


Figure 6.4: The lower symbol $\check{q}$ depicted for various values of the regulator $\rho = \hbar\pi\vartheta/L = \vartheta$ in units $\hbar = 1$, $L = \pi$. Note the way the mean value fits the function q when ρ is large, and approaches the classical average in the well for low values of the parameter.


$\rho = \frac{1}{10}$
p̌
0
q
L
p


$\rho = \frac{1}{\sqrt{10}}$
p̌
0
q
L
p


ρ =1
p̌
0
q
L
p


ρ =√10
p̌
0
q
L
p

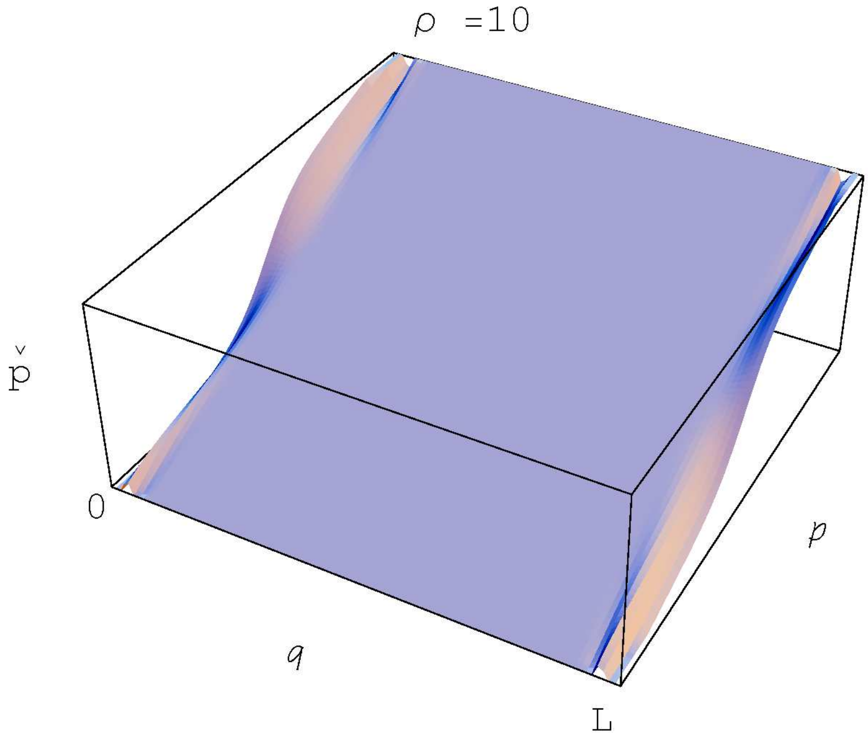
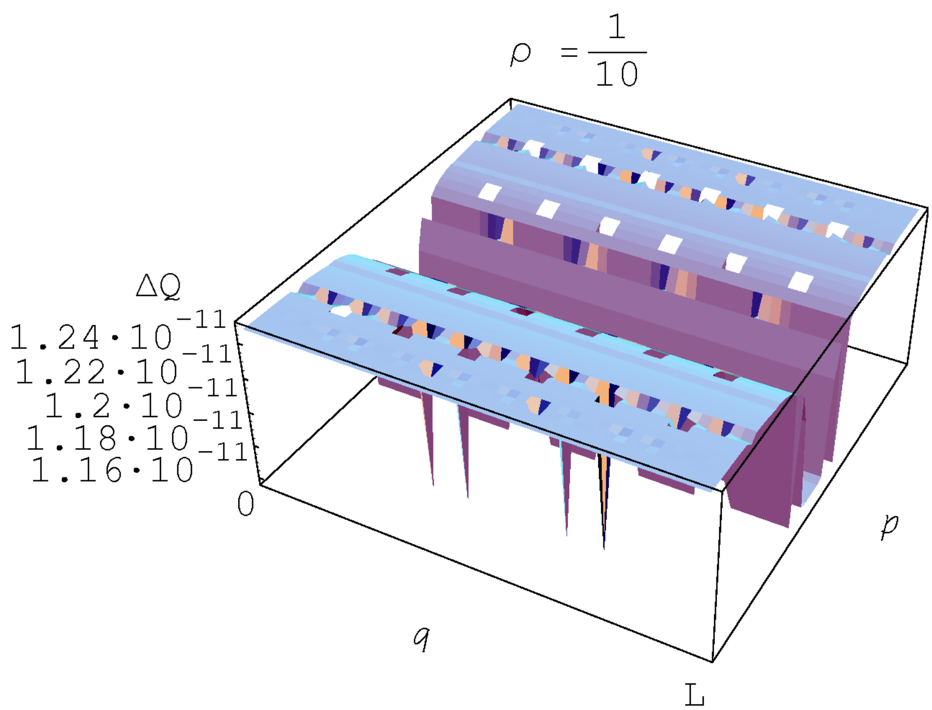
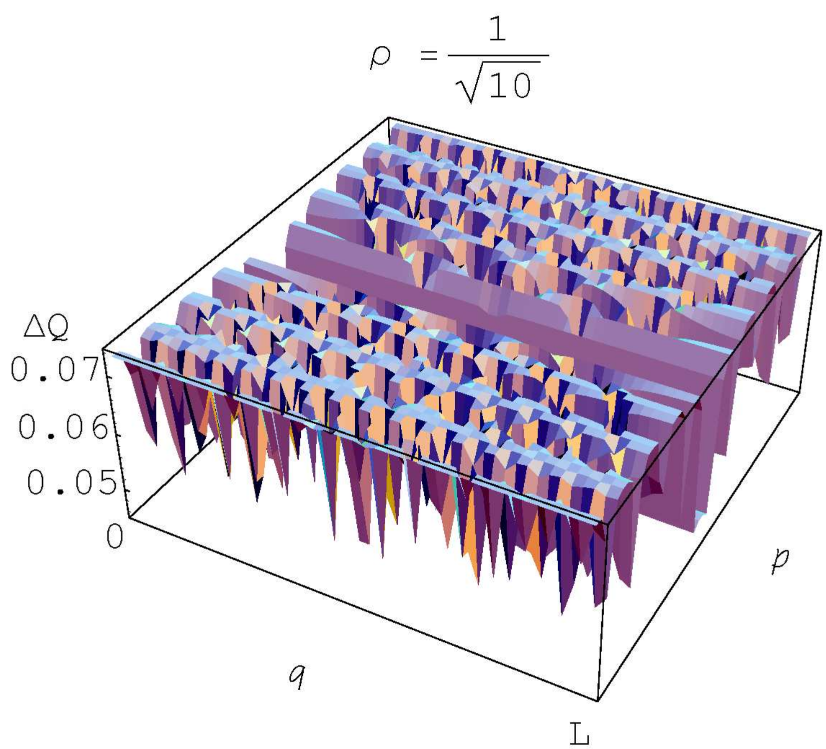


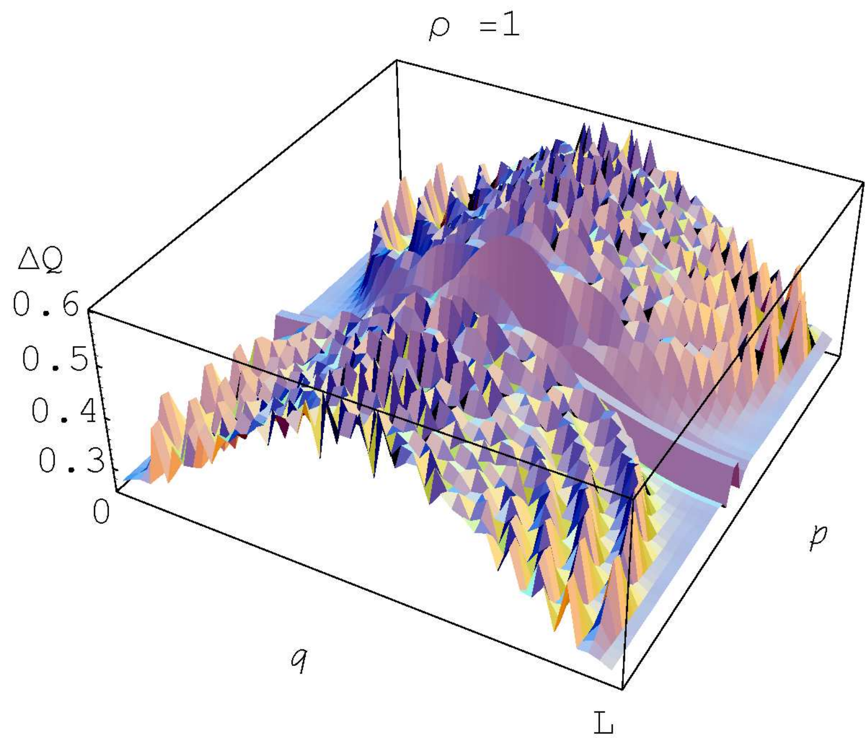
Figure 6.5: The lower symbol $\check{p}$ depicted for various values of $\rho = \hbar\pi\vartheta/L = \vartheta$ in units $\hbar = 1$, $L = \pi$. The function becomes smoother when ρ is large.

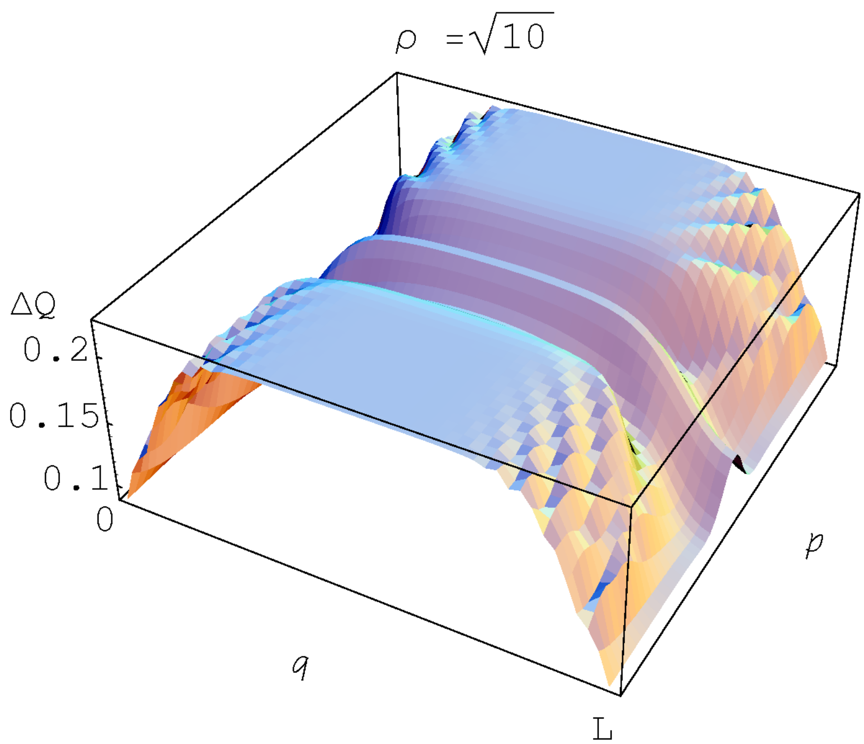


ρ = 1/10
ΔQ
1.24·10^-11
1.22·10^-11
1.2·10^-11
1.18·10^-11
1.16·10^-11
0
q
L
p



ρ = 1/√10
ΔQ
0.07
0.06
0.05
0
q
L
p


ρ =1
ΔQ
0.6
0.5
0.4
0.3
0
p
q
L


ρ =√10
ΔQ
0.2
0.15
0.1
0
p
q
L

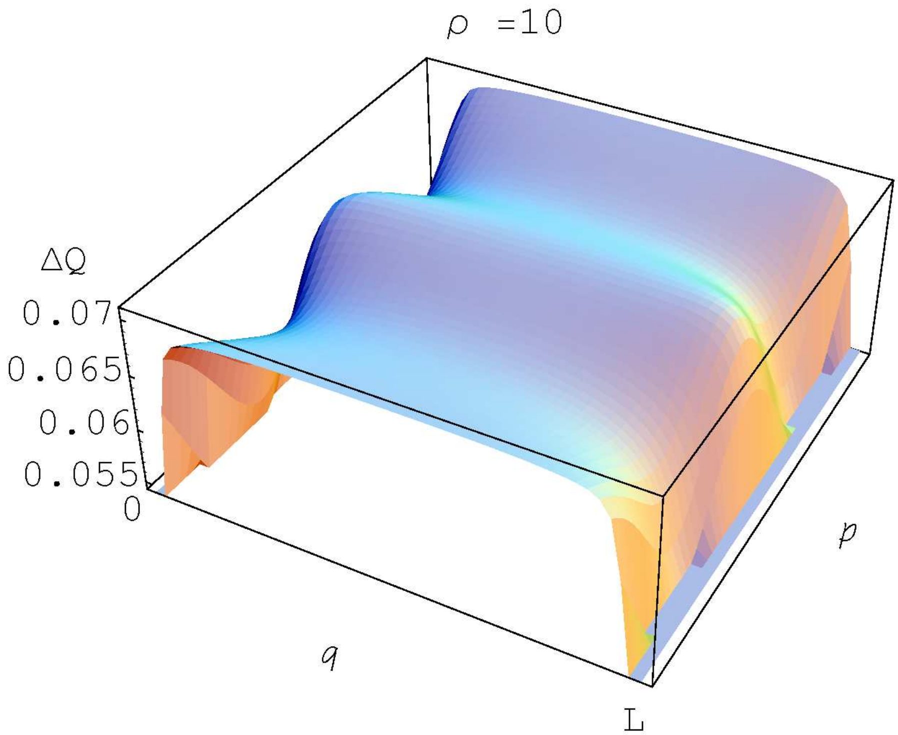
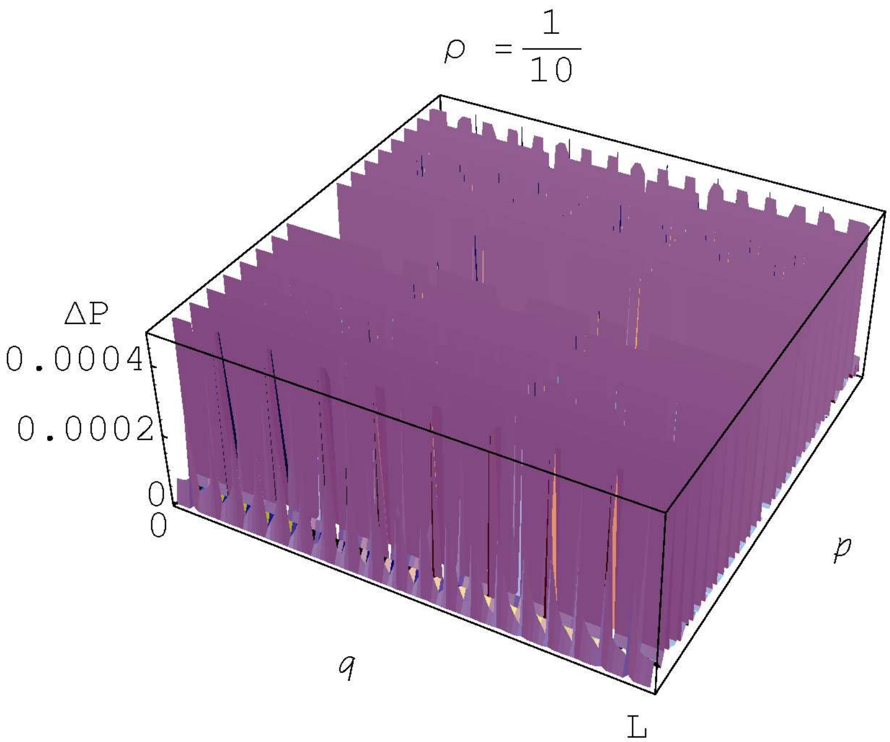
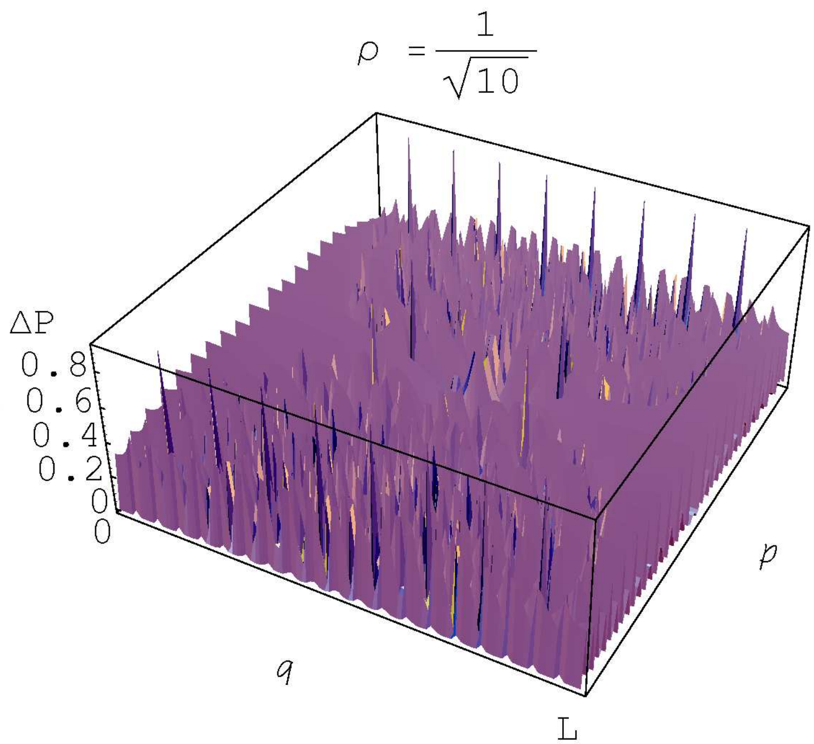


Figure 6.6: Variance of q depicted for various values of $\rho = \hbar\pi\vartheta/L = \vartheta$ in units $\hbar = 1$, $L = \pi$. Note how different dispersions are revealed just by changing the width of the Gaussian function of the p variable. Low dispersion, close to classical, is found for ϑ near 0 and the quantum behaviour is recovered at large values of the parameter.

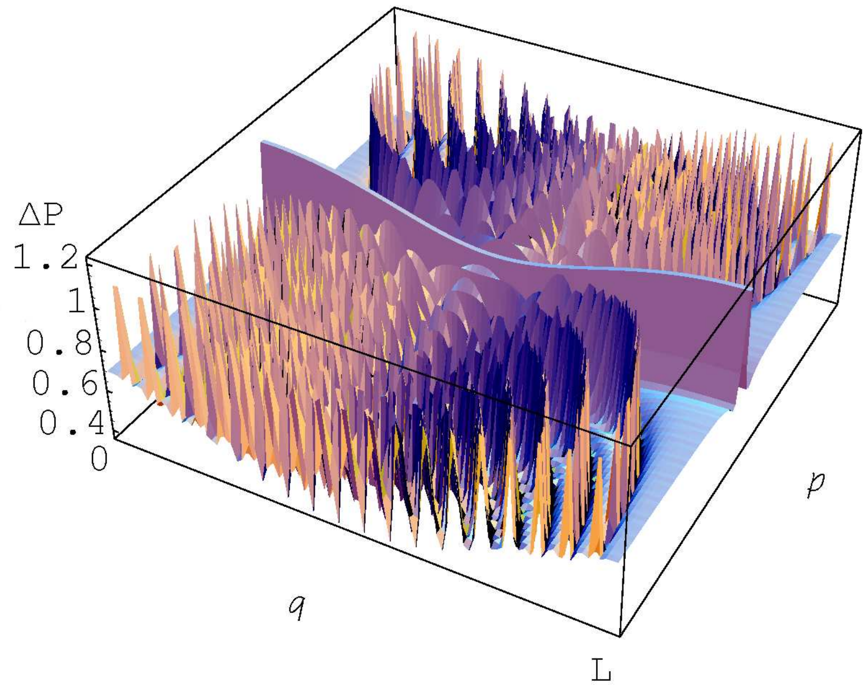


ρ = 1/10
ΔP
0.0004
0.0002
0
0
q
L
p

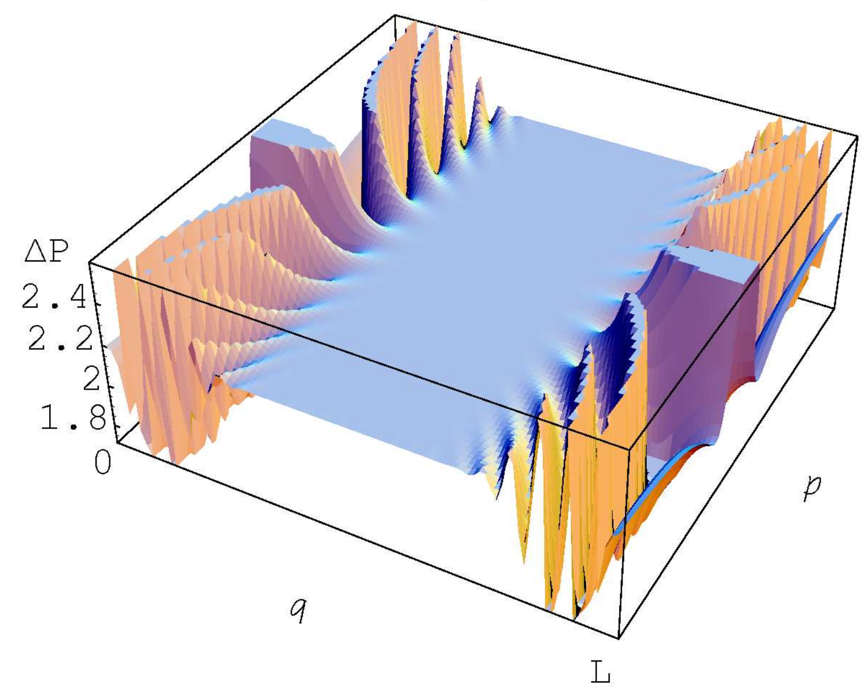


ρ = 1/√10
ΔP
0.8
0.6
0.4
0.2
0
0
q
L
p

$\rho = 1$



$\rho = \sqrt{10}$



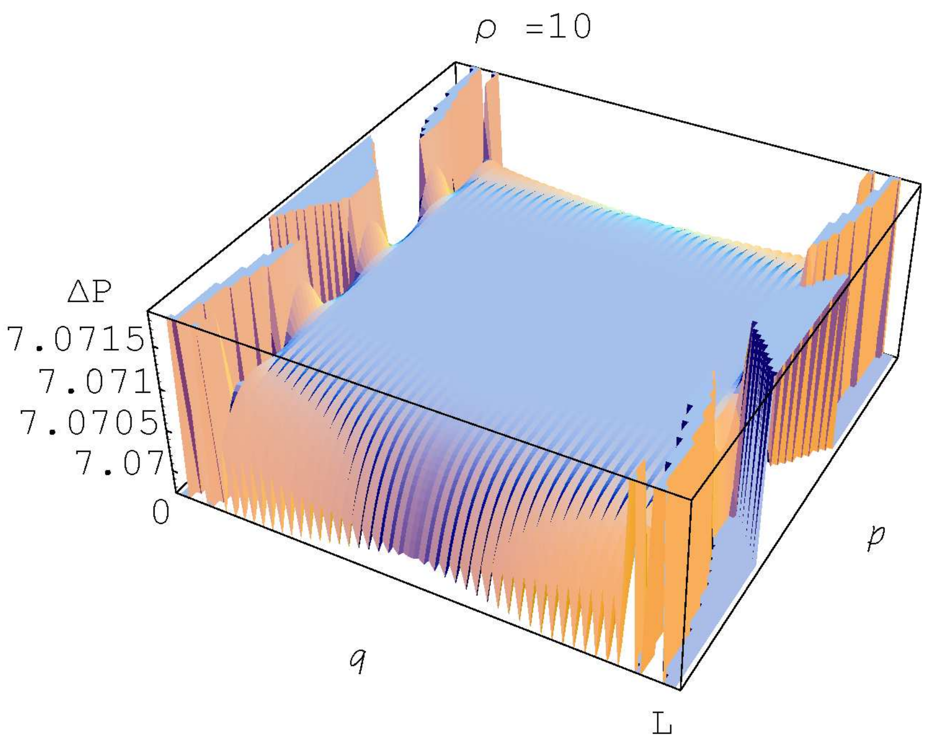
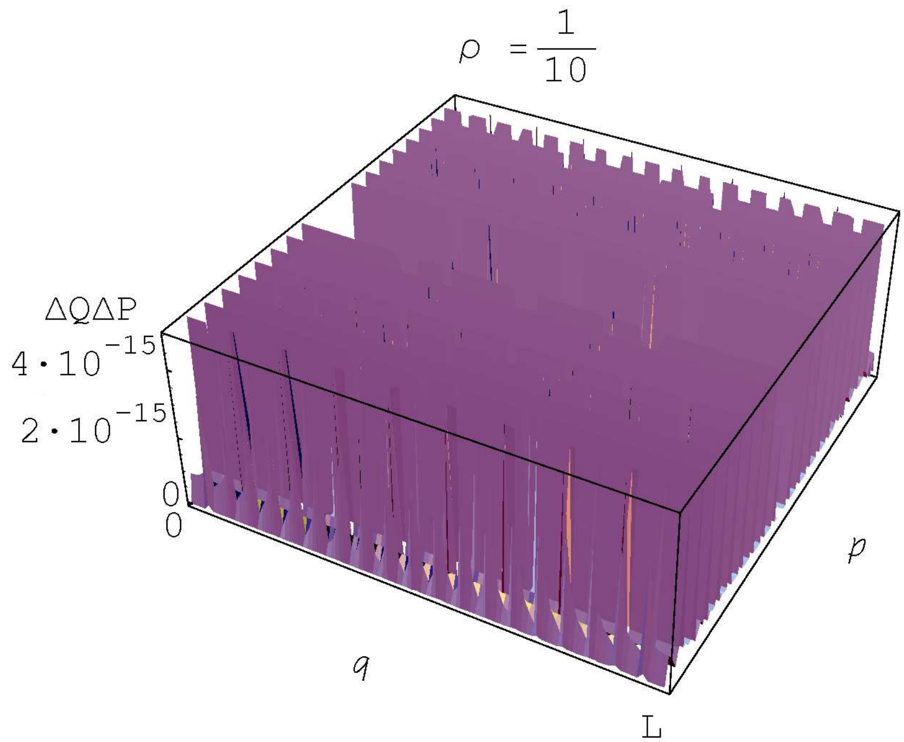
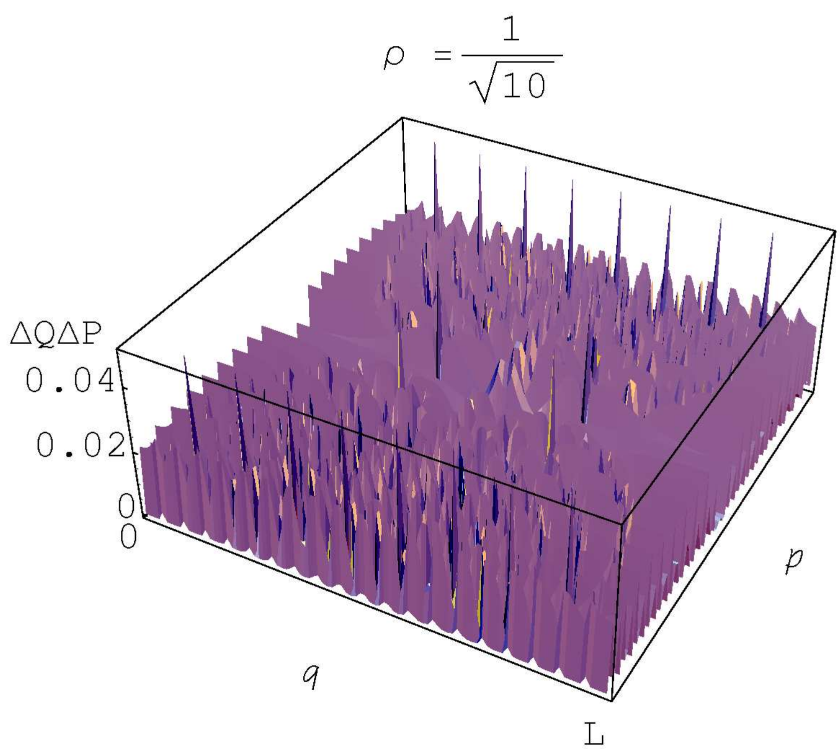
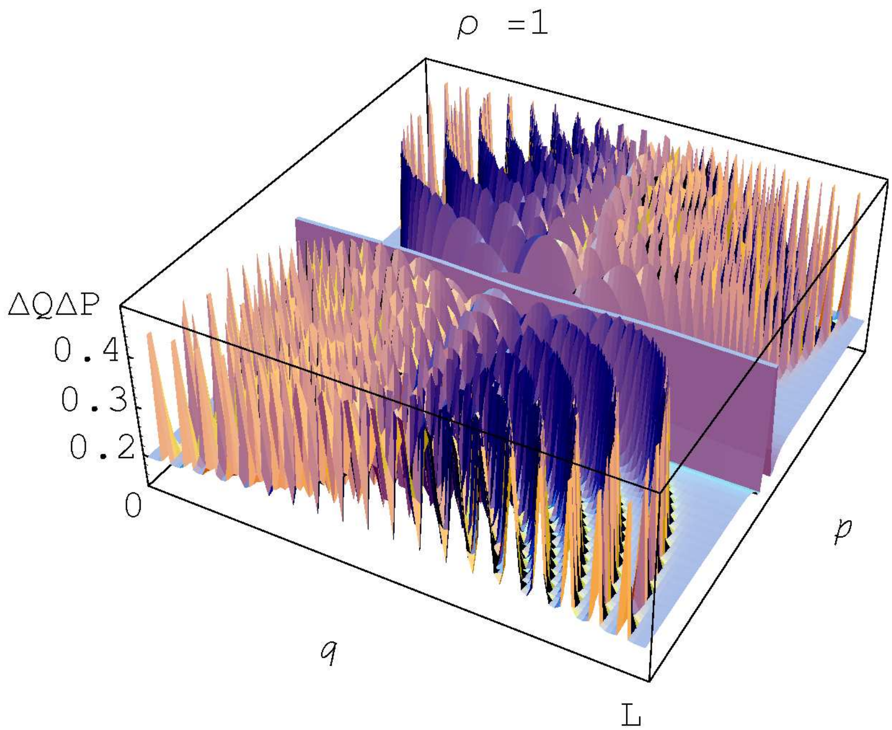
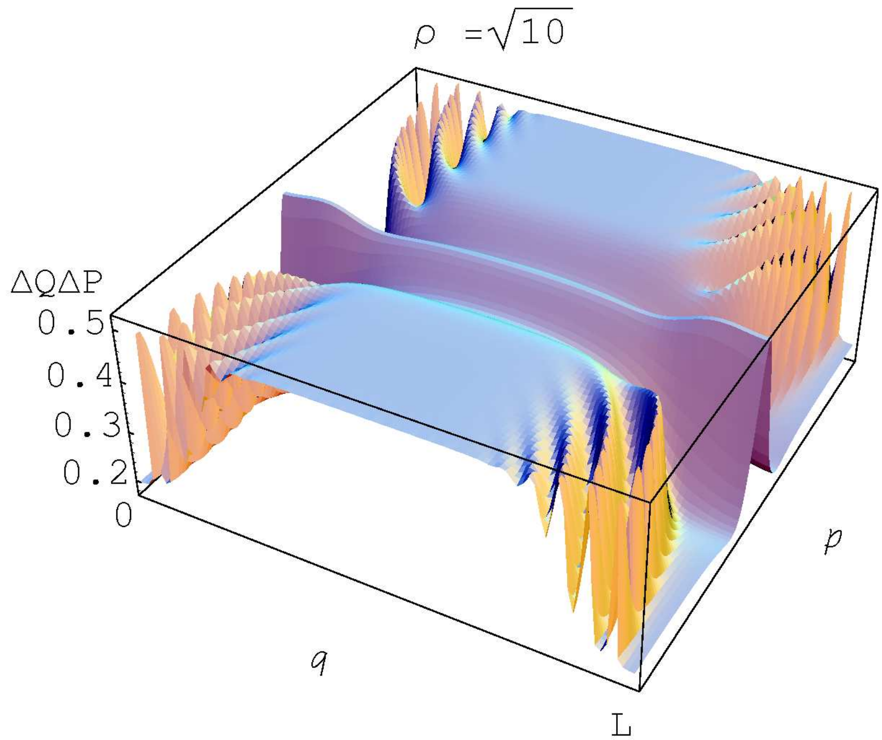


Figure 6.7: Variance of p depicted for various values of $\rho = \hbar\pi\vartheta/L = \vartheta$ in units $\hbar = 1$, $L = \pi$. Consistently with $\check{q}$, a well localized momentum is found for low values of the parameter. This is actually expected since the Gaussian becomes very narrow.


ρ = 1/10
ΔQΔP
4·10^-15
2·10^-15
0
0
q
L
p


ρ = 1/√10
ΔQΔP
0.04
0.02
0
0
q
L
p


ρ =1
ΔQΔP
0.4
0.3
0.2
0
p
q
L


ρ =$\sqrt{10}$
ΔQΔP
0.5
0.4
0.3
0.2
0
p
q
L

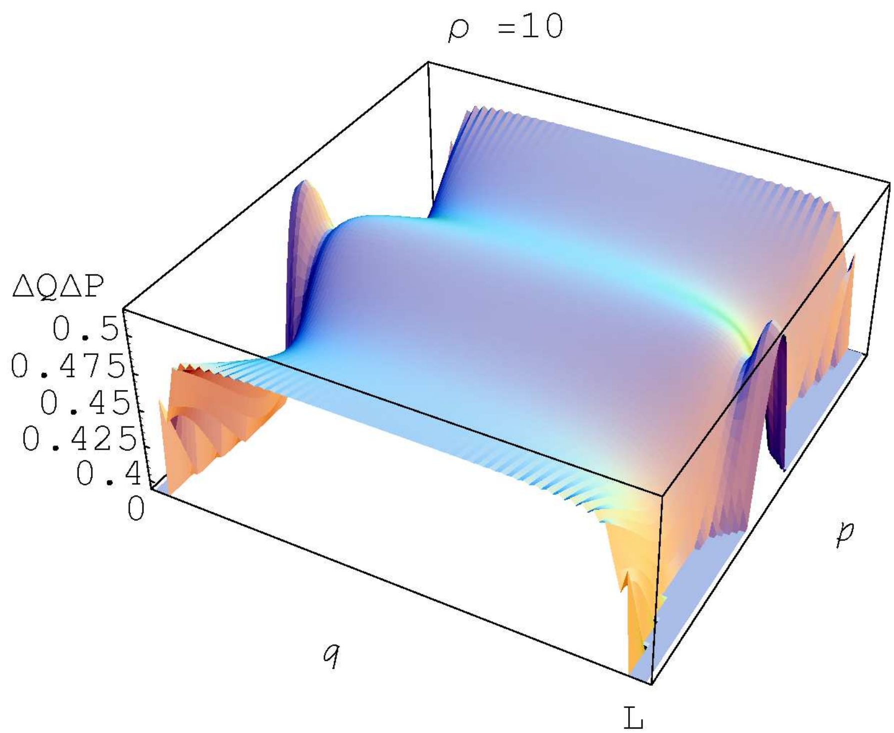


Figure 6.8: Product $\Delta Q \Delta P$ for various values of $\rho = \hbar\pi\vartheta/L = \vartheta$ in units $\hbar = 1$, $L = \pi$. Note the modification of the vertical scale from one picture to another. Again, the pair position-momentum tends to decorrelate at low values of the parameter, as they should do in the classical limit. On the other hand it approaches the usual quantum-conjugate pair at high values of the regulator ρ.

7 Time Operator

7.1 Introduction

A quantum time observable conjugate to the energy, as it naturally arises from the quantum mechanics formalism, deals with questions about its interpretation and its formal definition, as has been pointed out in [39] and [13]. The commutation relation $[T, H] = i$ and its subsequent uncertainty relation suggest that time is an intrinsic observable of a quantum system. In that way it must be distinguished from an external time, an observer time, than would enter just as a parameter of the system dynamics. Instead, a quantum time could be the interval that determines the occurrence of an event in the system, such as a radioactive decay, or its duration as a time of flight. It must be pointed that this observable will be specific for each system and has to be defined in correspondence to the Hamiltonian.
If time observable is conceived as a spectral representation of a unique self-adjoint operator, the covariance with the Hamiltonian contradicts the semi-bounded energy spectrum. As is stated in a theorem by Pauli [43], this excludes the existence of a self-adjoint operator. This is a common problem with phase operator [41] which in fact is proportional to a time operator for harmonic oscillator. Still, self-adjoint operators that are covariant with the Hamiltonian can be constructed using Positive Operator-Valued Measures (POVM). In the later measures, the observable is defined as a statistical mean value of an operator and not as an eigenvalue of the operator. Moreover, the eigenstates of the operator are not needed to be orthogonal whenever they permit a probability distribution on them. In this sense, coherent states, initially used in quantum optics, can be useful in the construction of a POVM. Here we will show a systematic procedure and apply it to the time operator for a free particle.

7.2 Positive Operator Valued Measure

If time is described as a PV measure, it will form a *system of imprimitivity* with a unitary representation U_g of a locally compact group if

$$U_g F(X) U_g^* = F(g \cdot X) \tag{7.1}$$

for every $X \in \mathcal{A}$ and every element of the group. If time is described as a POVM, the pair is a *system of covariance*. Take the G as the group of time translations and the generator H from the unitary representations $U_g = e^{-itH}$. The conjecture stated by Pauli implies that H cannot be an operator of semi-bounded spectrum, as the Hamiltonian of the system, since this would create a contradiction. Some care has to be taken on the domains of the operators for this to be true and to ensure

7.3 Coherent states and POVM

Coherent states, historically introduced for the harmonic oscillator in the context of quantum optics, can be defined upon different properties. But most importantly they provide resolution of the identity and as such give a good frame of reference in which to express other states on the Hilbert space. Resolution of the identity is precisely what is asked as a main property of a POVM, it is natural then to use coherent states as a basis to define it. Here we present a general method to link both formalisms.

7.4 Time operator

The specific case we will develop is a quantum clock model based on the one exposed in [24]. The time observable we choose [49] is the conjugate variable of the Hamiltonian for the motion of a free particle

$$H = \frac{p^2}{2}, \tag{7.2}$$

i.e. a system with one degree of freedom represented by the Hilbert space $\mathcal{H} = L^2(\mathbb{R})$. By [7.2] the classical time reads as

$$T = \frac{q}{p}, \quad p \neq 0\,. \tag{7.3}$$

It is indeed straightforward to check that $\{T, H\} = 1$ and we expect that a quantum time operator should, to a certain extent, satisfy a commutation rule of this kind with the quantum Hamiltonian consistent with (7.3). Note first of all that the singularity on $p = 0$ gives a natural cut of the phase space and forbids the use of standard coherent states in the POVM definition.

7.4.1 Using the Poincaré half-planes

To overcome the singularity at $p = 0$ we can separate the phase space into the upper and lower half-planes, for $p > 0$ and $p < 0$. We can work then on the unit disk on the complex plane if we take the homographic transformation, namely de Cayley transform, that maps the real line stereographically as $S^1 \longrightarrow \mathbb{R}$

$$[0, 2\pi) \ni \theta \longrightarrow q = \frac{e^{i\theta} + i}{ie^{i\theta} + 1} \in \mathbb{R}\,, \tag{7.4}$$

where $\theta = 0 \rightarrow q = 1$, $\theta = \pi/2 \rightarrow q = \pm\infty$, $\theta = \pi \rightarrow q = -1$ and $\theta = \frac{3\pi}{2} \rightarrow q = 0$, and more generally, for the rest of the half-plane, the transformation that maps the open unit disk $\mathcal{D}$ to the upper half-plane P_+ in the complex plane $\mathbb{C}$

$$\mathcal{D} \ni z \longrightarrow Z = \frac{z + i}{iz + 1} \in \mathrm{P}_+. \tag{7.5}$$

The inverse transformation is

$$z = \frac{Z - i}{1 - iZ}\,. \tag{7.6}$$

Symmetrically, the relation

$$\mathcal{D} \ni \bar{z} \longrightarrow \bar{Z} = \frac{\bar{z} - i}{-i\bar{z} + 1} \in \mathrm{P}_- \;\Leftrightarrow\; \bar{z} = \frac{\bar{Z} + i}{1 + i\bar{Z}} \tag{7.7}$$

maps the open unit disk $\mathcal{D}$ to the lower half-plane P_- in the complex plane $\mathbb{C}$.

First let us define our coherent states on the upper plane, we introduce the (q, p), $p > 0$ variables as the real and imaginary parts of Z : $Z = q + i/p$. These coordinates are expressed in terms of the pre-image z of Z as :

$$q = \frac{2\Re(z)}{1 + |z|^2 - 2\Im(z)}, \quad p = \frac{1 + |z|^2 - 2\Im(z)}{1 - |z|^2}\,, \tag{7.8}$$

the following relations are useful

$$|z|^2 = \frac{(q^2 + \frac{1}{p^2}) + 1 - \frac{2}{p}}{(q^2 + \frac{1}{p^2}) + 1 + \frac{2}{p}} \qquad z = \frac{2q + i(q^2 + \frac{1}{p^2} - 1)}{1 + (q^2 + \frac{1}{p^2}) + \frac{2}{p}} \tag{7.9}$$

and the measures are related as

$$d^2Z = \frac{4}{(|z|^2 + 1 + 2\Im(z))^2} d^2z = \frac{dqdp}{p^2} = \frac{4dz^2}{p^2(1 - |z|^2)^2}\,. \tag{7.10}$$

and

$$dz \wedge d\bar{z} = \frac{(1 - |z|^2)^2}{4} dqdp \tag{7.11}$$

Let η be a real parameter such that $\eta > \frac{1}{2}$ and let us equip the unit disk $\mathcal{D}$ with the $SU(1,1)$ invariant measure

$$\mu_\eta(dz\, d\bar{z}) \stackrel{\text{def}}{=} i\,\frac{2\eta - 1}{2\pi}\,\frac{dz \wedge d\bar{z}}{(1 - |z|^2)^2} = \frac{2\eta - 1}{8\pi} dqdp\,. \tag{7.12}$$

Note that, on the half-plane, the symplectic measure is recovered as is needed for the integration on the phase space. Consider now the Hilbert space $\mathrm{L}^2_\eta = \mathrm{L}(\mathcal{D}, \mu_\eta)$ of all functions $f(z, \bar{z})$ on $\mathcal{D}$ which are square integrable with respect to μ_η. Within this "large" Hilbert space we select all functions of the form

$$\phi_+(z, \bar{z}) = (1 - |z|^2)^\eta g(\bar{z})\,, \tag{7.13}$$

where $g(\bar{z})$ is antiholomorphic $\mathcal{D}$. The closure of the linear span of such functions is a Hilbert subspace of L^2_η denoted here by $\mathcal{H}_+$. An orthonormal basis of $\mathcal{H}_+$ is given by the countable set of functions

$$\phi_n(z, \bar{z}) \equiv \sqrt{\frac{(2\eta)_n}{n!}} (1 - |z|^2)^\eta \bar{z}^n \text{ with } n \in \mathbb{N}, \tag{7.14}$$

where $(2\eta)_n = \frac{\Gamma(2\eta+n)}{\Gamma(2\eta)}$ is the Pochhammer symbol. Note that

$$\sum_{n=0}^{\infty} |\phi_n(z, \bar{z})|^2 = 1\,. \tag{7.15}$$

Similarly, in the lower half-plane, we select all functions of the form

$$\phi_-(z,\bar z) = (1-|z|^2)^\eta g(z)\,, \tag{7.16}$$

where $g(z)$ is holomorphic in $\mathcal{D}$. The closure of the linear span of such functions is now denoted by $\mathcal{H}_-$. An orthonormal basis of $\mathcal{H}_-$ is given by the countable set of functions

$$\overline{\phi}_n(z,\bar z) \equiv \sqrt{\frac{(2\eta)_n}{n!}}(1-|z|^2)^\eta z^n \text{ with } n\in\mathbb{N}, \tag{7.17}$$

Now, to define coherent states on the whole phase space, instead of considering the direct sum $\mathcal{H}_+\oplus\mathcal{H}_-$, we will deal with the Hilbert space $\mathbb{C}^2\otimes \mathrm{L}^2_\eta$ with vector elements

$$\Phi(z,\bar z) = \begin{pmatrix}\phi(z)\\ \psi(\bar z)\end{pmatrix}\,, \tag{7.18}$$

provided with the inner product

$$\langle\Phi|\Phi'\rangle = \sum_{\pm}\int_{\mathcal{D}}\Phi^\dagger(z,\bar z)\Phi'(z,\bar z)\,\mu_\eta(dz\,d\bar z)\,. \tag{7.19}$$

Here the sum is done over both half-planes and the integration over their correspondent unit disks. We then introduce the Hilbert subspace of spinors spanned by the orthonormal system

$$\Phi_n(z,\bar z) = \frac{1}{\sqrt{2}}\begin{pmatrix}\phi_n\\ \overline{\phi}_n\end{pmatrix}\,,\quad \langle\Phi_n|\Phi'_{n'}\rangle = \delta_{nn'}\,. \tag{7.20}$$

Again, we note here that

$$\sum_{n=0}^{\infty}\Phi_n^\dagger(z,\bar z)\Phi_n(z,\bar z) = 1\,. \tag{7.21}$$

For simplicity let us associate each element of this system to the elements of the orthonormal basis in some separable Hilbert space of the type $\mathbb{C}^2\otimes\mathcal{H}\equiv\mathbb{K}$

$$|n,\pm\rangle \equiv |\pm\rangle\otimes|n\rangle\,,\qquad |+\rangle = \begin{pmatrix}1\\0\end{pmatrix},\quad |-\rangle = \begin{pmatrix}0\\1\end{pmatrix}, \tag{7.22}$$

We are now in measure of defining our vector coherent states. The following set of 2×2 diagonal real matrices is needed for the construction :

$$\mathrm{F}_n(z,\bar z) = \frac{1}{\sqrt{2}}\begin{pmatrix}\phi_n(z,\bar z) & 0\\ 0 & \overline{\phi}_n(z,\bar z)\end{pmatrix} \tag{7.23}$$

We can define the following two orthogonal coherent states, as vectors in $\mathcal{K}$

$$|z,k\rangle \equiv \sum_{n=0}^{\infty}\overline{\mathrm{F}}_n(z,\bar z)|k\rangle\otimes|n\rangle\quad k=\pm\,. \tag{7.24}$$

One easily verifies their normalization and the resolution of the identity as

$$\sum_{k=\pm}\langle z,k|z,k\rangle = 1\,,\qquad \sum_{k=\pm}2\int_{\mathcal{D}}\mu_\eta(dz\,d\bar z)\,|z,k\rangle\langle z,k| = \mathbb{I}_{\mathcal{K}}\,. \tag{7.25}$$

The components of states (7.24) coincide respectively with Perelomov coherent states of $SU(1,1)$ and their conjugates, in the corresponding unit disks, and after proper transformations to coherent states of $SL(2,\mathbb{R})$ on the half-planes.

7.4.2 Berezin-Toeplitz quantization of classical observables

Quantization of a general classical observable $f(z,\bar{z},k)$ is given by the operator

$$\mathbf{A}_f = 2\sum_{k=\pm}\int_{\mathcal{D}} f(z,\bar{z},k)|z,k\rangle\langle z,k|\mu_\eta(dzd\bar{z}) \equiv \begin{pmatrix} A_f^+ \\ A_f^- \end{pmatrix} \tag{7.26}$$

If we quantize $f(q,p,k)$ defined by $f(q,p,+) = q/p$, $p>0$, $f(q,p,-) = (-1)^\epsilon q/p$, $p<0$, $\epsilon = 0$ or 1 (to be made precise later, but we leave it for an option at the moment), we hope to get the quantum counterpart of the classical time. Let us take for now on just the upper half-plane, the corresponding results on the lower half-plane will be joined together later. For this, we just use the normalized $SU(1,1)$ coherent states $|z\rangle = \sum_n \overline{\phi_n(z,\bar{z})}|n\rangle$. Time operator will be the result of the following integral

$$\widehat{\Theta}^+ = A^+_{q/p} = \frac{2\eta-1}{\pi}\int_{\mathcal{D}} \frac{r^{n+n'+1}\cos\phi}{(1+r^2-2r\sin\phi)^2}(1-r^2)^{2\eta-1} \times \sum_{n,n'=0}^{\infty} \alpha_n\alpha_{n'}|n\rangle\langle n'|, \tag{7.27}$$

where

$$\alpha_n = \sqrt{\frac{(2\eta)_n}{n!}}. \tag{7.28}$$

After some calculation we get the time operator

$$\widehat{\Theta}^+ = i(2\eta-1)\left[\sum_{n\geq n'}^{\infty} \alpha_n\alpha_{n'}(n'-n)i^{n-n'}\mathrm{B}(2\eta-1,n+1)|n\rangle\langle n'| + \sum_{n'\geq n}^{\infty} \alpha_n\alpha_{n'}(n'-n)i^{n-n'}\mathrm{B}(2\eta-1,n'+1)|n\rangle\langle n'|\right]. \tag{7.29}$$

If we do a eigenvalue analysis of this operator we find, as is shown on figure 7.1, that, the eigenvalues give a regular pattern and tends to a dense set over the real line at the limit $\eta \longrightarrow \infty$. This recovers the continuous spectrum for the time variable.

The form of the physical observable has to be recovered through the lower symbol, that taken in coherent states $|z\rangle$ gives

$$\langle z|\widehat{\Theta}^+|z\rangle = \frac{4q}{p^2q^2+(1+p)^2} = \frac{q}{p}(1-r^2)\,, \tag{7.30}$$

where $r = |z^2|$. As we can see in figure 7.2 the form of the quantized variable is the one of the classical observable but is regularized at infinity. Note that this manifold doesn't depend on the parameter η.

To obtain an operator proportional to the classical Hamiltonian we must quantize p^2 which corresponds to use the function $f(z,\bar{z},+) = p^4 = \frac{(1-r^2)^4}{(1+r^2-2r\sin\phi)^4}$ in

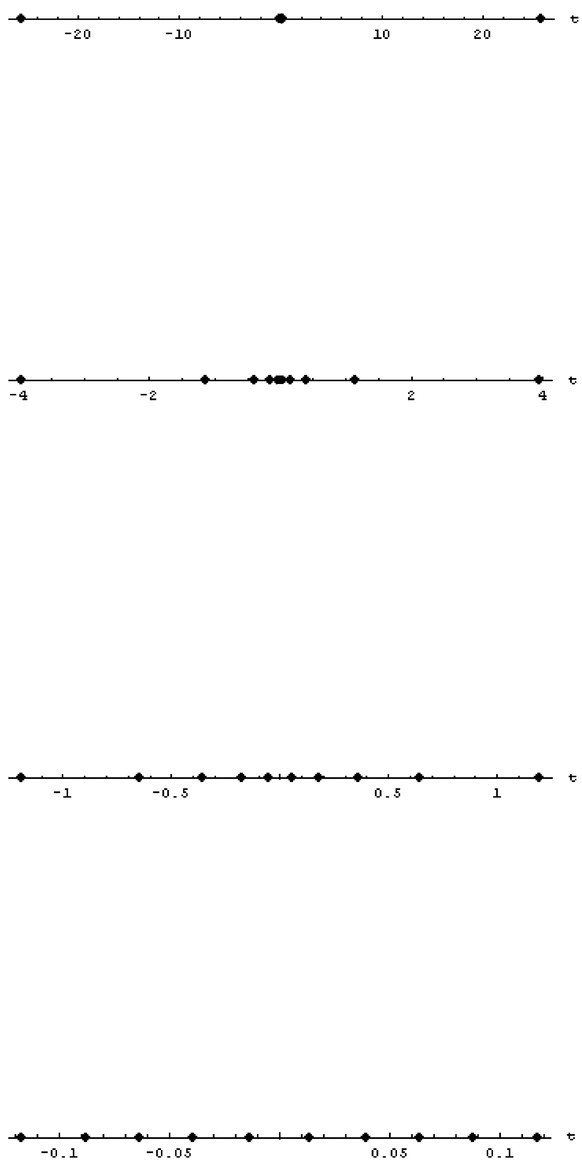


Figure 7.1: Finite matrix approximation of the eigenvalues of time operator for $\eta = 0.6, 5, 20, 1000$ respectively. Note how the points tend to spread regularly and to become dense for high values of the parameter.

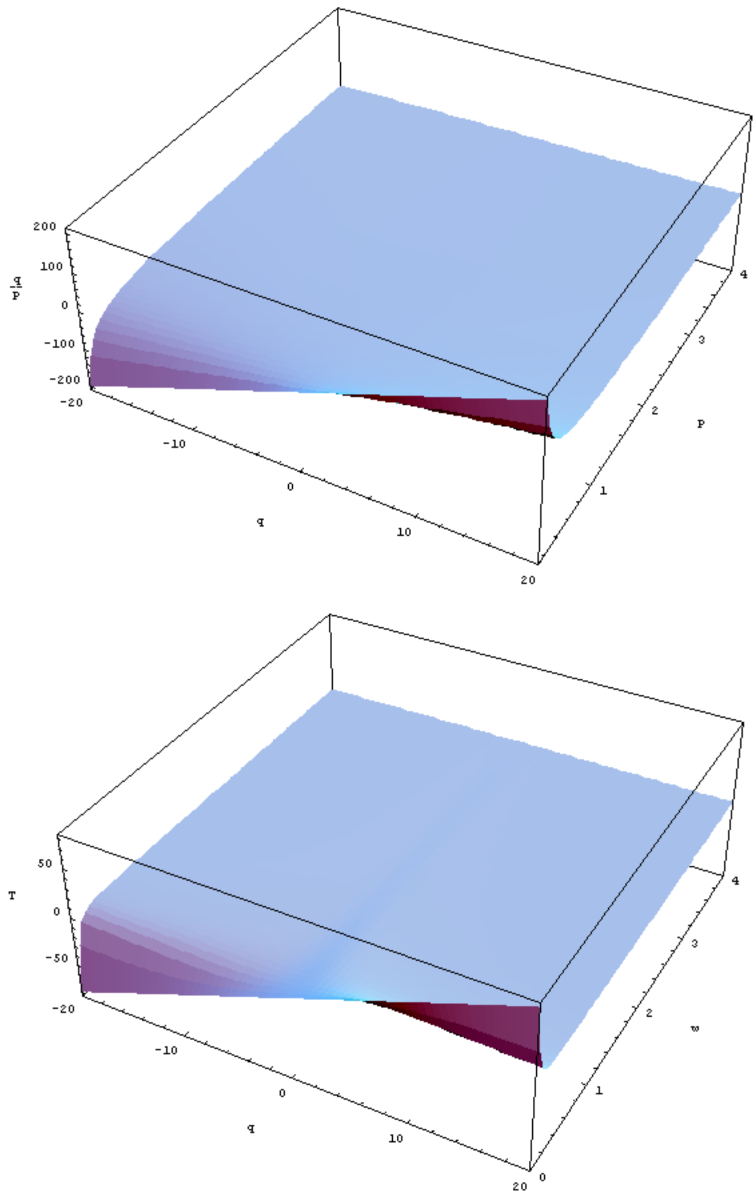


Figure 7.2: Classical time function compared with the mean value of time operator

(7.26), this is,

$$A^+_{p^2} = 4\int dz^2 \frac{(1-|z|^2)^2}{(1+|z|^2-2\Im(z))^2}\frac{(1-|z|^2)^2}{(1+|z|^2-2\Im(z))^2}\frac{2\eta-1}{4\pi}\times$$
$$\times\sum_{n,n'=0}^{\infty}\alpha_n\alpha_{n'}(1-|z|^2)^{2\eta-2}(1+|z|^2-2\Im(z))^2 z^n\bar{z}^{n'}|n\rangle\langle n'|\,. \tag{7.31}$$

We obtain the following penta-diagonal operator

$$\begin{aligned}A^+_{p^2} =&(2\eta-1)\sum_{n=0}^{\infty}\{\alpha_n^2\,[\mathrm{B}(n+1,2\eta-3)+4\mathrm{B}(n+2,2\eta-3)+\mathrm{B}(n+3,2\eta-3)]\,|n\rangle\langle n|\\ &+2\,i\,\alpha_{n+1}\alpha_n\,[\mathrm{B}(n+2,2\eta-3)+\mathrm{B}(n+3,2\eta-3)]\,(|n\rangle\langle n+1|-|n+1\rangle\langle n|)\\ &-\alpha_{n+1}\alpha_n\mathrm{B}(n+3,2\eta-3)\,(|n\rangle\langle n+2|+|n+2\rangle\langle n|)\}\,.\end{aligned} \tag{7.32}$$

Its lower symbol has the form:

$$\langle z|\,A^+_{p^2}\,|z\rangle = \frac{2\eta(2\eta-1)}{(2\eta-2)(2\eta-3)}\,p^2\,, \tag{7.33}$$

which gives the classic energy, modulated by a factor depending on the group representation linked to η. At the infinite limit of η, the concordance with the classical variable is found.

Now, let us take the commutator between this two variables. After some calculation we find the diagonal operator

$$[\widehat{\Theta}^+, A^+_{p^2}] = i\frac{1}{(2\eta-2)(2\eta-3)}\sum_{n=0}^{\infty}4n(2\eta+2n-1)|n\rangle\langle n| \tag{7.34}$$

and its expected value:

$$\langle z|\,[\widehat{\Theta}^+, A^+_{p^2}]\,|z\rangle = \frac{i8\eta^2(2\eta+1)}{(2\eta-2)(2\eta-3)}(2r^4+r^2). \tag{7.35}$$

The quantization procedure can be extended to other conjugate variables as momentum and position. For the first quantity we simply use the function $f=p$ to find the following:

$$A^+_p = \frac{1}{\eta-1}\sum_{n=0}^{\infty}\left\{(\eta+n)|n\rangle\langle n| + \frac{i}{2}\,\alpha_{n+1}\alpha_n\,(|n\rangle\langle n+1|-|n+1\rangle\langle n|)\right\}, \tag{7.36}$$

Similarly, position operator will be given by:

$$A^+_q = -\sum_{n>n'} i^{n-n'+1}\frac{\alpha_{n'}}{\alpha_n}|n\rangle\langle n'| + \sum_{n'>n} i^{n-n'+1}\frac{\alpha_n}{\alpha'_n}|n\rangle\langle n'|. \tag{7.37}$$

Once again, taking the lower symbols we find for the momentum:

$$\langle z|\,A^+_p\,|z\rangle = \frac{\eta}{\eta-1}\,p \tag{7.38}$$

which recalls the result for $\widehat{p^2}$. And for the position:

$$\langle z|\,A^+_q\,|z\rangle = q. \tag{7.39}$$

We can see that for the position, this coherent state quantization is exact without regard of the particular representation of the group that is used. Nevertheless parameter η still control the distribution of the eigenvalues of A_q^+ operator. As is shown in figure 7.3, for a finite matrix numerical approximation, for large values of the parameter, the values tend to spread regularly on the real line more and more densely, a similar result than for time operator.

This result is also seen in the commutator $[\,A_q^+, A_p^+\,]$, which, after some rearrangement has the following matrix form

$$[\,A_q^+, A_p^+\,] = \frac{i}{\eta - 1}\sum_{n=0}^{\infty}(\eta + n + \frac{1}{2})|n\rangle\langle n|. \tag{7.40}$$

For the lower symbol we find the following expression

$$\begin{aligned} \langle z|[\,A_q^+, A_p^+\,]|z\rangle &= \frac{i}{\eta - 1}\left(\eta\frac{1+r^2}{1-r^2} - \frac{1}{2}\right) \\ &= \frac{i}{\eta - 1}\left(\eta\frac{1+q^2+p^2}{2p} - \frac{1}{2}\right). \end{aligned} \tag{7.41}$$

One can see that this function is equal to i on the circle centered in $q = 0$ and $p = 1$ with radius $1/2\eta$. As $\eta > \frac{1}{2}$ the circle remains in the upper half-plane and for the limit $\eta \to \infty$ it contracts to a point.

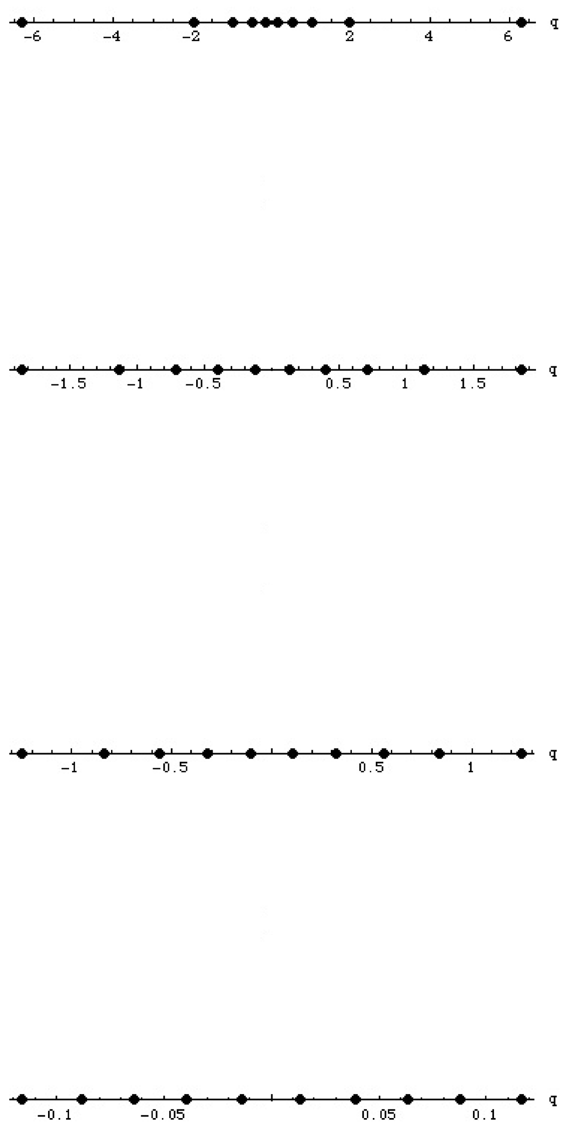


Figure 7.3: Finite matrix approximation of the eigenvalues of position operator for $\eta = 0.5, 5, 10, 1000$ respectively. Note the variation on the scale of the range covered by the eigenvalues. As for time operator, the set tends to be uniformly distributed and dense at the limit where $\eta \longrightarrow \infty$.

8

Conclusions

We have seen through the treated examples that coherent state quantization gives an useful tool to construct quantum operators. Self-adjointness is ensured by definition from the beginning for the quantization of any real function. The method is quite general allowing the use of a broad class of states, among them, coherent states defined by other means. In this way we have avoided the restriction posed by the Pauli theorem on conjugated pairs of observables remaining in a well defined Hilbert space context.

8.1 On these examples

In the phase operator case, the advantages of having a larger set of states on which to represent the phase are clear. The convergence of the commutator at the classical limit is more natural, analytical, than in previous proposals and the expected value of the phase operator leads to the 2π-periodical sawtooth profile of the classical phase.
Creation and annihilation operators can be found by quantizing the exponential of the angle and their commutator converges to the usual one when the mean value is taken on states with vanishing components at high energies. In concodance to intuition, the limit is found by enlarging the dimension of the Hilbert space.

On the infinite well case, the definition of momentum, done by quantizing the classical p function on the phase space instead of assuming the differential form that contradict the Hilbert space imposed by the boundary conditions, give some interesting results. This new operator is diagonal in the set of orthogonal states chosen for the coherent state construction, with eigenvalues given by the possible discrete values of momentum and energy operator, resulting from the p^2 function quantization, reproduces the expected spectrum.
The orthogonal functions, with sinusoidal shape on the position and gaussian functions in the momentum, can be modulated to be as narrow or broad as we want and thus modify the output of the lower symbol.
For position operator, which is not diagonal in these states, the numerical mean value converges to the function to the classical mean value of position in the well for sufficiently narrow functions, and reproduces the position q for functions with a broad profile. That is, the coherent states allow a fair localisation in the well.
In the same way, the modulation of initial functions can show either a total decorrelation of position and momentum through the product $\Delta Q\Delta P$, or approach the

quantum value for a region in the well as large as we want.

Quantization of time for a free particle, taken as the function q/p, shares with the last example the use of vector coherent states. In this case the choice is imposed by the singularity on $P = 0$ and in each component, corresponding respectively to different halves of the complex plane coherent states where chosen as the ones for $SU(1,1)$. Different representations of this group, labeled by a continuous parameter μ were used to recover the classical limit.
The states used reveal to be useful in the quantization of other observables and notably, give an exact quantization of position and a good convergence of the mean value of momentum and energy to their classical values.
The mean value of time operator, has a shape close to the original q/p function quantized as can be seen in figures.

8.2 Interpretation of CS quantization

Various questions arise from the application of this method. It clearly gives a good alternative in problematic cases since everything is well defined in the respective Hilbert spaces. First of all, in the choice of the coherent states used, we dont have a unique possibility but just some normalization constraints. So what is the physical relevance of these states? In the phase problem the choice seems to be more direct, Fourier series being a natural way of decomposing periodical quantities, the addition of vectors within these functions to enlarge the frame on which represent operators has a correspondance on the functional properties of the classical observable. This can be a clue to optimize the quantization method. For the motion on the infinite well, we dont have such a “natural” choice. The same can be said for time operator but these first results give a notion on how this mechanism can be tuned to reveal the desired quantum counterpart of relevant classical observables. This suggests that quantization is not unique but can be used as a filter, a tool, to bring to light particular characteristics in the quantum realm. Another interesting question is the appearance of non-commutativity. This can be attributed to the operator domains within the Hilbert space and is a matter that opens the way to further explorations.

8.3 Challenges

The perspectives of this approach could be validated in the future through specifical examples in physical systems. The construction of coherent states of the type used here could be useful for specific experimental applications. The procedure can find in this way a systematization that can rely on the configuration of particular physical systems.

A
Mathematical tools

In order to have the mathematical tools for the definition of physical relevant quantities let me introduce the mathematical framework of complex functional analysis. This introduction will follow the program of the book of W. Rudin for complex analysis [53], Simon and Reed [35] for functional analysis Akhiezer Glazman [6], von Neumann [28] and A.Peres [4] for the measuring precess in quantum theory, J.P. Dirac for standard formulation of quantum mechanics and coherent states, Klauder and Sudarskan [29] and J.P. Antoine, T. Ali and J.P. Gazeau [8] for generalized coherent states. Basic concepts will be exposed as a list of definitions and theorems without proof that will allow to set the theoretical frame on which coherent state quantization lies.

A.1 Measure theory

Definition A.1.1 *Let X be a set. A* **σ-algebra** *$\mathcal{F}$ on X is a nonempty subset of the powerset (the set of subsets) of X, closed under countable intersections and countable unions with the following properties:*
1) X belongs to $\mathcal{F}$.
2) if $A \in \mathcal{F}$, then the complement of A with respect to X, $\bar{A} \in \mathcal{F}$, then $\bar{X} = \emptyset \in \mathcal{F}$.
3) If a collection of $A_n \in \mathcal{F}$ with $n = 1, 2, 3, \ldots$, then the union $\bigcup_n A_n = A \in \mathcal{F}$. As a consequence of this and 2), $\bigcup_n \bar{A}_n \in \mathcal{F}$ and its complement is also in the σ-algebra,

$$\overline{\left(\bigcup_n \bar{A}_n\right)} = \bigcap_n A_n \in \mathcal{F}. \tag{A.1}$$

Definition A.1.2 *A* **measurable space** *is the pair $(X, \mathcal{F})$, and a* **measurable set** *is any element of $\mathcal{F}$.*

Definition A.1.3 *A* **topology** *τ is a nonempty set of subsets of X that satisfy:*
1) $\emptyset \in \tau$ and $X \in \tau$.
2) Taken a collection of $V_n \in \tau$ with $n = 1, 2, 3, \ldots$, the unions $\bigcap_n V_n \in \tau$.
3) The union of an arbitrary collection V_α of elements of τ is also in τ.

Definition A.1.4 *The pair (X, τ) is called a* **topological space***, the members of τ are called open sets. A common example of a topological space is a metric space.*

Definition A.1.5 *A* **measurable function** f *is a mapping of a measurable space* X *into a topological space* Y *given that* $f^{-1}(V)$ *is a measurable set for every open sets* V *in* Y*.*

Definition A.1.6 *Given a topological space* X*, a* **Borel set** *is an element of the smallest* σ*-algebra that contains all the open sets in* X*. This makes* X *a measurable space and the Borel sets are the corresponding measurable sets.*

Definition A.1.7 *Any continuous mapping* f *from* X *to the real line or the complex plane is called a* **Borel function***.*

Definition A.1.8 *A function that maps* X *to a finite number of points in* $[0, \infty)$ *is called a* **simple function***.*

Definition A.1.9 *A* **positive measure***, or just a* **measure***, is a mapping* μ *from a* σ*-algebra* $\mathcal{F}$ *to the interval* $[0, \infty)$ *such that*

$$\mu(\emptyset) = 0\,. \tag{A.2}$$

If the measure of the whole set X *is*

$$\mu(X) = 1 \tag{A.3}$$

then the measure is a **probability measure***. In all cases monotonicity holds, that is, if If* $A, B \in \mathcal{F}$ *and* $A \subset B$ *then*

$$\mu(A) \leq \mu(B)\,. \tag{A.4}$$

The measure of the union of countable disjoint sets U_n *gives*

$$\mu(\bigcup_n U_n) = \sum_n \mu(U_n)\,, \tag{A.5}$$

that is, the countable additivity property is satisfied. Moreover, the measure of pairwise disjoint members $A_1, A_2, \ldots, A_n$ *of* $\mathcal{F}$

$$\mu(A_1 \cap A_2 \cap \cdots \cap A_n) = \mu(A_1) + \mu(A_2) + \cdots + \mu(A_n)\,. \tag{A.6}$$

Definition A.1.10 *If a measure* μ *maps the* σ*-algebra into the complex plane* $\mathbb{C}$ *it is quite naturally a* **complex measure**

Definition A.1.11 *A* **measure space** *is just a space that has a measure defined on the* σ*-algebra of its measurable sets. It is defined sometimes as a triplet* $(X, \mathcal{F}, \mu)$*.*

Definition A.1.12 *Let* s *and* f *measurable simple functions on a set* X *such that* $0 \leq s \leq f$*, and* $E \in \mathcal{F}$*, the* **Lebesgue integral** *of a particular* f *is defined as*

$$\int_E f d\mu = sup \int_E s d\mu\,. \tag{A.7}$$

This integral is also a measure on $\mathcal{F}$*. The analog definition can be made for complex measures and complex functions.*

A.2 Some topological notions

Definition A.2.1 *X is a* **Hausdorff space** *if for any two elements $a, b \in X$ one can define a neighborhood $V(a)$ and $V(b)$ such that $V(a) \bigcap V(B) = \emptyset$.*

Definition A.2.2 *Let us suppose for simplicity that a topological space X is a Hausdorff space. Then X is* **locally compact** *if we can define a compact neighborhood for every point in it.*

Definition A.2.3 *If a set X contains a countable dense subset, it is said to be* **separable**. *This property is usually assumed ensure the validity of results in bounded dimensional spaces to infinite ones as will be exposed later.*

Definition A.2.4 *A measure defined on the a σ-algebra of all Borel sets in a locally compact Hausdorff space X is called a* **Borel measure** *on X.*

A.3 Hilbert spaces

Definition A.3.1 *A set V is called a* **vector space** *and its elements* **vectors** *if two operations, commutative and distributive addition and multiplication are defined.*

Definition A.3.2 *A* **linear transformation** *T maps a vector space V into another vector space V' as*

$$T(\alpha a + \beta b) = \alpha T a + \beta T b\,, \tag{A.8}$$

for all scalars α and β and all elements $a, b \in V$. If V' is the field of scalars, T is called a **linear functional**.

Definition A.3.3 *The space of all linear functionals on a vector space V is called the* **dual space** *V^*. As an example, the Lebesgue integral is a linear functional.*

Definition A.3.4 *The space $L^p(\mu)$ consists in all the functions f such that the Lebesgue integral*

$$\left(\int |f|^p d\mu \right)^{1/p} = ||f||_p < \infty\,. \tag{A.9}$$

Here $||f||_p$ is called the L^p **norm** *of f.*

Definition A.3.5 *$L^p(\mu)$ is a* **complete metric space**, *that is, every cauchy sequence converges to an element in L^p, for $1 \le p \le \infty$ and every positive measure μ.*

Theorem A.3.6 *L^p is a vector space*

Definition A.3.7 *A complex vector space V is an* **inner product space** *if we can define an operation called inner product on it that satisfies the following properties given $x, y \in V$:*
1) $(x, y) = \overline{(y, x)}$

2) $(x + y, z) = (x, z) + (y, z)$ *i.e. it is distributive in the sum*
3) $(\alpha x, y) = \alpha(x, y)$
4) $(x, x) \geq 0$ *for all* $x \in V$*, the equality holds only when* $x = 0$
This properties lead to the definition of the norm as $||x|| = (x, x)^{\frac{1}{2}}$

Definition A.3.8 *The* **Schwartz inequality** *derives from these properties*

$$|(x, y)| \leq ||x||||y|| \tag{A.10}$$

Definition A.3.9 *As well as the* **triangle inequality**

$$||x + y|| \leq ||x|| + ||y|| \tag{A.11}$$

Definition A.3.10 *An inner product vector space* H *where every Cauchy sequence converges to elements in* H *(i.e. complete) is called a* **Hilbert space***.*

Definition A.3.11 *Let* V *be a vector space and* A *a set in it, now take two elements* $x, y \in A$*,* A *is a* **convex set** *if*

$$A \ni z = ax + by = (1 - t)x + ty \tag{A.12}$$

for any $t \in [0, 1]$*. Note that* $a + b = 1$*. This is extendable to the sum*

$$z = \sum_{n=1}^{N} a_n x_n \tag{A.13}$$

where all $x_n \in V$*, and*

$$\sum_{n=1}^{N} a_n = 1. \tag{A.14}$$

Note that the set of a_n *is a probability measure.*

Theorem A.3.12 L^2 *is the only* L^p *space that is a Hilbert space. The "square integrable" space function has an inner product defined as*

$$\langle f, g \rangle = \int f * g d\mu \tag{A.15}$$

where f *and* g *are complex measurable functions.*

Definition A.3.13 *For* $x, y \in \mathcal{H}$*, if the inner product gives* $(x, y) = 0$*, then they are said to be* **orthogonal***.*

Definition A.3.14 *If* $\mathcal{A}, \mathcal{B} \subset \mathcal{H}$ *and* $(x, y) = 0$ *for every* $x \in \mathcal{A}$ *and* $y \in \mathcal{B}$*, then* $\mathcal{A}$ *and* $\mathcal{B}$ *are* **orthogonal subsets** *of* $\mathcal{H}$*.*

Definition A.3.15 *If* S *is an orthogonal set in* $\mathcal{H}$ *and no other set contains* S *as a proper subset then* S *is an* **orthogonal basis** *for* $\mathcal{H}$*.*

Definition A.3.16 *The set of vectors that are orthogonal to a subset* $M \in \mathcal{H}$ *is called the* **orthogonal complement** $M^{\perp}$*.* M *and* $M^{\perp}$ *are both Hilbert spaces and have only the* 0 *vector in common. The whole space* $\mathcal{H}$ *can be written as*

$$\mathcal{H} = M + M^{\perp} \tag{A.16}$$

Theorem A.3.17 *Projection theorem*
If M is a closed subset in a Hilbert space $\mathcal{H}$, and $z \in M$, $w \in M^{\perp}$ then any $x \in \mathcal{H}$ can be decomposed uniquely as $x = z + w$.

Theorem A.3.18 *Every Hilbert space has an orthonormal basis and if this basis is countable, $\mathcal{H}$ is separable.*

A.4 Operators:

Definition A.4.1 *A linear transformation T from a Hilbert space $\mathcal{H}$ to another $\mathcal{H}'$ is* **bounded** *if there exist a positive number $\alpha \in \mathbb{R}$ such that $||Ax|| \leq \alpha ||x||$.*

Definition A.4.2 *A linear transformation A defined in a dense subspace $D(A) \subset \mathcal{H}$ is called, in quantum mechanics, an* **operator**. *The set $D(A)$ is the* **domain** *of the operator. Two operators A and B are said to be equal if their action on vectors is the same and if their domains coincide*

$$A\phi = B\phi \qquad \phi \in D(A) = D(B) \tag{A.17}$$

Definition A.4.3 *The infimum of all possible values of α determines the* **operator norm** *of A*

$$||A|| = inf \alpha |||Ax|| \leq \alpha ||x|| \forall x \in \mathcal{H}. \tag{A.18}$$

Theorem A.4.4 *Riesz for bounded transformations. A linear functional γ on a Hilbert space $\mathcal{H}$ is bounded if and only if there exist a unique vector $y \in \mathcal{H}$ such that $\gamma(x) = (x, y)$ for all $x \in \mathcal{H}$.*

Definition A.4.5 *An operator A is said to be* **symmetric** *if*

$$(Ax, y) = (x, Ay) \tag{A.19}$$

for all $x, y \in D(A)$

Definition A.4.6 *If A is an operator, there exists a unique operator A^* called the* **adjoint** *of A such that*

$$(Ax, y) = (x, A^* y) \tag{A.20}$$

for all x and y. $||A|| = ||A^*||$.

Theorem A.4.7 *If A is an operator, x is a vector and $\{x_i\}$ a family of vectors such that $\sum_i x_i = x$, then $\sum_i Ax_i = Ax$.*

Definition A.4.8 *An operator P is called a* **projection** *if it maps a separable Hilbert space into another and $P^2 = P$. If in addition $P = P^*$ it is an* **orthogonal projection**.

Definition A.4.9 *The* **spectrum** *$\Lambda(T)$ of an operator T is the set of all complex numbers λ such that $T - \lambda I = 0$.*

Theorem A.4.10 *If T is self-adjoint then $\Lambda(T)$ is a subset of the real axis.*

Theorem A.4.11 *Spectral theorem*
For a bounded self-adjoint operator A on a Hilbert space $\mathcal{H}$ and a bounded real measurable function F on a measure space M, we can always find a measure μ on M and a unitary operator U such that

$$(UAU^{-1}f)(x) = F(x)f(x) \tag{A.21}$$

Theorem A.4.12 *Every bounded self-adjoint operator is a multiplication operator.*

Theorem A.4.13 *Riesz representation theorem*
Let X be a locally compact Hausdorff space and T a positive linear functional. Then there is a σ-algebra $\mathcal{F}$ in X such that it contains all the Borel sets and there is a unique positive measure μ such that it represents T as

$$Tf = \int_X f d\mu \tag{A.22}$$

Theorem A.4.14 *Stone theorem*
Let A be a self-adjoint operator on a Hilbert space $\mathcal{H}$, there exists a unique unitary family of operators U_t parametrized by t, such that

$$U_t \equiv e^{iAt} \, . \tag{A.23}$$

The unitary operators are strongly continuous, that is

$$\lim_{t\longrightarrow t_0} ||U_t - U_{t_0}|| = 0 \, . \tag{A.24}$$

Definition A.4.15 *Let X be a non-empty set, and G a group acting on it, X is a* **homogeneous space** *if G acts continuously and transitively*[1] *on X. If X is a topological space, transitivity implies the indistinguishability of the elements in X under the action of G and gives a structure to the set as a single orbit of G.*

In particular, if X is the real line, it is homogeneous for the group of translations since we can cover ?? all the set continuously through the application of the group and there is always a $g \in G$ that maps two points in the set. Note that a finite interval is not homogeneous for the group of translations.

A.4.1 Self-adjoint extensions

If an operator A is Hermitian but not self-adjoint, we can measure how far is A from being self-adjoint operator by analyzing the part of its spectrum that is imaginary. That is, from the eigenvalue equation

$$A\phi = \pm i\phi \, , \tag{A.25}$$

we want to know the dimension of the set of states such that

$$(A \mp i1)\phi = 0 \, , \tag{A.26}$$

[1] G acts transitively in X if for any x and $y \in X$ there is some $g \in G$ such that $g \cdot x = y$

and this will give a **deficiency index** $n_\pm$

$$\begin{aligned} n_+ &= \dim Ker(A - i1) \\ n_- &= \dim Ker(A + i1) \end{aligned} \tag{A.27}$$

on which to apply a criterion.

Theorem A.4.16 *Von Neumann criterion*
For an Hermitian operator with deficiency indices n_+ *and*
1) If $n_+ = n_- = 0$ *then* A *is self-adjoint and only in this case the spectrum of* A *is a subset of the real axis.*
2) If $n_+ = n_-$, A *the domain of* A *can be extended so as to have a self adjoint operator. The spectrum 3) If* $n_+ \neq n_-$ *there is no self-adjoint extension to* A.

But these extensions have to be chosen regarding the correspondence that they have in the physical conditions they imply. We will return to the problem of higher dimensional extensions in chapter 6 when we analyze the infinite well problem.

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