Semiclassical approximation to the propagator of the Wigner function for particles in confined spaces

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A.1 For an even potential the distance between the turning points is $2q_l$. Adding a distance of $2\lambda$ in the forbidden region in each turning point gives a total distance $D = 2q_l + 4\lambda$, where $\lambda$ is the de Broglie wavelength corresponding to the energy $E_m$. 

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Introduction

Since their introduction quantum phase space distribution functions have served as important tools in the study of quantum phenomena. They provide a complementary point of view in the physical interpretation of quantum states and their evolution. For this reason, these functions constitute a valuable framework for research on new physical systems as well as in the interpretation and explanation of systems and phenomena already studied from standard quantum mechanics.

The aim of the phase space representation of quantum mechanics is to describe quantum systems directly in phase space using number functions rather than operators and state vectors. This representation was introduced by Wigner in 1932 \cite{1} and it grew to form a family of quantum phase space distribution functions \cite{2}. It is important to say that this formalism was devised for systems with a classical counterpart (however there is a recent attempt to generalize the Wigner function to include systems with spin \cite{3}). Among other reasons, the Wigner function has a special place in this family because it is the basis for the phase space representation of quantum mechanics, which translates not only quantum states but also the equations of motion, eigenvalue equations and propagators from the standard framework of quantum mechanics. In addition, one important advantage of the Wigner function is that it allows for semiclassical approximations that are superior in various respects to those based, e.g., on the configuration space representation.

Semiclassical physics can be seen from two perspectives: From a practical point of view, it collects different approximations which construct quantum quantities (as wavefunctions, phases, cross sections, etc.) from classical concepts. From a fundamental point of view it studies the classical contributions existing in the quantum realm. In this sense, semiclassical physics explores the intriguing borderline between the quantum and the classical world.

Semiclassical approximations are widely known in position representation of quantum mechanics. In the energy domain, we have the WKB method (Wentzel, Kramers, Brillouin) for the construction of wavefunctions and the EBK method (Einstein, Brillouin, Keller) which allows the quantization of chaotic systems. In the time domain, the semiclassical propagation of wavepackets is achieved by the van-Vleck propagator (the semiclassical limit of Feynman’s path integral) and the Herman-Kluk propagator \cite{4}. A notable example of the success of semiclassical physics is the Gutzwiller trace formula in which the quantum density of states is expressed in terms of classical periodic orbits \cite{5}. This formula emphasises the important role of unstable periodic orbits in the quantization of chaotic systems \cite{4}.
In phase space, semiclassical propagation of Wigner functions presented difficulties as pointed out by Heller [6]. The main issue was related with the correct treatment of the non-diagonal terms of the density matrix or the “dangerous cross-terms”. This problem was resolved by semiclassical propagation in terms of pairs of neighboring trajectories instead of one guiding orbit [7]. With this development we can study the semiclassical approximation for quantum systems directly in phase space.

Particles in confined spaces, that is, restricted by infinitely high potential walls on one or two sides, were studied since the beginning of quantum mechanics (some historical notes about this problem are found in [8]) and rich dynamical behavior has been found in these systems (mainly in the case of two walls). Despite their simplicity, particles in confined spaces constitute highly nonlinear systems. For example, it was shown that the infinitely deep potential well (particle confined within two walls) can exhibit chaotic dynamics in the presence of an external field [9]. On the other hand, highly regular patterns in the space-time representation of probability distribution, known as quantum carpets, have been observed in this system [10]. Their formation have been explained in terms of interference between individual eigenmodes [11] [12]. These patterns have been observed in other potentials, for example the harmonic oscillator potential. In the case of the infinitely deep potential well, the zones of high and low amplitude (sometimes called ridges and tunnels, respectively) are clearer and form straight lines. The phase space formulation of quantum mechanics has been useful in the study of these examples [13]. In the former example its quantum counterpart was studied by means of the Husimi function [14] and in the latter quantum carpets can be explained from the interference terms of the Wigner function [15].

For the classical system, we know that trajectories of particles interacting with one or two walls can be thought of in terms of the mirror image method, that is, the reflected trajectory is seen as a free-particle trajectory between the starting point and a mirror image of the final point in a replica of the original confined region. In the quantum version of these systems, this periodic approach was used in order to derive the Feynman propagator from the path integral formalism [16] [17]. In analogy with the classical case, the Feynman propagator is constructed from the free-particle propagator between the starting point and the mirror images of the final point.

Both approaches assume a different nature of the walls. While the periodic approach considers thin walls (δ-functions) between each replica of the original region, in the confined approach the walls are assumed thick (θ-functions), which means that wavefunctions (or particles, in the classical system) cannot go through the walls. Different walls impose different boundary conditions for the wavefunctions. This boundary conditions will be translated into the phase space formalism and, in particular, they have to be taken into account not only for the construction of the Wigner function but also in its time evolution [18]. Moreover, the boundary conditions in the infinitely deep potential well (particle with two walls) has been used to illustrate some paradoxes related with the self-adjoint condition of quantum operators [19]. These examples show the important role of the boundary conditions in the dynamical evolution and the physical interpretation of quantum systems.

The box with thin walls has been used in optics as a model of diffraction gratings. In this way, a diffraction grating can be regarded as infinite series of δ-functions with a separation of twice the width of the strips. On the other hand, the box with thick walls has been applied as a model of quantum dots in solid state physics because it captures the main characteristics for one-dimensional confinement potentials in general [20]. Additionally, in
numerical solutions of the Schrödinger equation, boundary conditions like those imposed by the thick walls are usually assumed.

The existing symmetry in the repetitions of the original box, facilitates the analysis of the box with thin walls. Without this symmetry, the box with thick walls imposes big technical challenges. Despite this difficulties, thick walls are closer to nonlinear classic systems (as a limit of potentials of the form $q^2$). These systems constitute an important research topic owing to their behaviour. The interpretation of the dynamics of these systems from the phase space formalism can offer a different perspective, and with the Wigner function formalism we have the tools to explore the semiclassical limit of the propagator of the Wigner function directly in phase space.

This work construct the exact propagator of the Wigner function in the case of thick walls, a novel result with a huge potential for both theory and applications. Although semiclassical approximation does not apply in this case, this work takes advantage of the limit of polynomial potentials so as to obtain the semiclassical approximation of smooth potentials close to the box with thick walls. With this approach, we want to confirm the closeness of this smooth potential approximation to the exact propagator of the infinitely deep potential well.

The document is organized as follows: In chapter 1 we present a review of the phase space formalism in terms of the Wigner function. In particular, we are interested in the exact propagator of the Wigner function. In chapter 2 we are going to derive the exact Wigner propagator in the case of a particle with one wall. We will do this derivation from the two approaches in order to identify the differences between both points of view. In chapter 3 we present the derivation of the exact Wigner propagator in the case of two walls following the same procedure as in the case of one wall. Due to their characteristics the infinitely high potential walls represents a challenge for semiclassical approximations. Moreover, we will see that in the periodic approach the semiclassical approximation has no sense. For this reason, to construct the semiclassical propagator of the Wigner function we are going to use an smooth potential approximation for the infinitely deep potential well. This potential will be studied in chapter 4. The Wigner eigenfunctions and the exact propagator will be found and compared with the case of two walls. Finally, in chapter 5 we construct the semiclassical propagator of the Wigner function for the smooth potential approximation of the infinitely deep potential well and compare this with the exact results.
The Wigner function and the phase space formalism

In the realm of quantum states that are not pure and of incoherent time evolution, the description of a quantum system is given by the density operator $\hat{\rho}$. This abstract operator can have different representations depending on the basis used to represent it. For example, common representations are $\langle q | \hat{\rho} | q' \rangle$, $\langle p | \hat{\rho} | p' \rangle$ and $\langle E | \hat{\rho} | E' \rangle$ [21]. The idea of the phase-space formalism is to give a representation of the density operator $\hat{\rho}$, and in general of any operator $\hat{A}(q, \hat{p})$, in terms of functions (real or complex) in phase space. In order to give a full picture of quantum mechanics in phase space, it is also necessary to describe the dynamical evolution of the state of the system directly in phase space. This can be accomplished by means of the appropriate translation of the equations of motion to phase space or in terms of propagators in phase space.

The uncertainty principle prevents a particle to have simultaneously a well defined position and momentum. For this reason, it is not possible to define a probability that a particle has a position $q$ and a momentum $p$ [2]. For quantum systems, it is possible to define quasiprobability functions which retain as much as possible the behaviour of real probability functions. On the other hand, due to the fact that, in general, operators do not commute, there is no a unique way to associate quantum operators with number functions [14]. As a result, there is a family of phase-space distribution functions, each one preserving part of the characteristics of a true probability distribution function.

The Wigner function $W(p, q)$ [1] is one of the members of this family which allows, with Weyl’s correspondence rule, a complete phase-space formulation of quantum mechanics [22] in the sense of an invertible (one-to-one) relation between the density operator and the Wigner function.

In this chapter we are going to briefly review the phase space formulation of quantum mechanics in terms of the Wigner function. In particular, we are going to show the construction of the exact propagator of the Wigner function and develop the expressions to be used in the next chapters. Due to the fact that the systems treated in this work are one-dimensional we restrict this review to this kind of systems.
1.1 The Wigner function

The Wigner function is a one-to-one representation of the density operator. It is defined by the expression

\[
W(r) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} du \exp\left(-\frac{i}{\hbar} pu\right) \langle q + \frac{u}{2} | \hat{\rho} | q - \frac{u}{2}\rangle.
\]

(1.1)

where we have introduced the notation \( r = (p, q) \).

The main properties of this function are [13]:

- The Wigner function is real and normalizable

\[
\int dr W(r) = 1
\]

(1.2)

- The Wigner function can take positive as well as negative values. For this reason the Wigner function cannot be interpreted as a true phase-space probability density.

- We can obtain the probability distribution of position and momentum from the integration of the Wigner function with respect to momentum and position, respectively

\[
\int dp W(p, q) = \langle q|\hat{\rho}|q\rangle = W(q) \quad \text{and} \quad \int dq W(p, q) = \langle p|\hat{\rho}|p\rangle = W(p).
\]

(1.3)

1.2 The Weyl Transform

The rule defined by the Wigner function can be extended to any quantum operator that depends on \( p \) and \( q \). The phase-space representation \( A_W(r) \) of the operator \( \hat{A}(\hat{p}, \hat{q}) \) is called the Weyl symbol of the operator and is given by

\[
A_W(r) = \int du \langle q + \frac{u}{2} | \hat{A}(\hat{p}, \hat{q}) | q - \frac{u}{2}\rangle \exp\left(-\frac{i}{\hbar} up\right).
\]

(1.4)

Denoting the transformation given by (1.4) as \( T_W[\hat{A}(\hat{p}, \hat{q})] \) we can see that the Wigner function is the Weyl symbol of the density operator times the normalization factor \( 1/(2\pi\hbar) \).

The rule to go from the phase-space representation to the quantum operator is defined by the inverse Weyl transform

\[
\hat{A}(\hat{p}, \hat{q}) = \int d\tau d\sigma d\tau A_W(r) \exp[i\tau(\hat{p} - p) + i\sigma(\hat{q} - q)].
\]

(1.5)

Despite the fact that it can be negative, a remarkable feature of the Wigner function is that the expectation value of the operator \( \hat{A}(\hat{p}, \hat{q}) \) in the phase space formalism is given by

\[
\langle \hat{A}(\hat{p}, \hat{q}) \rangle = \int dr A_W(r) W(r)
\]

(1.6)

which is identical to the method of evaluation of average values in classical statistical physics.
An important quantity in the construction of the propagator of the Wigner function is the Weyl symbol of the unitary time evolution operator

\[ \hat{U}(t) = \exp\left(-\frac{i}{\hbar} \hat{H}t\right) \]  

(1.7)

where \( \hat{H} \) is the time-independent Hamiltonian of the system.

The Weyl symbol of \( \hat{U}(t) \) (sometimes called the Weyl propagator) is

\[ U_W(r, t) = \int du \langle q + \frac{u}{2} | \hat{U}(t) | q - \frac{u}{2} \rangle \exp\left(-\frac{i}{\hbar} up\right) \]

(1.8)

where \( K(q'', t; q', 0) \) is the Feynman propagator of the system. The main properties of the Weyl propagator are reviewed in [23].

### 1.3 The propagator of the Wigner Function

The density operator at time \( t \), \( \hat{\rho}(t) \), is obtained from the initial density operator \( \hat{\rho}(0) \) from the relation

\[ \hat{\rho}(t) = \hat{U}^\dagger(t) \hat{\rho}(0) \hat{U}(t) \]  

(1.9)

In order to isolate the propagator of the Wigner function, we need to apply the Weyl transform to (1.9)

\[ T_W[\hat{\rho}(t)] = W(p'', q'', t) = T_W[\hat{U}^\dagger(t) \hat{\rho}(0) \hat{U}(t)], \]

(1.10)

but in the right-hand side of the previous equation we have the Weyl transform of the product of three operators, which is not equal to the product of the Weyl symbol of each operator.

If we have an operator \( \hat{A}(\hat{r}) = \hat{A}_1(\hat{r}_1)\hat{A}_2(\hat{r}_2)\hat{A}_3(\hat{r}_3) \), its Weyl symbol is given by

\[ A_W(r) = \frac{1}{(\pi\hbar)^2} \int dr_1 dr_2 dr_3 A_{W_1}(r_1)A_{W_2}(r_2)A_{W_3}(r_3) \exp\left[\frac{i}{\hbar} (r_1 \wedge r_2 + r_3 \wedge r) \right] \delta(r_1 - r_2 + r_3 - r), \]

(1.11)

where \( r_1 \wedge r_2 = r_1^T J r_2 \) is the symplectic product, with the symplectic matrix \( J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \).

Using the equation (1.11) with the right-hand side of (1.10) we can identify the propagator of the Wigner function as

\[ G_W(r'', t; r', 0) = \frac{1}{(\pi\hbar)^2} \int d^2r_1 d^2r_2 U_W(r_1, t)U_W^*(r_2, t) \exp\left[\frac{i}{\hbar} (r_1 \wedge r' + r_2 \wedge r'') \right] \delta(r_1 + r_2 - (r'' + r')). \]

(1.12)
CHAPTER 1. THE WIGNER FUNCTION AND THE PHASE SPACE FORMALISM

Using the new variables \( r = r_2 - r_1 \) and \( R = (r_2 + r_1)/2 \) the last equation takes the form

\[
G_W(r''; t; r', 0) = \frac{1}{(\pi \hbar)^2} \int d^2r d^2RU_W(R - r/2, t)U^*_W(R + r/2, t) \exp \left[ \frac{i}{\hbar} (R - r/2) \land r' + (R + r/2) \land r'') \right] \delta(2R - (r'' + r')).
\]

(1.13)

Performing the integral with respect to \( R \) and defining a new set of variables \( r_{\pm} = (r'' + \pm r)/2 \) we obtain

\[
G_W(r'', t; r', 0) = \frac{1}{(2\pi \hbar)^2} \int d^2r U_W(r-, t)U^*_W(r+, t) \exp \left[ \frac{i}{\hbar} (r \land (r'' - r')) \right].
\]

(1.14)

Therefore, the propagator of the Wigner function is obtained as the convolution of two Weyl propagators [24].

Like the Wigner function, its propagator is real. From this expression it can be shown that the propagator of the Wigner function satisfies the initial condition

\[
G_W(r'', 0; r', 0) = \delta(r'' - r')
\]

(1.15)

and the composition rule

\[
G_W(r'', t''; r', 0) = \int d^2r G_W(r'', t''; r, t')G_W(r, t'; r', 0)
\]

(1.16)

1.3.1 Propagator of the Wigner function in the energy basis

If the system under consideration has a set of energy eigenstates \( \hat{H}|\alpha\rangle = E|\alpha\rangle \) we can expand the Weyl propagator in terms of these states, obtaining for the propagator of the Wigner function

\[
G_W(r'', t; r', 0) = \sum_{\alpha, \beta} \exp \left[ -\frac{i}{\hbar} (E_\alpha - E_\beta)t \right] \int d^2r \exp \left[ \frac{i}{\hbar} (r \land (r'' - r')) \right]
\]

\[
\times \int du_+ \langle q_+ + \frac{u_+}{2} | \alpha \rangle \langle \alpha | q_+ - \frac{u_+}{2} \rangle \exp \left(-\frac{i}{\hbar} u_+ p_+ \right)
\]

\[
\times \int du_- \langle q_- + \frac{u_-}{2} | \beta \rangle \langle \beta | q_- - \frac{u_-}{2} \rangle \exp \left(-\frac{i}{\hbar} u_- p_- \right).
\]

(1.17)

The integral with respect to \( r \) gives the result \((2\pi \hbar)^2 \delta(r'' - r')\). Using this result and rearranging terms we arrive to the expression

\[
G_W(r'', t; r', 0) = (2\pi \hbar)^2 \sum_{\alpha, \beta} \exp \left[ -\frac{i}{\hbar} (E_\alpha - E_\beta)t \right] W^*_\alpha,\beta(r')W_{\alpha,\beta}(r'')
\]

(1.18)

which involves the non-diagonal Wigner functions

\[
W_{\alpha,\beta}(r) = \frac{1}{2\pi \hbar} \int du \exp \left(-\frac{i}{\hbar} pu \right) \langle q + \frac{u}{2} | \alpha \rangle \langle \beta | q - \frac{u}{2} \rangle
\]

(1.19)
In contrast to the diagonal elements, the operator $|\alpha\rangle \langle \beta|$ is not an hermitian operator. Consequently, the non-diagonal Wigner functions are not generally real.

The expression (1.18) allows the numerical calculation of the exact propagator of the Wigner function once we have the energy eigenfunctions. This expression will be used in the next chapters to obtain the exact propagator for the infinitely deep potential well and its smooth approximation.

1.3.2 Wigner function for discrete phase space

In numerical applications, the wavefunctions are usually known only in certain discrete values of the position (or momentum). This implies working in a discrete spatial basis $|n\rangle, n = 0, 1, \ldots, N$. Due to the fact that the momentum and position are related with a Fourier transform, the periodicity of position implies a discretization of momentum and vice versa. This structure corresponds to a cylindrical phase space. If there exists also a periodicity in the position the topology of phase space will be that of a torus. The definition of the Wigner function in these phase spaces was derived by Berry [25]. For a cylindrical phase space with periodic position of period $Q$, the Wigner function is given by

$$W(p_\lambda, q) = \frac{1}{2\pi} \sum_{\lambda=\infty}^{\infty} \frac{1 + (-1)^{\lambda-L}}{2} \left( \frac{\lambda + \lambda'}{2} \right) \left| \hat{\rho} \left( \frac{\lambda + \lambda'}{2} \right) \right| \exp \left( 2\pi i \frac{\lambda q}{Q} \right)$$

(1.20)

with $\hat{p} |\lambda\rangle = p_\lambda |\lambda\rangle$ and $p_\lambda = \pi \lambda / Q$. In the case of periodic momentum, the expression is the same, we only have to interchange $Q \rightarrow P$ and $\lambda \rightarrow n$ where $|n\rangle$ are the discrete position eigenstates.

Nevertheless, this definition of the Wigner function contains redundant information. A possible definition of a non-redundant version of the Wigner function is [26], [27]

$$W(n, p) = \sum_{n'=-\infty}^{\infty} W_{n,n'} \exp \left\{ -2\pi i n' \frac{p}{P} \right\}$$

(1.21)

where the coefficients $W_{n,n'}$ are of the form

$$W_{n,n'} = \frac{1}{2\pi \hbar} \left\{ \begin{array}{ll}
\left( n + \frac{n'}{2} \right) \left| \hat{\rho} \left( n - \frac{n'}{2} \right) \right| & \text{if } n' \text{ is even} \\
\frac{1}{\pi} \sum_{m=-\infty}^{\infty} (-1)^m \left( n + \frac{n'}{2} + m + \frac{1}{2} \right) \left| \hat{\rho} \left( n - \frac{n'}{2} + m + \frac{1}{2} \right) \right| & \text{if } n' \text{ is odd}
\end{array} \right.$$

(1.22)

1.3.3 Propagator of the Wigner function for discrete spaces

The transformation given by (1.21) and (1.22) is used to construct the propagator of the Wigner function for discrete spaces. If we call this transformation $T_{W_d}$ the Wigner function propagator is obtained from [28]

$$G_W(r_n^\prime, t; r_n^\prime, 0) = T_{W_d} K(n^\prime, t; n^\prime, 0) T_{W_d}^{-1}$$

(1.23)

where $r_n = (p, n)$. With the help of the energy eigenstates we can write (1.23) in the same way as (1.18) in terms of the non-diagonal Wigner functions, given in this case by
the transformation $T_{W_d}$

$$G_W(r'', t; r', 0) = \frac{1}{N} \sum_{\alpha, \beta} \exp \left[ -\frac{i}{\hbar} (E_\alpha - E_\beta) t \right] W^*_{\alpha, \beta}(r'_n) W_{\alpha, \beta}(r''_n).$$  \hspace{1cm} (1.24)$$

This expression for the Wigner function propagator will be used in the chapter where we will have to obtain the energy eigenfunctions numerically.
CHAPTER 2

Particle in a half-space

We are going to start the study of particles in confined spaces with the case of a particle restricted by one infinitely high potential wall or a particle in a half-space. In this chapter we shall focus in the exact propagator and we will obtain it directly without mention of the Wigner eigenfunctions.

The main difference between this system and the system with two walls relies in the quantization. Here we have a continuous energy and momentum spectrum while these are quantized in the case of two walls.

We are going to use two different approaches: the periodic and confined approach. Although both options describe the same system, there are differences in the physical interpretation, in particular, the propagator of the Wigner function has a distinct form and a particular time evolution in each case.

2.1 Potential

If the wall is located at $q = 0$ the potential for this system is

$$V(q) = \begin{cases} \infty & q \leq 0, \\ 0 & \text{else}. \end{cases}$$ (2.1)

This potential splits the coordinate space in two parts, the forbidden ($q \leq 0$) and the allowed region ($q > 0$). Although in the allowed region the particle behaves as a free particle, due to the boundary condition, the wavefunctions for this systems differ from the free-particle case

$$\psi_k(q) = \begin{cases} \frac{1}{\sqrt{\pi \hbar}} \sin(kq) & q > 0, \\ 0 & q \leq 0 \end{cases}$$ (2.2)

$$= \sin(kq) \Theta(q)$$

with $k \in \mathbb{R}$.
As we will see, the free-particle propagation emerges from the symmetric approach to the particle in a half-space. For this reason, it is useful to know the form of the free-particle Wigner propagator.

### 2.2 The Wigner free-particle propagator

In this case we can obtain the propagator of the Wigner function for free-particle propagation by direct application of Eq. (1.14). The Hamiltonian of the system is $\hat{H} = \hat{p}^2 / 2m$ and its Weyl propagator is

$$U_W(p, q, t) = \exp \left( -\frac{i}{\hbar} \frac{p^2}{2m} t \right).$$

Substitution of (2.3) in (1.14) gives

$$G_W(r'', t; r', 0) = \frac{1}{(2\pi \hbar)^{2}} \int dp dq \exp \left( -\frac{i}{\hbar} \frac{(p'' + p') pt}{2m} \right) \exp \left[ -\frac{i}{\hbar} (q(p'' - p') - p(q'' - q')) \right]$$

$$= \delta(p'' - p') \delta(q'' - (q' + \frac{p'}{m} t)).$$

This result indicates that the Wigner function propagates following the classical trajectory under the action of the free-particle Hamiltonian.

### 2.3 Wigner propagator for a particle in a half-space

As was mentioned before, we have to distinguish between two approaches to the propagator. The first is to consider a thin wall which allows the wavefunctions go through it but imposing a symmetry between the left and right sides of the wall. In this approach we can interpret the wall as a mirror. On the other hand, we can consider a thick wall and restrict the wavefunctions to certain region of the space, in other words, divide the space in the forbidden and allowed region.

#### 2.3.1 Thin wall (Symmetric approach)

In order to derive the Wigner propagator in the case of a thin wall, we are going to compare the initial Wigner function at $t = 0$ with the Wigner function at time $t$. To begin with, consider an initial wavefunction $\psi(q, 0)$ and the wavepacket in terms of the antisymmetric
wavefunctions \((\psi(-q) = -\psi(q))\) \(\text{(2.2)}\)

\[
\psi(q, 0) = \frac{1}{\sqrt{\pi \hbar}} \int_0^\infty dk a(k) \sin(kq) \\
= \frac{1}{2i \sqrt{\pi \hbar}} \int_0^\infty dk a(k)(e^{ikq} - e^{-ikq}) \\
= \frac{1}{2i \sqrt{\pi \hbar}} \int_{-\infty}^\infty dk a(k)e^{ikq}
\] \(\text{(2.5)}\)

where we have assumed the property for the coefficients \(a(-k) = -a(k)\). Notice the change of the integration limits, so there is no forbidden region.

Now we want to construct the initial density matrix

\[
\rho(q_1, q_2, 0) = \psi_{k_1}(q_1)\psi^*_{k_2}(q_2) \\
= \frac{1}{2\pi} \int_{-\infty}^{\infty} dk_1 dk_2 a(k_1)a^*(k_2)e^{i(k_1q_1-k_2q_2)}.
\] \(\text{(2.6)}\)

The coefficients \(a(k_1)a^*(k_2)\) can be written in terms of the initial density matrix

\[
a(k_1)a^*(k_2) = \frac{\hbar}{2\pi} \int_{-\infty}^{\infty} dq_1 dq_2 \rho(q_1, q_2, 0)e^{-ik_1q_1+ik_2q_2}.
\] \(\text{(2.7)}\)

Applying an inverse Weyl transform we can write the initial density matrix as

\[
\rho(q_1, q_2, 0) = \int_{-\infty}^{\infty} dp W \left(p, \frac{q_1 + q_2}{2} \right) e^{-\frac{i}{\hbar}(\rho(q_2-q_1))}
\] \(\text{(2.8)}\)

and the coefficients take the form

\[
a(k_1)a^*(k_2) = \frac{\hbar}{2\pi} \int_{-\infty}^{\infty} dq_1 dq_2 e^{-ik_1q_1+ik_2q_2} \int_{-\infty}^{\infty} dp W \left(p, \frac{q_1 + q_2}{2} \right) e^{-\frac{i}{\hbar}(\rho(q_2-q_1))}.
\] \(\text{(2.9)}\)

**Figure 2.1.** The thick wall (a) prevents the particle of being in the left side of the plane while the thin wall (b) works like a mirror between the left an right sides.
The time-evolved density matrix is obtained from the substitution of the time-dependent coefficients
\[ a(k_1, t) a^*(k_2, t) = a(k_1) a^*(k_2) e^{-\frac{i}{\hbar} (E_{k_1} - E_{k_2}) t}, \]
with \( E_k = (\hbar k)^2 / 2m \), in (2.6) and together with the expression (2.9) it gives
\[ \rho(q_1, q_2, t) = \frac{\hbar}{(2\pi)^2} \int_{-\infty}^{\infty} dk_1 dk_2 \int_{-\infty}^{\infty} dq_1 dq_2 e^{-ik_1(q_1 - q_1')} e^{ik_2(q_2 - q_2')} e^{-\frac{i}{\hbar} (E_{k_1} - E_{k_2}) t} \]
\[ \int_{-\infty}^{\infty} dp W \left[ p, \frac{q_1^2 + q_2^2}{2} \right] e^{-\frac{i}{\hbar} (p(q_2 - q_1))}. \]

We apply a forward Weyl transform to get the time-evolved Wigner function
\[ W(r'', t) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} du'' \rho \left( q'' + \frac{u''}{2}, q'' - \frac{u''}{2}, t \right) e^{-\frac{i}{\hbar} p''u''} \]
\[ \times \left( e^{-ik_1(q'' - u'')} e^{ik_2(q'' + u'')} e^{\frac{i}{\hbar} p''u''} \right) \]
\[ \times \left( e^{ik_1(q'' + u'')} e^{-ik_2(q'' - u'')} e^{-\frac{i}{\hbar} p''u''} \right) \]
\[ = \int_{-\infty}^{\infty} dp' dq' G_W(r'', t; r', 0) W(r') \]

with the Wigner propagator given by
\[ G_W(r'', t; r', 0) = \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} dk_1 dk_2 \int_{-\infty}^{\infty} du'' \int_{-\infty}^{\infty} dp' dp'' e^{-\frac{i}{\hbar} (E_{k_1} - E_{k_2}) t} \]
\[ \times \left( e^{-ik_1(q'' - u'')} e^{ik_2(q'' + u'')} e^{\frac{i}{\hbar} p''u''} \right) \]
\[ \times \left( e^{ik_1(q'' + u'')} e^{-ik_2(q'' - u'')} e^{-\frac{i}{\hbar} p''u''} \right). \]

To solve the integrals in the previous expression we transform to new variables \( k = \frac{1}{2}(k_1 + k_2) \) and \( K = k_1 - k_2 \) and rearranging terms we have
\[ G_W(r'', t; r', 0) = \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} dk dK \int_{-\infty}^{\infty} du'' \int_{-\infty}^{\infty} dp e^{-\frac{i}{2m} kK t} e^{iu' \left( \frac{K}{2} + k' \right)} e^{-iu'' \left( \frac{K}{2} + k'' \right)} e^{-ik(q'' - q')} \]
\[ = \delta(p'' - p') \delta \left( q'' - \left( q' + \frac{p'}{m} t \right) \right). \]

As we can see, with a thin wall we have a classical free-particle propagation. For this reason, there is no point in attempting a semiclassical approximation in this approach.
Furthermore, as a consequence of this classical propagation, the quantum features are encoded in the quantum initial state.

For instance, for a Gaussian wavepacket

\[ \psi(q) = (\sqrt{\pi} \Delta q)^{-\frac{1}{2}} \exp \left[ -\frac{1}{2} \left( \frac{q - q_0}{\Delta q} \right)^2 \right] \exp \left[ i \frac{\hbar}{p_0} (q - q_0) \right]. \] (2.16)

its Wigner function in the half-space is composed of three terms \[ W(r) = W_+(r) + W_-(r) + W_{\text{int}}(r) \] (2.17)

where

\[ W_{\pm}(r) = \frac{1}{\pi \hbar} \exp \left[ -\left( \frac{q \pm q_0}{\Delta q} \right)^2 \right] \exp \left[ -\left( \frac{p \pm p_0}{\Delta p} \right)^2 \right] \] (2.18)

and

\[ W_{\text{int}}(r) = -\frac{2}{\pi \hbar} \cos \left( \frac{2}{\hbar} (p_0 q + p q_0) \right) \exp \left[ -\left( \frac{q}{\Delta q} \right)^2 \right] \exp \left[ -\left( \frac{p}{\Delta p} \right)^2 \right] \] (2.19)

As we can see, from the initial Gaussian wavepacket we have, in its Wigner function, two Gaussian contributions with opposite amplitude. One is centred at \( r_0 = (p_0, q_0) \) and the other at \( r_0 = (-p_0, -q_0) \). These contributions will move along free-particle trajectories in opposite directions. The third contribution in this Wigner function is given by the interference term (2.19) and it is located in the middle of the two Gaussian contributions. The thin wall works like a mirror because it splits the initial distribution in two main contributions which gives rise to an additional interference pattern in the Wigner representation.

### 2.3.2 Thick wall (Confined approach)

Now we are going to consider the approach with a thick wall. As was mentioned before, in this case the wavefunctions vanish in the forbidden region \( q \leq 0 \). Using the same procedure as in the case of a thin wall, we can isolate the propagating integration kernel

\[ G(r'', t; r', 0) = \frac{1}{\pi^2 \hbar} \int_0^\infty dk_1 dk_2 \exp \left[ -\frac{\hbar}{2m} (k_1^2 - k_2^2) t \right] \]

\[ \times \int_{-2q'}^{2q'} du' e^{ik_1 u'} \sin \left[ k_1 \left( q' - \frac{u'}{2} \right) \right] \sin \left[ k_2 \left( \frac{u' + q'}{2} \right) \right] \]

\[ \times \int_{-2q''}^{2q''} du'' e^{-ik_2 u''} \sin \left[ k_1 \left( q'' - \frac{u''}{2} \right) \right] \sin \left[ k_2 \left( \frac{q'' + u''}{2} \right) \right]. \] (2.20)

The effective range of integration for the variables \( u' \) and \( u'' \) is obtained by considering the boundary condition imposed by the wall. Solving the integrals with respect to these variables we arrive to
\[ G_w(q'', t; q', 0) = \frac{q'' q'}{\pi \hbar} \int_0^\infty dk_1 dk_2 \exp \left[ -\frac{i\hbar}{2m} (k_1^2 - k_2^2)t \right] \]
\[
\{ \exp[i(k_1 - k_2)q'] \text{sinc} [(2k' + k_1 + k_2)q'] + \exp[-i(k_1 - k_2)q'] \text{sinc} [(2k' - k_1 - k_2)q'] \\
- \exp[i(k_1 + k_2)q'] \text{sinc} [(2k' + k_1 - k_2)q'] - \exp[-i(k_1 + k_2)q'] \text{sinc} [(2k' - k_1 + k_2)q'] \}
\]
\[
\{ \exp[i(k_1 - k_2)q''] \text{sinc} [(2k'' + k_1 + k_2)q''] + \exp[-i(k_1 - k_2)q''] \text{sinc} [(2k'' - k_1 - k_2)q''] \\
- \exp[i(k_1 + k_2)q''] \text{sinc} [(2k'' - k_1 + k_2)q''] - \exp[-i(k_1 + k_2)q''] \text{sinc} [(2k'' + k_1 - k_2)q''] \}
\]

Figure 2.2 shows the quantum spot of the Wigner propagator (2.21). This structure is a graphic representation of the naked propagator. The plots were obtained from numerical integration of the propagator. Two cases were considered: a negative and positive initial momentum corresponding to a particle launched towards the wall and a particle moving to the right without interaction with it, respectively. We can see that the initial distribution moves along the classical trajectory. However, the time evolution splits the initial distribution into two main contributions. It is remarkable that the initial distribution is already divided even though the distribution does not interact directly with the wall. This is a non-local effect in the sense that the distribution “feels” the wall without a direct interaction.
Figure 2.2. Quantum spot of the half-space system in the confined space approach, with negative initial momentum (left column) and positive initial momentum (right column), at times $t = 0$ (first row), $t = 0.2$ (second row) and $t = 2.0$ (third row). The initial conditions were $(p, q) = (\pm 5.0, 0.1)$. Color code ranges from negative (red) through zero (white) through positive (blue).
Wigner propagator for particles confined between two walls

In this chapter we are going to apply the phase space formalism in terms of the Wigner function to particles confined between two infinitely high potential walls (infinitely deep potential well). The main objective of this chapter is to obtain the exact Wigner propagator for these systems.

As in the previous chapter, we shall derive it for the two approaches: for a potential that defines a forbidden region for the system or for repetitions of the allowed region.

We start describing the main characteristics of the infinitely deep potential well. In the next section we obtain the Wigner functions for the energy eigenstates and finally we are going to find the Wigner propagator for the two alternatives described above.

3.1 Infinitely deep potential well

The one-dimensional particle between two infinitely high potential walls is one of the simplest systems used to demonstrate the main characteristics of quantum mechanics. The quantization of momentum and energy in this system is a consequence of the spatial boundary conditions imposed by the potential.

For an infinitely deep potential well of width $a$ with the walls located in $q = 0$ and $q = a$, the potential is given by

$$V(q) = \begin{cases} 0 & 0 < q < a, \\ \infty & \text{else}. \end{cases} \quad (3.1)$$

The wavefunctions vanish everywhere outside the region defined by the potential, that is, the wavefunctions must satisfy the boundary conditions

$$\psi(q) = \langle q|\psi \rangle = 0, \quad q \leq 0 \quad \text{or} \quad q \geq a \quad (3.2)$$

As we will see, the Wigner function must satisfy the same spatial boundary conditions. Solving the time-independent Schrödinger equation with the boundary conditions (3.2)
gives the energy eigenfunctions

\[
\psi_\lambda(q) = \langle q | \psi_\lambda \rangle = \begin{cases} 
\sqrt{\frac{2}{a}} \sin(k_\lambda q) & 0 < q < a \\
0 & \text{else}
\end{cases}
\]

\[
= \sqrt{\frac{2}{a}} \sin(k_\lambda q) \Theta \left( \frac{a}{2} - |q - \frac{a}{2}| \right),
\]

where \( k_\lambda = \lambda \pi / a \) and \( \lambda \in \mathbb{N} \). The energy eigenvalues are of the form

\[
E_\lambda = \frac{p_\lambda^2}{2m} = \frac{(\hbar k_\lambda)^2}{2m} = \frac{1}{2m} \left( \frac{\lambda \hbar \pi}{a} \right)^2.
\]

For this system the state with the lowest energy is obtained for \( \lambda = 1 \). The energy eigenfunctions have the symmetry

\[
\psi_\lambda(a - q) = \begin{cases} 
\psi_\lambda(q) & \lambda \text{ odd,} \\
-\psi_\lambda(q) & \lambda \text{ even.}
\end{cases}
\]

The momentum representation of the eigenfunctions will give us some idea of the functional form of the corresponding Wigner eigenfunctions

\[
\tilde{\psi}_\lambda(p) = \langle p | \psi_\lambda \rangle = \frac{1}{2\pi \hbar} \int dq \psi_\lambda(q) \exp \left(-\frac{i}{\hbar} pq \right)
\]

\[
= \sqrt{\frac{a}{\pi \hbar}} \text{sinc} \left( \frac{\lambda \pi + pa / \hbar}{2} \right) \exp \left(-\frac{ipa}{2\hbar} \right).
\]

### 3.2 Wigner energy eigenfunctions

The Wigner energy eigenfunctions were derived first in [30]. In order to obtain the Wigner representation of the energy eigenfunctions we substitute the eigenfunctions \((3.3)\) into the
Figure 3.2. For a system restricted to the interval $0 \leq q \leq a$, the Wigner function is calculated by integrating along the diagonals as shown in the figure.

Wigner function (1.1)

$$W_\lambda(p,q) = \frac{1}{2\pi \hbar} \int du \exp\left(-\frac{i \hbar}{\hbar} pu\right) \sin\left(k_\lambda \left(q - \frac{u}{2}\right)\right) \sin\left(k_\lambda \left(q + \frac{u}{2}\right)\right) \Theta\left(\frac{a}{2} - \left|q - \frac{u + a}{2}\right|\right) \Theta\left(\frac{a}{2} - \left|q + \frac{u - a}{2}\right|\right)$$ \hspace{1cm} (3.7)

We need to evaluate the integral in (3.7) over a region where the wavefunctions do not vanish (Fig. 3.2). To determine the appropriate limits of integration, we split the full length $a$ into two regions, namely, $0 < q \leq a/2$ and $a/2 \leq q < a$ [18].

For the first region we have that the argument of the integral vanishes unless

$$0 < q + \frac{u}{2} \leq \frac{a}{2} \quad \text{and} \quad 0 < q - \frac{u}{2} \leq \frac{a}{2}.$$ \hspace{1cm} (3.8)

Joining both conditions we get the limits $-2q < u < 2q$. In the same way we get for the second region the effective integration range $2(a-q) < u < 2(q-a)$.

The integral can be written in the form

$$\int_{-q_e}^{q_e} du \exp\left(-\frac{i \hbar}{\hbar} pu\right) \sin\left(k_\lambda \left(q - \frac{u}{2}\right)\right) \sin\left(k_\lambda \left(q + \frac{u}{2}\right)\right) =$$

$$\int_{-q_e}^{q_e} du \exp\left(-\frac{i \hbar}{\hbar} pu\right) \left[\cos(k_\lambda u) - \cos(2k_\lambda q)\right]$$
with \( q_e = 2q \) for the first region and \( q_e = 2(a - q) \) for the second. Solving the integral we get for the Wigner eigenfunctions

\[
W_\lambda(p, q) = \frac{q_e}{2\pi\hbar} \left[ -2\cos(2k_\lambda q) \text{sinc} \left( \frac{p}{\hbar} q_e \right) + \text{sinc} \left( \left( \frac{p}{\hbar} + k_\lambda \right) q_e \right) + \text{sinc} \left( \left( \frac{p}{\hbar} - k_\lambda \right) q_e \right) \right].
\] (3.9)

Figure 3.3 shows the first four Wigner energy eigenfunctions obtained from (3.9). These functions are symmetric in both position and momentum. In Figure 3.4 we have the Wigner eigenfunctions for higher values of \( \lambda \). The Wigner function concentrates in the quantized momentum \( p_\lambda = \pm \hbar k_\lambda \), with an interference pattern in the middle. The interference pattern is smaller for higher values of \( \lambda \).

\[\text{Figure 3.3. Wigner eigenfunctions for (a) } \lambda = 1, \text{ (b) } 2, \text{ (c) } 3, \text{ (d) } 4. \text{ Color code ranges from negative (red) through white (zero) through positive (blue). Parameters values were } \hbar = 0.1 \text{ and } a = 1.\]
3.3 Propagator of the Wigner function infinitely deep potential well

For the classical system, a particle between two walls will be bouncing between them. The interaction with the walls produces an inversion of the momentum but once the particle leaves the wall it behaves as a free particle. As in the case of the particle in a half-space, we expect that for the quantum system the existence of the two walls affects the dynamic evolution of the Wigner propagator.

As was mentioned before, there are two ways to describe the infinitely deep potential well: with periodic repetitions or in terms of the confined potential. In order to illustrate
the equivalence between both alternatives, imagine that you draw one free-particle classical trajectory from $q'$ to $q''$ in one paper sheet as is depicted in Fig. 3.5 (c). If you fold the sheet as in Fig. 3.5 (b) you will obtain the reflected trajectory in the box of length $a$ as in Fig. 3.5 (a). So, you can think of the trajectory reflected in the box or you can view it as a free particle moving from the initial point $q'$ to one of the mirror images of the point $q''$ in one of the repetitions of the original box.

**Figure 3.5.** The equivalence between the confined interpretation and the periodic repetitions interpretation is understood as the process of folding and unfolding of a paper sheet.

### 3.3.1 Periodic repetitions

Consider the general initial state in position representation $\psi(q, 0)$. It can be expanded in terms of the energy eigenfunctions (3.3)

$$\psi(q, 0) = \sum_{\lambda=1}^{\infty} c_{\lambda} \psi_{\lambda}(q).$$

(3.10)
Using the exponential form of the sine function we can express the last equation as

$$\psi(q,0) = \frac{1}{2i} \sum_{\lambda = -\infty}^{\infty} c_\lambda \exp(ik_\lambda q)$$  \hspace{1cm} (3.11)

where the coefficients $c_\lambda$ fulfill the property $c_{-\lambda} = -c_\lambda$. We can express the expansion of the initial state in terms of the momentum representation

$$\psi(q,0) = \frac{1}{\sqrt{2a}} \sum_{\lambda = -\infty}^{\infty} \tilde{\psi}_\lambda \exp\left(i \frac{p_\lambda}{\hbar} q\right)$$  \hspace{1cm} (3.12)

with $p_\lambda = \hbar k_\lambda$ and

$$\tilde{\psi}_\lambda = \frac{1}{2\sqrt{a}} \int_0^{2a} dq \psi(q,0) \exp(-ik_\lambda q).$$

The coefficients $\tilde{\psi}_\lambda$ satisfy the property $\tilde{\psi}_{-\lambda} = -\tilde{\psi}_\lambda$. The wavefunctions are not confined in the box and in this case have a period of $2a$. Now we want to propagate the initial state till time $t$ by means of

$$\psi(q'',t) = \int_0^{2a} dq' K(q'',t'';q',0) \psi(q',0)$$

where the Feynman propagator $K(q'',t'';q',0)$ is given by

$$K(q'',t'';q',0) = -\frac{1}{8a} \sum_{\lambda = -\infty}^{\infty} \exp\left(-i \frac{E_\lambda t}{\hbar}\right) \left[\exp(i k_\lambda (q'' + q')) + \exp(-i k_\lambda (q'' - q')) - \exp(-i k_\lambda (q' - q')) - \exp(i k_\lambda (q'' - q'))\right].$$  \hspace{1cm} (3.13)

Applying the propagator (3.13) to the initial state gives

$$\psi(q'',t) = \frac{1}{4a} \sum_{\lambda = -\infty}^{\infty} \left( \int_0^{2a} dq' \exp(i k_\lambda (q'' - q')) + \int_0^{2a} dq' \exp(-i k_\lambda (q'' - q')) \right) \psi(q',0).$$  \hspace{1cm} (3.14)

With the time-evolved state, we can construct the density matrix at time $t$

$$\rho(q''_1, q''_2, t) = \psi^*(q''_2, t) \psi(q''_1, t)$$

$$= \frac{1}{16a^2} \sum_{\lambda_1 = -\infty}^{\infty} \exp\left(i \frac{k_{\lambda_1}^2 h}{2m} t\right) \times \left( \int_0^{2a} dq_2' \exp(-i k_{\lambda_1} (q''_2 - q_2')) + \int_0^{2a} dq_2' \exp(i k_{\lambda_1} (q''_2 - q_2')) \right) \times \sum_{\lambda_2 = -\infty}^{\infty} \exp\left(i \frac{k_{\lambda_2}^2 h}{2m} t\right) \times \left( \int_0^{2a} dq_1' \exp(i k_{\lambda_2} (q''_1 - q_1')) + \int_0^{2a} dq_1' \exp(-i k_{\lambda_2} (q''_1 - q_1')) \right) \times \rho(q''_1, q''_2, 0).$$  \hspace{1cm} (3.15)
The last expression can be reduced in the momentum representation of the density matrix

\[ \tilde{\rho}_{\lambda', \lambda''} (t) = \frac{1}{2a} \int_0^{2a} dq_1'' dq_2'' \rho(q_1'', q_2'', t) \exp \left( -i k_{\lambda'} q_1'' + i k_{\lambda''} q_2'' \right) \] (3.16)

Substituting Eq. (3.15) in (3.16) and deforming the integrals with respect to \( q_1'' \) and \( q_2'' \) we get

\[ \tilde{\rho}_{\lambda', \lambda''} (t) = \tilde{\rho}_{\lambda', \lambda''} (0) \exp \left( \frac{i \hbar}{2m} \left( k_{\lambda''}^2 - k_{\lambda'}^2 \right) t'' \right) \] (3.17)

with

\[ \tilde{\rho}_{\lambda', \lambda''} (0) = \frac{1}{2a} \int_0^{2a} dq_1'' dq_2'' \rho(q_1'', q_2'', 0) \exp \left( -i k_{\lambda'} q_1'' + i k_{\lambda''} q_2'' \right). \] (3.18)

The redundant Wigner function (1.20) can be written as

\[ W(p_{\lambda''}, q'', t'') = \frac{1}{2a} \sum_{\lambda=-\infty}^{\infty} \tilde{\rho}_{\lambda', -\lambda, \lambda} (t'') \exp \left( i \pi ( k_{\lambda''} - 2k_{\lambda}) q'' \right) \] (3.19)

and together with (3.17) gives for the Wigner function at time \( t'' \)

\[ W(p_{\lambda''}, q'', t'') = \frac{1}{2a} \sum_{\lambda=-\infty}^{\infty} \tilde{\rho}_{\lambda', \lambda''} (0) \exp \left( \frac{i \hbar}{2m} \left( k_{\lambda''}^2 - k_{\lambda'}^2 \right) t'' \right) \exp \left( i ( k_{\lambda''} - 2k_{\lambda}) q'' \right). \] (3.20)

Writing the initial density matrix as

\[ \tilde{\rho}_{\lambda', \lambda''} (0) = 2 \int_0^a dq' W(p_{\lambda''}, q', 0) \exp \left[ i ( 2k_{\lambda}' - k_{\lambda''} ) q' \right] \] (3.21)

we have

\[ W(p_{\lambda''}, q'', t'') = \frac{1}{2a} \sum_{\lambda=-\infty}^{\infty} 2 \int_0^a dq' W(p_{\lambda''}, q', 0) \exp \left[ i ( 2k_{\lambda}' - k_{\lambda''} ) q' \right] \exp \left( \frac{i \hbar}{2m} \left( k_{\lambda''}^2 - k_{\lambda'}^2 \right) t'' \right) \exp \left( i ( k_{\lambda''} - 2k_{\lambda}' ) q'' \right) \]

\[ = \int_0^a dq W(p_{\lambda''}, q', 0) \exp \left( -i \pi \lambda'' \frac{q'}{a} \right) \exp \left[ i \pi \lambda'' \left( \frac{q''}{a} - \lambda'' \frac{\pi \hbar t'}{2ma^2} \right) \right] \delta \left( q' - \left( q'' - \lambda'' \frac{\pi \hbar t'}{2ma} \right) \right) \] (3.22)

and finally

\[ W(p_{\lambda''}, q'', t) = W(p_{\lambda''}, q'' - \frac{p_{\lambda''}}{m} t, 0). \] (3.23)

Equation (3.23) relates the final Wigner function at time \( t \) with the initial Wigner function at \( t = 0 \). From this equation, it is clear that the propagator has the form

\[ G_W (p_{\lambda''}, q'', t; p_{\lambda''}, q', 0) = \delta_{\lambda'' - \lambda} \delta \left( q' + \frac{p_{\lambda''}}{m} t \right). \] (3.24)
3.3.2 Confined Potential

For the confined potential we are going to derive the propagator of the Wigner function using the equation (1.18). The non-diagonal Wigner functions are given by

\[
G_W(p'', q'', t; p', q', 0) = \frac{1}{2\pi^2} \frac{4}{a^2} \sum_{\lambda_1, \lambda_2=1}^{\infty} \exp\left( -\frac{i}{\hbar} (E_{\lambda_1} - E_{\lambda_2}) t \right) \\
\times \int du' \exp\left( \frac{i}{\hbar} p' u' \right) \sin\left( k_{\lambda_1} \left( q' + \frac{u'}{2} \right) \right) \sin\left( k_{\lambda_2} \left( q' - \frac{u'}{2} \right) \right) \\
\times \int du'' \exp\left( -\frac{i}{\hbar} p'' u'' \right) \sin\left( k_{\lambda_1} \left( q'' + \frac{u''}{2} \right) \right) \sin\left( k_{\lambda_2} \left( q'' - \frac{u''}{2} \right) \right)
\]

Solving the integrals in the previous expression with the effective range of integration for the same regions taken for the Wigner eigenfunctions we obtain for the non-diagonal Wigner functions

\[
W_{\alpha, \beta}(r'') = \frac{\hbar}{2} \left[ e^{-i(k_{\lambda_1} - k_{\lambda_2})r''} \sin\left( (2k'' + k_{\lambda_1} + k_{\lambda_2}) \frac{r''}{2} \right) + e^{i(k_{\lambda_1} - k_{\lambda_2})r''} \sin\left( (2k'' - k_{\lambda_1} - k_{\lambda_2}) \frac{r''}{2} \right) \\
- e^{i(k_{\lambda_1} + k_{\lambda_2})r''} \sin\left( (2k'' - k_{\lambda_1} + k_{\lambda_2}) \frac{r''}{2} \right) - e^{-i(k_{\lambda_1} + k_{\lambda_2})r''} \sin\left( (2k'' - k_{\lambda_1} + k_{\lambda_2}) \frac{r''}{2} \right) \right]
\]

with \( k_{\lambda_1/2} = \frac{p_{\lambda_1/2}}{\hbar} \), \( k'' = \frac{p''}{\hbar} \) and

\[
q'' \begin{cases} 
2q'' & 0 < q'' < a/2, \\
2(a - q'') & a/2 < q'' < a.
\end{cases}
\]

The propagator of the Wigner function for the confined potential has the form

\[
G_W(p'', q'', t; p', q', 0) = \frac{q'' q'}{\pi \hbar a} \sum_{\lambda_1, \lambda_2=1}^{\infty} \exp\left( -\frac{i}{\hbar} (E_{\lambda_1} - E_{\lambda_2}) t \right)
\]

\[
\times \left[ e^{i(k_{\lambda_1} - k_{\lambda_2})r''} \sin\left( (2k' + k_{\lambda_1} + k_{\lambda_2}) \frac{r''}{2} \right) + e^{-i(k_{\lambda_1} - k_{\lambda_2})r''} \sin\left( (2k' - k_{\lambda_1} - k_{\lambda_2}) \frac{r''}{2} \right) \\
- e^{-i(k_{\lambda_1} + k_{\lambda_2})r''} \sin\left( (2k' - k_{\lambda_1} + k_{\lambda_2}) \frac{r''}{2} \right) - e^{i(k_{\lambda_1} + k_{\lambda_2})r''} \sin\left( (2k' - k_{\lambda_1} + k_{\lambda_2}) \frac{r''}{2} \right) \right]
\]

To our best knowledge, the propagator of the Wigner function for the system with thick walls has not been derived before. It constitutes a contribution of the present work. Figures 3.6 and 3.7 were obtained by numerical evaluation of the propagator (3.27). In this evaluation, we have truncated the sums to a finite value \( n \in \mathbb{N} \). A higher upper bound improves the quality of the quantum spot but implies a longer time of evaluation.
3.3.3 Classical vs. Quantum period

The time dependence of the propagator (3.27) relies on the first exponential factor. The argument of this term can be written as

\[ \frac{i}{\hbar}(E_{\lambda_1} - E_{\lambda_2})t = \frac{\hbar\pi^2}{2ma^2}(\lambda_1^2 - \lambda_2^2)t \]

Taking into account that the difference between the squares of two integers is an integer we can see a recurrence of the Wigner propagator for a time \( T_Q = \frac{4ma^2}{\pi\hbar} \). It is interesting to compare this quantum period with the classical period \( T_{Cl} = \frac{2ma}{p_{\lambda}} = \frac{2ma}{\hbar k_\lambda} \) for a particle with initial momentum \( p_{\lambda} = \hbar k_\lambda \).

![Figure 3.6. Wigner propagator in one classical period at (a) \( t = 0 \), (b) \( t = T_{Cl}/4 \), (c) \( t = T_{Cl}/2 \) and (d) \( t = T_{Cl} \). Color ranges from negative (red) through zero (white) through positive (blue). Parameter values were \( \hbar = 0.1 \), \( m = 1 \) and \( a = 1 \). The initial conditions were \( q' = 0.5 \) and \( p' = \hbar k_{15} \), with \( T_{Cl} \approx 0.4 \).]

The classical period equals the quantum period for a wavenumber \( k_\lambda = \pi/2a \). However, the least wavenumber for the infinitely deep potential well is \( k_1 = \pi/a \), as a consequence, for all physical admissible wavenumbers we have \( T_Q > T_{Cl} \). Therefore, the system will complete the classical cycle several times before it complete one quantum period.

In Fig. 3.6 we have the quantum spot of the Wigner propagator in one classical period. The quantum spot follows the classical trajectory for the initial conditions assumed. Nevertheless, after the first collision with the right wall the main distribution splits in three, one on the left and one on the right of the main distribution. These two “companion” distributions have the same sign of the main distribution.
A second distribution emerges in the top-left corner. Compared with the initial distribution, this “twin” distribution moves with opposite momentum and the accompanying spots in its left and right side have negative amplitude, indicated by red color. These companions will keep their sign after each period but the separation between the center distribution and its companions increases after each classical period. On the other hand, with higher initial momentum the quantum spot can follow the classical trajectory without the appearance of the twin distribution for longer time.

**Figure 3.7.** Wigner propagator in one quantum period at (a) $t = 0$, (b) $t = T_Q/4$, (c) $t = T_Q/2$ and (d) $t = 3T_Q/4$. Color ranges from negative (red) through zero (white) through positive (blue). Parameter values were $\hbar = 0.1$, $m = 1$ and $a = 1$. The initial conditions were $q' = 0.5$ and $p' = h k_{15}$, with $T_Q \approx 12.7$.

In the quantum period we can see that at $t = T_Q/4$ and $t = 3T_Q/4$ the quantum spot is divided in two distributions moving with opposite momentum and they recompose at $t = T_Q/2$. Notice the absence of the accompanying distributions in these parts of the quantum period.
Smooth Potential Approximation

In this chapter we shall use a smooth potential as an approximation to the infinitely deep potential well. This potential will be used to construct the semiclassical propagator of the Wigner function in the next chapter.

In order to verify the performance of the semiclassical propagator we need to obtain the exact Wigner propagator for the smooth potential. To begin with, we need to find the energy eigenfunctions for this system. To do this we will solve numerically the Schrödinger equation for this system. With the numerical values of the energy eigenfunctions it is possible to construct the corresponding Wigner function using the expressions (1.21) and (1.22). Finally we will obtain the exact Wigner propagator for this system and compare it with the infinitely deep potential well.

4.1 Potential

The infinitely deep potential well can be considered as the limit of a smooth symmetric potential of the form

\[ V(x) = \lim_{j \to \infty} V_0 \left( \frac{2q}{a} - 1 \right)^{2j}, \]

(4.1)

where \( a \) is the length of the infinite potential well and \( j \) is an integer.

\[ \begin{array}{cccc}
0 & 0.2 & 0.4 & 0.6 \\
V(x) & 0 & \text{blue} & \text{orange} & \text{green}
\end{array} \]

\[ \begin{array}{cccc}
0.5 & 1 & 1.5 & 2 \\
\text{length of the box is 1 and the walls are located in } q = 0 \text{ and } q = 1.
\end{array} \]

**Figure 4.1.** Plot of the potential (4.1) for \( j = 2 \) (blue), \( j = 5 \) (orange) and \( j = 20 \) (green). The length of the box is 1 and the walls are located in \( q = 0 \) and \( q = 1 \).
The Hamiltonian of this problem for a finite value \( j \in \mathbb{N} \) is

\[
\hat{H}_j = \frac{\hat{p}^2}{2m} + V_0 \left( \frac{2q}{a} - 1 \right)^{2j},
\]

and the time-independent Schrödinger equation in position representation is

\[
\left( \frac{p^2}{2m} + V_0 \left( \frac{2q}{a} - 1 \right)^{2j} \right) \psi(q) = E_n \psi(q)
\]

where \( \hat{q} \to q \) and \( \hat{p} \to p = i\hbar d/dq \).

In order to solve numerically the Schrödinger equation, it is useful to write this equation in terms of dimensionless variables. Ignoring the horizontal displacement in the potential (which implies that the potential will be symmetric around \( q = 0.5 \)) and defining the variables

\[
p_d = \frac{p}{\sqrt{mV_0}}, \quad q_d = \frac{2q}{a} \quad \text{and} \quad \epsilon_n = \frac{E_n}{V_0},
\]

the equation (4.3) takes the form

\[
\left( \frac{p_d^2}{2} + \frac{q_d^{2j}}{2} \right) \psi(q_d) = \epsilon_n \psi(q_d).
\]

Notice that equation (4.4) reduces to the time-independent Schrödinger equation of the harmonic oscillator for \( j = 1 \) and \( V_0 = \frac{1}{2}m\omega^2q \).

It is important to note that the potential in (4.4) is an approximation to the infinite potential well of length \( a = 2 \) and centered at the origin. So, after solving the equation, we will have to adjust the eigenfunctions accordingly to the potential (4.1).

Numerically, the differential equation (4.4) can be solved using different methods, like the Runge-Kutta method; however, the eigenvalue \( \epsilon_n \) it is not known analytically, in fact, is one of the values that we want to obtain. In general the searching of the eigenvalues is based on physical grounds. Usually, the eigenvalue is picked as a trial between an interval where it is thought to be. Then, the eigenfunction is obtained solving numerically the differential equation and if the eigenfunction does not blow up for large values, the numeric trial is a good approximation for the real eigenvalue.

A simple method to find the eigenfunctions as well as the eigenvalues based on the Numerov method was developed in [31]. This method was used to solve the equation (4.4) and it is explained the appendix A.

### 4.2 Energy eigenfunctions

The Schrödinger equation with the smooth potential was solved using the matrix Numerov method for four different values of the exponent \( j \), namely, \( j = 1 \) (harmonic oscillator), \( j = 5 \), \( j = 10 \) and \( j = 20 \).

Figure (4.2) shows the ground state obtained for each exponent \( j \). With higher values of \( j \) the ground state of the smooth potential gets closer to the ground state eigenfunction of the infinitely deep square potential well. While the eigenfunction shrinks along the horizontal axis, it stretches along the vertical axis. The eigenvalues also tend to those of the potential well for higher values of \( j \), starting from the minimum values of \( j = 1 \) of the harmonic oscillator.

In figure (4.3) the ground and first exited state are shown. With higher values of \( j \) the eigenfunctions are closer to be confined in the interval \((0, 1)\).
CHAPTER 4. SMOOTH POTENTIAL APPROXIMATION

Figure 4.2. Comparison of the ground state for different values of $j$ in the smooth potential and the infinitely deep potential well. Vertical dashed lines indicate the walls of the square potential well. The energy of the ground state $\epsilon_0$ for each case is $\epsilon_0 = 0.5$ ($j = 1$), $\epsilon_0 = 0.64$ ($j = 5$), $\epsilon_0 = 0.78$ ($j = 10$), $\epsilon_0 = 0.91$ ($j = 20$) and $\epsilon_0 = 1.57$ (potential well). The numerical values of the parameters were $\hbar = 1, m = 1, V_0 = 1, a = 1$.

Figure 4.3. Ground (blue) and first exited (red) states for the smooth potential for different values of $j$. a) $j = 1$, b) $j = 5$, c) $j = 10$ and d) $j = 20$. The numerical values of the parameters were $\hbar = 1, m = 1, V_0 = 1, a = 1$.

4.3 Wigner eigenfunctions

Figure 4.5 shows the Wigner eigenfunction of the ground state for the smooth potential. In the same way as the energy eigenfunctions, the Wigner function is closer to the potential well for higher values of $j$.

Figure 4.6 shows the Wigner function for the fortieth energy eigenfunction. We can see the same pattern of the potential well with the Wigner function located around the quantized momentum $p_n = \pm \sqrt{2m\epsilon_n}$ with an interference pattern in the middle. As the energy increases
with the exponent $j$, the quantized momentum also increases and tends to the quantized momentum of the infinitely deep potential well when $j \to \infty$.

### 4.4 Wigner propagator

The Wigner propagator for the smooth potential approximation was obtained using equation (1.24) for $j = 5$, $j = 10$ and $j = 20$. The number of eigenfunctions used to construct the propagator was 30.
Figure 4.6. Wigner function for the fortieth state for (a) $j = 5$, (b) $j = 10$, (c) $j = 20$ and (d) potential box. The vertical dashed lines are located in the classical turning points. The horizontal dashed lines are located in the momentum $p_n = \pm \sqrt{2m\epsilon_n}$. Color code ranges from red (negative) through white (zero) through blue (positive).

The evolution of the quantum spot is shown in Figure 4.7 in a classical period $T_{Cl}$. The initial distribution at $t = 0$ follows the classical trajectory indicated by the smooth potential. With $j = 5$ the initial distribution does not split and the “twin” distribution is not seen at $t = T_{Cl}/2$. This situation changes with bigger value of $j$.

With $j = 10$ the “twin” distribution with its accompanying is formed and moves with opposite momentum like in the infinitely deep potential well. However, the division of the initial distribution is not seen with this exponent. This division is obtained with the exponent $j = 20$.

As was expected, the formation of the structures in the quantum spot is faster and closer to the infinitely deep potential well with higher values of $j$. This validates the smooth potential approximation in the classical period $T_{Cl}$.
Figure 4.7. Wigner propagator for the smooth potential at $t = 0$ (left column) and $t = T_C/2$ (right column) for $j = 5$ (a) and (b), $j = 10$ (c) and (d), $j = 20$ (e) and (f). Parameter values were $\hbar = 1$, $m = 1$, $V_0$ and $a = 1$. Color code ranges from red (negative) through white (zero) through blue (positive).
CHAPTER 5

Semiclassical propagator of the Wigner function

In this chapter we are going to construct the semiclassical propagator of the Wigner function for the smooth potential approximation for a particle confined between two walls. As mentioned before, although the semiclassical approximation does not work for the box with thick walls, we can approach this limit with higher exponents in the potential (4.1).

First, we shall review the construction of the propagator from the van-Vleck propagator and then, we will show the steps needed in order to obtain the semiclassical propagator for the system considered.

5.1 From van-Vleck propagator to Semiclassical Wigner propagator

There are two routes towards the semiclassical propagator of the Wigner function: from Marinov’s path integral and from the van-Vleck propagator. We are going to use the expression obtained from the latter. A comprehensive review of the derivation and applications of the semiclassical propagator is given in [24]. Further details of the derivation can be found in [23],[27].

As we saw in chapter 1, the Wigner propagator involves the convolution of two Weyl propagators. The starting point of this semiclassical approximation is to replace in equation (1.14) the Weyl transform of the van-Vleck propagator

\[ U_W(r, t) = 2 \sum_j \exp\left[iS_j(r, t)/\hbar - i\mu_j\pi/2\right] \sqrt{|\det(M_j(r, t) + I)|} \]  

(5.1)

where \( M_j \) and \( \mu_j \) are the stability matrix and the Maslov index of the \( j \)th trajectory, respectively. The action \( S_j(r, t) = A_j(r_j, t) - H_j(r_j, t) \) depends on the symplectic area \( A_j(r_j, t) \) enclosed by the trajectory and the chord connecting the initial \( r_j' \) and final \( r_j'' \) points. The sum in (5.1) runs over all the trajectories such that the midpoint condition \( r = (r_j'' + r_j')/2 \) is fulfilled.

The next step is to evaluate the corresponding integral for the propagator using the stationary phase approximation. Together with the midpoint condition, stationary points are defined by

\[ r' = \frac{r_{j+} + r_{j-}}{2}, \quad r'' = \frac{r_{j''+} + r_{j''-}}{2} \]  

(5.2)
From equation (5.2) we can see that contributions to the semiclassical propagator are given by trajectory pairs \( j^+ \) and \( j^- \) which have the initial argument \( r' \) in the middle of their respective initial points and likewise for the final argument \( r'' \). Notice that any trajectory pair that fulfills this requirement will contribute to the semiclassical propagator and for this reason the trajectories need not to be identical.

The final result of this route is the expression for the semiclassical Wigner propagator

\[
G_{\text{sc}}(r'', r', t) = \frac{2}{\pi \hbar} \sum_j 2 \cos \left[ \frac{1}{\hbar} S^v_j (r'', r', t) - \frac{f \pi}{2} \right] \left| \det (M^+_j - M^-_j) \right|^{1/2}
\]

with the action

\[
S^v_j (r'', r', t) = \int_0^t ds [\frac{\dot{r}_j (s) \wedge R_j (s)}{2} - H_j (r_j^+ + H_j (r_j^-)],
\]

where \( \dot{r}_j (s) = [r_{j^+} (s) + r_{j^-} (s)]/2 \) and \( R_j (s) = r_{j^+} (s) - r_{j^-} (s) \). The additional term \( f = \mu_j^+ - \mu_j^- \) is an integer obtained from the difference of the number of positive and negative eigenvalues of the matrix \( M^+_j - M^-_j \).

The action (5.4) involves the symplectic area enclosed between the classical trajectories \( r_{j^+} \) and \( r_{j^-} \), together with the area between each trajectory and its corresponding chord joining the initial and final points.

With the time evolution of the trajectories, the midpoints form a cone-like structure which is the support of the semiclassical propagator (5.3). Trajectory pairs contribute to the upper and lower shells of the cone according to the criteria

\[
\text{trajectories pair is} \begin{cases} \text{ell.} & \text{if} \quad \det [M^+_j - M^-_j] > 0, \\ \text{hyp.} & \text{if} \quad \det [M^+_j - M^-_j] < 0. \end{cases}
\]

Inside the cone we have two trajectory pairs contributions, one of them elliptic and the other hyperbolic. The boundary between both shells forms a caustic where the two contributions collapse into one.

### 5.2 Algorithm to compute the naked propagator

In order to obtain the propagator as an independent quantity, that is, before operating on any admissible initial Wigner function, we need to follow the next steps:

- Define pairs of initial points \( r'_\pm \) with common midpoint the initial argument of the propagator \( r' \). This step can be done with random points \( r'_\pm \) uniformly distributed in a circle with center at \( r' \) and their counterparts \( r'_\pm \) resulting from reflection with respect to \( r' \).
- Evolve the trajectory pairs according to classical equations of motion taking into account the ingredients of the semiclassical propagator, to obtain endpoints \( r''_\pm \).
- For the amplitude of the propagator, the stability matrices \( M^+_j \) and \( M^-_j \) have to be obtained at time \( t \). The evolution equation of the stability matrix is

\[
\dot{M} = J^T \frac{\partial^2 H[r]}{\partial^2 r^2} M.
\]

It is suggested to merge the classical equations of motion for the trajectories and the equation for the stability matrix in a single system of equations. Once the stability matrices are obtained at time \( t \), the trajectory pairs are separated according to (5.5).
CHAPTER 5. SEMICLASSICAL PROPAGATOR OF THE WIGNER FUNCTION

5.3 Numerical results

We have implemented the algorithm outlined above with the smooth potential approximation for $j = 2$ and $j = 3$. The initial conditions were $p' = 0.15$ and $q' = 0.0$. Around this point, we have generated random points inside a circle with center in the initial point $r'$ and we assigned the corresponding pair to each point. The radius of the circle has been chosen with respect to the time of propagation. A helpful plot for the selection of the radius is shown in Figure 5.2. In this figure, the points of the initial distributions have been coloured according to the nature of the trajectory pair. We can see the two regions that form the shells of the cone and the boundary between them marked with coloured pixels, according to the nature (elliptic-blue, hyperbolic-red) of the trajectory pair.

The semiclassical propagator of the Wigner function was obtained at times $T_{Cl}/8$, $3T_{Cl}/8$ and $c) T_{Cl}/2$ of the classical period. The propagator of the trajectory pair has been calculated as the superposition of the elliptic and hyperbolic contributions. We can see each contribution and the final result in Figure 5.3.

The evolution of the quantum spot for $j = 2$ and $j = 3$ is shown in Figure 5.4. The checkerboard pattern of the quantum spot is similar at $t = T_{Cl}$. The difference between the quantum spots, for the values of $j$ considered, emerges after the underlying classical trajectory for $r'$ passes through the right turning point. This is the corresponding version of an interaction with the thick wall in the smooth potential approximation. Note also the change in the shape of the cone formed by the midpoints of the trajectory pairs.
The construction of the semiclassical propagator for the initial conditions chosen for higher values of $j$ is more difficult because, between the edges of the trajectory, the dynamical evolution is closer to that of the free particle. As a consequence, the contribution of hyperbolic pairs is very small compared with the contribution of elliptic pairs and this affects the formation of the cone structure needed for the semiclassical propagator.
Figure 5.4. Semiclassical propagator of the Wigner function for $j = 2$ (left column) and $j = 3$ (right column) at $t = T_{CI}/8$ (panels (a) and (b)), $t = 3T_{CI}/8$ (panels (c) and (d)) and $t = T_{CI}/2$ (panels (e) and (f)). Parameter values were $\hbar = 0.005$, $a = 1$ and $m = 1$. Color code ranges from red (negative) through white (zero) through blue (positive).
The Numerov method

A simple method to find the eigenfunctions as well as the eigenvalues based on the Numerov method was developed in [31]. This method was used to solve the Schrödinger equation in chapter 3 and it is explained in the next section.

A.0.1 The Numerov method

The Numerov method is a numerical method to solve equations of the form

\[ \psi''(q) + k(q)\psi(q) = 0. \]  

(A.1)

In the case of the Schrödinger equation \( k(q) = (E_n - V(q))2m/\hbar^2 \).

The first step is to discretize the q-axis with a step size \( d \). The Taylor expansion for the points \( n-1 \) and \( n+1 \) will be given in terms of the point \( n \)

\[ \psi_{n\pm1} = \psi_n \pm d\psi_n' + \frac{d^2}{2} \psi_n'' + \frac{d^3}{6} \psi_n''' + \frac{d^4}{24} \psi_n^{(4)} + O(d^5) \]  

(A.2)

with \( \psi_n = \psi(n) \), \( \psi_n' = \psi'(n) \) and so on for higher derivatives.

The sum of both expansions gives

\[ \psi_{n+1} + \psi_{n-1} = 2\psi_n + \frac{d^2}{2} \psi_n'' + \frac{d^4}{12} \psi_n^{(4)} + O(d^6). \]  

(A.3)

From (A.1) the second derivative can be replaced by \( \psi''_n = -k_n\psi_n \) and the fourth derivative is written as

\[ \psi_n^{(4)} = \frac{d^2}{dq^2} \psi_n'' = -\frac{d^2}{dq^2} k_n\psi_n \].

Using the discrete form of the second derivative

\[ \left. \frac{d^2\psi}{dq^2} \right|_n = \frac{\psi_{n+1} - 2\psi_n + \psi_{n-1}}{d^2} \]

the fourth derivative takes the form

\[ \psi_n^{(4)} = -\frac{k_{n+1}\psi_{n+1} - 2k_n\psi_n + k_{n-1}\psi_{n-1}}{d^2}. \]  

(A.4)
Replacing (A.4) in (A.3)

\[ \psi_{n+1} + \psi_{n-1} = 2\psi_n - d^2k_n\psi_n - \frac{d^2}{12}(k_{n+1}\psi_{n+1} - 2k_n\psi_n + k_{n-1}\psi_{n-1}) + O(d^6) \]

\[ \psi_{n+1} \left(1 + \frac{d^2}{12}k_{n+1}\right) - 2\psi_n \left(1 - \frac{5}{12}d^2k_n\right) + \left(1 + \frac{d^2}{12}k_{n-1}\right) = 0 + O(d^2). \]  

(A.5)

The equation (A.5) is the key result of the Numerov method and it allows to calculate the complete set of \( \psi_n \) values from two adjacent initial values.

A.0.2 The matrix Numerov method

The main idea of the algorithm developed in [31] is to write the equation (A.5) in terms of matrices. In order to do this, let's assume a column vector with the elements \( \psi_{n-1}, \psi_n \) and \( \psi_{n+1} \):

\[ \psi = \begin{pmatrix} \psi_{n-1} \\ \psi_n \\ \psi_{n+1} \end{pmatrix} \]

and define the matrices

\[ I_{-1} = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \quad I_0 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \text{and} \quad I_1 = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}. \]

The \( I_0 \) matrix is the identity matrix and the \( I_{-1} \) and \( I_1 \) matrices are obtained by replacing the zeros by ones in the diagonal below and above the main diagonal of the identity matrix, respectively.

The elements of the potential are arranged in the diagonal matrix

\[ V = \begin{pmatrix} V_{n-1} & 0 & 0 \\ 0 & V_n & 0 \\ 0 & 0 & V_{n+1} \end{pmatrix}. \]

With the help of the previous definitions, the equation (A.5) can be written in the form

\[ -\frac{\hbar^2}{2m} A\psi + BV\psi = E_n B\psi, \]

where

\[ A = \frac{l_{-1} - 2l_0 + l_1}{d^2} \]  

(A.7)

and

\[ B = \frac{l_{-1} + 10l_0 + l_1}{12}. \]  

(A.8)

Explicitly, the equation (A.6) gives

\[ -\frac{\hbar^2}{2m} \frac{1}{d^2} \begin{pmatrix} -2\psi_{n-1} + \psi_n \\ \psi_{n-1} - 2\psi_n + \psi_{n+1} \\ \psi_n - 2\psi_{n+1} \end{pmatrix} + \frac{1}{12} \begin{pmatrix} 10V_{n-1}\psi_{n-1} + V_n\psi_n \\ V_{n-1}\psi_{n-1} + 10V_n\psi_n + V_{n+1}\psi_{n+1} \\ V_n\psi_n + 10V_{n+1}\psi_{n+1} \end{pmatrix} \]

\[ = \frac{E_n}{12} \begin{pmatrix} 10\psi_{n-1} + \psi_n \\ \psi_{n-1} + 10\psi_n + \psi_{n+1} \\ \psi_n + 10\psi_{n+1} \end{pmatrix}. \]  

(A.9)
Figure A.1. For an even potential the distance between the turning points is $2q_t$. Adding a distance of $2\lambda$ in the forbidden region in each turning point gives a total distance $D = 2q_t + 4\lambda$, where $\lambda$ is the de Broglie wavelength corresponding to the energy $E_m$.

Notice that equation (A.5) is the second row of the equation (A.9) and the first and third rows are the equations for the points $\psi_{n-2}, \psi_{n-1}, \psi_n$ with $\psi_{n-2} = 0$, and $\psi_n, \psi_{n+1}, \psi_{n+2}$ with $\psi_{n+2} = 0$, respectively.

For a grid of $N$ points, $A$ and $B$ are $N \times N$ matrices and the boundary conditions $\psi_{n+1} = \psi_0 = 0$ are assumed. The boundary conditions can be interpreted as though the potential of interest were inside a infinitely high potential box.

The product of (A.6) from the left with $B^{-1}$ gives

$$-\frac{\hbar^2}{2m} B^{-1} A \psi + V \psi = E_n \psi \quad \Rightarrow \quad H \psi = E_n \psi$$

(A.10)

with $H = -\frac{\hbar^2}{2m} B^{-1} A + V$.

The eigenvalues of $H$ are the energy eigenvalues of the system and the entries of each eigenvector give the values of the eigenfunction with eigenvalue $E_n$ in the points of the grid.

A.0.2.1 Selection of the grid

First, an upper limit for the energy is selected and only the states below this limit will be obtained. Pillai et al. found that sufficient accuracy is obtained with a grid spacing of $d = \lambda/2\pi$, where $\lambda = 2\pi \hbar/\sqrt{2mE_m}$ is the De Broglie wavelength for the upper limit for the energy $E_m$. The grid points needed are estimated using the classical turning points $q_t(V(q_t) = E_m)$.

The division of the distance $D = 2q_t + 4\lambda$ between the grid spacing $d$ gives the number of points $N$ of the grid

$$N = \frac{2q_t + 4\lambda}{d} = \frac{2q_t + 4\pi d}{d} = 2 \left( \frac{q_t}{d} + 4\pi \right)$$

rounded to the nearest integer.
Conclusions

In this document we have studied particles with one and two infinitely high potential walls in the phase-space formalism of the Wigner function. Two approaches were considered according to the nature of the walls, namely, thin walls or thick walls. In the former, we have seen that with one and two walls, the propagator of the Wigner function is that of a free particle and the quantum features of these systems are contained in the initial state. This work contributes to the understanding of the less studied case of confinement with thick walls. We have derived the propagator of the Wigner function in the case of one and two thick walls and then we have evaluated these expressions numerically. Our results show a different time evolution of the Wigner propagator with this kind of walls. This time evolution bears a resemblance to the movement of a classical particle in the box but, in contrast with the case of thin walls, the quantum nature of the system arise in the propagator itself. This is seen in the emergence of the twin and accompanying contributions for the particle with two walls and the division of the initial spot in the case of one wall. It is remarkable that non-local features can be seen in a clear way in this kind of confinement. One can consider the propagation of smooth localized initial states, for example Gaussian wavepackets, as a task for future research. Another topic for future work could be the extension to further dimensions and its possible application in models of quantum dots.

We confirmed the close relation between the box with thick walls and the smooth potential approximation in the quantum domain. We have obtained the Wigner eigenfunctions for this approximation and we found qualitatively the same pattern compared with those of the infinitely deep potential well. Furthermore, we have seen the asymptotic behaviour, towards the box with thick walls, of this polynomial potential with higher values of the exponent. As was expected, the higher is the exponent the closer are the behaviour of the smooth potential to the box. On the other hand, with the Wigner eigenfunctions, we constructed the propagator of the Wigner function and we verified that the smooth potential can reproduce the structures of the quantum spot in the regime of a classical period. The twin and accompanying contributions emerge faster and clearer with higher values of $j$.

Finally, we have constructed the semiclassical propagator of the Wigner function using its van-Vleck-based expression for the smooth potential approximation of the box. The plot used in chapter 5 to define the initial distribution of points is a helpful tool in the construction of the semiclassical propagator. We showed the effect of a different exponent in the smooth potential on the shape of the cone structure and the interference pattern.
Bibliography


