

Explicit Solution of the Time Evolution of the Wigner Function[†]

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Abstract. Previously, an explicit solution for the time evolution of the Wigner function was presented in terms of auxiliary phase space coordinates which obey simple equations of motion. These equations of motion are analogous with, but not identical to, the classical equations of motion. They can be solved easily and their solutions can be utilized to construct the time evolution of the Wigner function. The usefulness of this explicit solution is demonstrated by solving a numerical example in which the Wigner function has strong spatial and temporal variation as well as regions with negative values. It is found that the explicit solution gives a correct description of the time evolution of the Wigner function.

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1. Introduction

It is a great pleasure for me to participate in the Wigner Centennial Conference at Pecs, Hungary in honor of the Centennial of Professor Eugene Wigner's birthday. I first met Professor Wigner in 1959 when I was an undergraduate student at Princeton. Professor Wigner taught us and our graduate school classmates Curtis Callen, Stephen Adler, and Alfred Goldhaber a course in Advanced Quantum Mechanics in 1961. We were at the celebration party at the Graduate College when Professor Wigner was awarded the Nobel Prize in Physics in 1963. After I obtained my Ph. D. degree at Princeton, I came to work at Oak Ridge National Laboratory, for which Professor Wigner was the founding Scientific Director. I saw Professor Wigner from time to time at Oak Ridge when he came to work on his civil defense project. It is therefore particularly meaningful to me to come and celebrate the Centennial in his native land to commemorate his many important contributions.

As a part of the "Junior Paper" research project at Princeton University, I went to see Professor Wigner in his office in Fine Hall in 1959 and inquired about the early history of Quantum Mechanics. He told me that the great thing about Schrödinger was that his wave equation was formulated in configuration space. However, to Professor Wigner, who was trained as a chemical engineer, dynamics could also be described in phase space. His formulation of quantum mechanics in phase space in 1932 led to the well-known Wigner description of quantum systems [1]. The joint function of coordinate and momentum $f(\mathbf{r}\mathbf{p})$ introduced in 1932, now known as the Wigner function, is analogous with the classical distribution function. This analogy has provided new insights and useful applications to many quantum systems. It is deservedly a subject of intense interest in this Wigner Centennial Conference [2].

The Wigner function is, however, not identical to the classical distribution function. The classical distribution function is always non-negative and can be described in terms of a collection of cell points with positive weights in phase space. The evolution of the classical distribution function can be followed by tracking these cell points using classical equations of motion [3].

The Wigner function can assume negative as well as positive values in some regions of phase space. How does a Wigner function with regions of negative values evolve as a function of time? The concept of a probability distribution function with positive weights is clearly not applicable here. The difficulty of propagating the Wigner function with negative values has been a barrier to the study of the dynamics of the Wigner function using the equation of motion of the Wigner function directly.

Previously, I formulated a simple method to propagate the Wigner function in time [3]. The ability to propagate the Wigner function with negative values arises from the fact that one deals with amplitudes in this method, and one does not need to use the concept of probabilities. The method contains three important components. First, one employs an auxiliary variable \mathbf{s} , which is allowed to span the whole configuration space. Second, using this auxiliary variable \mathbf{s} , the Wigner function can be represented

in terms of auxiliary phase space coordinates \mathbf{R} and \mathbf{P} . The equations of motion for these auxiliary coordinates \mathbf{R} and \mathbf{P} are quite simple. They are analogous with, but not identical to, the classical equations of motion, as $\partial\mathbf{P}/\partial t$ depends on the auxiliary coordinate \mathbf{s} . They can be solved easily and their solutions can be utilized to construct the Wigner function at the next time step. The third component consists of providing the correct amplitude function for the evolution. For each value of \mathbf{s} and the evolution of phase space coordinates, one associates an amplitude factor $\exp\{i\mathbf{s} \cdot (\mathbf{p} - \mathbf{P})/\hbar\}$. After the amplitudes for all possible values of \mathbf{s} have been obtained at the end of one time step, one adds all these amplitudes together coherently (Huygen Principle) to give the Wigner function $f(\mathbf{r}\mathbf{p})$ at the next time step. This explicit solution overcomes the difficulty of propagating a Wigner function with negative values.

Recently, with the rapid advances in quantum information technology and the reduction in the size of micro-electronic devices, there has been renewed interest in experimental and theoretical studies of the Wigner function [4]-[15]. Experimental measurements of the Wigner function have been carried out using many different techniques [4]-[9]. Regions of negative Wigner function were observed in many experiments [5, 8]. The time evolution of the Wigner function has been studied by many authors [10]-[15]. It is instructive to review the explicit solution for the time evolution of the Wigner function obtained previously and to demonstrate its usefulness by a numerical example. We choose to examine an example in which the time evolution of the Wigner function can be readily evaluated by using wave functions and eigenvalues. The Wigner function in the example should have significant spatial and temporal variations as well as regions of negative values to test whether the explicit solution obtained previously is capable of treating these non-classical features. The success in providing a correct time evolution of the Wigner function using this explicit solution will pave the way for its applications in the future.

2. Explicit Solution of the Time Evolution of the Wigner Function

We shall first review the explicit solution obtained in 1982 [3]. We consider a particle in the potential V

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r}, t) = \left\{ -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}, t) \right\} \psi(\mathbf{r}, t). \quad (1)$$

The Wigner function is

$$f(\mathbf{r}\mathbf{p}, t) = \int d\mathbf{s} e^{i\mathbf{p}\cdot\mathbf{s}/\hbar} \psi\left(\mathbf{r} - \frac{\mathbf{s}}{2}, t\right) \psi^*\left(\mathbf{r} + \frac{\mathbf{s}}{2}, t\right). \quad (2)$$

From the Schrödinger equation, we obtain the equation of motion for the Wigner function [1]

$$\frac{\partial f(\mathbf{r}\mathbf{p}, t)}{\partial t} + \frac{\mathbf{p}}{m} \cdot \nabla_{\mathbf{r}} f(\mathbf{r}\mathbf{p}, t) - \frac{2}{\hbar} \sin \left\{ \frac{\hbar}{2} \nabla_{\mathbf{r}}^V \cdot \nabla_{\mathbf{p}}^f \right\} V(\mathbf{r}, t) f(\mathbf{r}\mathbf{p}, t) = 0, \quad (3)$$

where $\nabla_{\mathbf{r}}^V$ acts on the potential V and $\nabla_{\mathbf{p}}^f$ acts on the Wigner function f .

Given the Wigner function $f(\mathbf{r}_0\mathbf{p}_0, t_0)$ at time t_0 , we wish to obtain the Wigner function at the next time step at $t = t_0 + \delta t$ with a small δt . To solve for the dynamics, we divide the phase space into cells. Consider one such cell centered at $\{\mathbf{r}_0 \mathbf{p}_0\}$ at time t_0 with volume element $d\mathbf{r}_0 d\mathbf{p}_0$ and amplitude $f(\mathbf{r}_0\mathbf{p}_0, t_0)$. We retain the auxiliary coordinate \mathbf{s} and follow the time dependence of each cell in the Lagrangian sense. For the phase space coordinates $\{\mathbf{r}_0\mathbf{p}_0\}$ initially at time t_0 , we label their phase space coordinates at subsequent time t by $\{\mathbf{R}(\mathbf{r}_0\mathbf{p}_0\mathbf{s}, t) \mathbf{P}(\mathbf{r}_0\mathbf{p}_0\mathbf{s}, t)\}$. In classical dynamics, the evolution of the phase space coordinates will not depend on \mathbf{s} . In quantum dynamics, they will depend on \mathbf{s} . The momentum coordinate \mathbf{P} can jump to the momentum coordinate \mathbf{p} at time t . We associate an amplitude of $\exp\{i\mathbf{s} \cdot [\mathbf{p} - \mathbf{P}(\mathbf{r}_0\mathbf{p}_0\mathbf{s}, t)]/\hbar\}$ for this momentum jump. This amplitude factor is chosen because for the classical case where \mathbf{P} is independent of \mathbf{s} this amplitude leads to the correct delta function propagator $\delta(\mathbf{p} - \mathbf{P}(\mathbf{r}_0\mathbf{p}_0, t))$ after we integrate over \mathbf{s} [see Eq. (14)]. We therefore express the Wigner function $f(\mathbf{r}\mathbf{p}, t)$ at the next time step as

$$f(\mathbf{r}\mathbf{p}, t) = \int \frac{d\mathbf{r}_0 d\mathbf{p}_0 d\mathbf{s}}{(2\pi\hbar)^3} \exp\{i\mathbf{s} \cdot [\mathbf{p} - \mathbf{P}(\mathbf{r}_0\mathbf{p}_0\mathbf{s}, t)]/\hbar\} \delta[\mathbf{r} - \mathbf{R}(\mathbf{r}_0\mathbf{p}_0\mathbf{s}, t)] f(\mathbf{r}_0\mathbf{p}_0, t_0). \quad (4)$$

Our task is to find solutions for the phase space coordinates $\mathbf{R}(\mathbf{r}_0\mathbf{p}_0\mathbf{s}, t)$ and $\mathbf{P}(\mathbf{r}_0\mathbf{p}_0\mathbf{s}, t)$ with initial conditions $\mathbf{R}(\mathbf{r}_0\mathbf{p}_0\mathbf{s}, t_0) = \mathbf{r}_0$ and $\mathbf{P}(\mathbf{r}_0\mathbf{p}_0\mathbf{s}, t_0) = \mathbf{p}_0$. If we can find these coordinates at the next time step, the above integral can then be carried out to give the Wigner function at the new time t .

To obtain the equations of motion for $\mathbf{R}(\mathbf{r}_0\mathbf{p}_0\mathbf{s}, t)$ and $\mathbf{P}(\mathbf{r}_0\mathbf{p}_0\mathbf{s}, t)$, we substitute Eq. (4) into Eq. (3). For the first term in Eq. (3), we get

$$\begin{aligned} \frac{\partial f(\mathbf{r}\mathbf{p}, t)}{\partial t} &= \int \frac{d\mathbf{r}_0 d\mathbf{p}_0 d\mathbf{s}}{(2\pi\hbar)^3} f(\mathbf{r}_0\mathbf{p}_0, t_0) \\ &\times \left[\frac{(-i\mathbf{s})}{\hbar} \cdot \frac{\partial \mathbf{P}}{\partial t} \exp\{i\mathbf{s} \cdot [\mathbf{p} - \mathbf{P}(\mathbf{r}_0\mathbf{p}_0\mathbf{s}, t)]/\hbar\} \delta[\mathbf{r} - \mathbf{R}(\mathbf{r}_0\mathbf{p}_0\mathbf{s}, t)] \right. \\ &\left. + \exp\{i\mathbf{s} \cdot [\mathbf{p} - \mathbf{P}(\mathbf{r}_0\mathbf{p}_0\mathbf{s}, t)]/\hbar\} (\nabla_{\mathbf{R}} \delta[\mathbf{r} - \mathbf{R}(\mathbf{r}_0\mathbf{p}_0\mathbf{s}, t)]) \cdot \partial \mathbf{R}(\mathbf{r}_0\mathbf{p}_0\mathbf{s}, t) / \partial t \right]. \end{aligned} \quad (5)$$

Noting that

$$\nabla_{\mathbf{R}} \delta[\mathbf{r} - \mathbf{R}(\mathbf{r}_0\mathbf{p}_0\mathbf{s}, t)] = -\nabla_{\mathbf{r}} \delta[\mathbf{r} - \mathbf{R}(\mathbf{r}_0\mathbf{p}_0\mathbf{s}, t)], \quad (6)$$

we can rewrite the second term inside the square bracket as

$$\begin{aligned} &\int \frac{d\mathbf{r}_0 d\mathbf{p}_0 d\mathbf{s}}{(2\pi\hbar)^3} f(\mathbf{r}_0\mathbf{p}_0, t_0) \\ &\times \exp\{i\mathbf{s} \cdot [\mathbf{p} - \mathbf{P}(\mathbf{r}_0\mathbf{p}_0\mathbf{s}, t)]/\hbar\} (-\nabla_{\mathbf{r}} \delta[\mathbf{r} - \mathbf{R}(\mathbf{r}_0\mathbf{p}_0\mathbf{s}, t)]) \cdot \partial \mathbf{R}(\mathbf{r}_0\mathbf{p}_0\mathbf{s}, t) / \partial t \\ &= -\frac{\partial \mathbf{R}(\mathbf{r}_0\mathbf{p}_0\mathbf{s}, t)}{\partial t} \cdot \nabla_{\mathbf{r}} f(\mathbf{r}\mathbf{p}, t), \end{aligned} \quad (7)$$

where we have used Eq. (4) to obtain the right-hand side. For the last term in Eq. (3), we substitute (4) into this term and find

$$\begin{aligned} \frac{2}{\hbar} \sin \left\{ \frac{\hbar}{2} \nabla_{\mathbf{r}}^V \cdot \nabla_{\mathbf{p}}^f \right\} V(\mathbf{r}, t) f(\mathbf{r}\mathbf{p}, t) &= \frac{1}{\hbar} \int \frac{d\mathbf{r}_0 d\mathbf{p}_0 d\mathbf{s}}{(2\pi\hbar)^3} f(\mathbf{r}_0\mathbf{p}_0, t_0) \\ &\times \exp\{i\mathbf{s} \cdot [\mathbf{p} - \mathbf{P}(\mathbf{r}_0\mathbf{p}_0\mathbf{s}, t)]/\hbar\} \delta[\mathbf{r} - \mathbf{R}(\mathbf{r}_0\mathbf{p}_0\mathbf{s}, t)] \frac{[V(\mathbf{r} - \frac{\mathbf{s}}{2}, t) - V(\mathbf{r} + \frac{\mathbf{s}}{2}, t)]}{i}. \end{aligned} \quad (8)$$

Putting Eqs. (5)-(8) into Eq. (3), we obtain

$$\begin{aligned} & \left[-\frac{\partial \mathbf{R}(\mathbf{r}_0 \mathbf{p}_0 \mathbf{s}, t)}{\partial t} + \frac{\mathbf{p}}{m} \right] \cdot \nabla_{\mathbf{r}} f(\mathbf{r} \mathbf{p}, t) \\ & + \int \frac{d\mathbf{r}_0 d\mathbf{p}_0 d\mathbf{s}}{(2\pi\hbar)^3} f(\mathbf{r}_0 \mathbf{p}_0, t_0) \left[\frac{(-i\mathbf{s})}{\hbar} \cdot \frac{\partial \mathbf{P}}{\partial t} - \frac{[V(\mathbf{r} - \frac{\mathbf{s}}{2}, t) - V(\mathbf{r} + \frac{\mathbf{s}}{2}, t)]}{i\hbar} \right] \\ & \times \exp\{i\mathbf{s} \cdot [\mathbf{p} - \mathbf{P}(\mathbf{r}_0 \mathbf{p}_0 \mathbf{s}, t)]/\hbar\} \delta[\mathbf{r} - \mathbf{R}(\mathbf{r}_0 \mathbf{p}_0 \mathbf{s}, t)] = 0. \end{aligned} \quad (9)$$

By comparing similar terms, the above equation leads to the equations of motion for \mathbf{R} and \mathbf{P} [3],

$$\frac{\partial \mathbf{R}}{\partial t} = \frac{\mathbf{p}}{m}, \quad (10)$$

$$\mathbf{s} \cdot \frac{\partial \mathbf{P}}{\partial t} = V\left(\mathbf{R} - \frac{\mathbf{s}}{2}, t\right) - V\left(\mathbf{R} + \frac{\mathbf{s}}{2}, t\right). \quad (11)$$

Note that because of the δ -function $\delta(\mathbf{r} - \mathbf{R})$ in Eq. (4), \mathbf{r} and \mathbf{R} are interchangeable in the above equations.

Equation (4) combined with the equations of motion (10) and (11) gives an explicit and exact solution of the time evolution of the Wigner function [3]. To apply it to the evolution of the Wigner function, one starts at an initial time t_0 and divides the phase space into cells with phase space coordinates \mathbf{r}_0 and \mathbf{p}_0 with amplitude $f(\mathbf{r}_0, \mathbf{p}_0)$. One samples the space of the coordinate \mathbf{s} . For a value of \mathbf{s} , one solves the equations of motion (10) and (11) for $\mathbf{R}(\mathbf{r}_0 \mathbf{p}_0 \mathbf{s}, t)$ and $\mathbf{P}(\mathbf{r}_0 \mathbf{p}_0 \mathbf{s}, t)$ with initial conditions $\mathbf{R}(\mathbf{r}_0 \mathbf{p}_0 \mathbf{s}, t_0) = \mathbf{r}_0$ and $\mathbf{P}(\mathbf{r}_0 \mathbf{p}_0 \mathbf{s}, t_0) = \mathbf{p}_0$. The equation of motion for \mathbf{R} is the same as the classical equation of motion. The equation of motion for \mathbf{P} coincides with the classical equation of motion for small \mathbf{s} but differs from the classical equation when \mathbf{s} is large. The latter difference distinguishes a quantum system from a classical system.

To describe quantum mechanics properly, Eq. (4) stipulates that one associates an amplitude factor $\exp\{i\mathbf{s} \cdot (\mathbf{p} - \mathbf{P})/\hbar\}$ with each value of \mathbf{s} . After the amplitudes for all possible values of \mathbf{s} have been obtained at the next time step, one adds these amplitudes together coherently, as given in the righthand side of Eq. (4). The resultant amplitude gives the Wigner function at the next time step. This coherent sum gives the correct phase and sign of the Wigner function in different regions of phase space. Carrying out this procedure repeatedly allows one to evolve the Wigner function forward in time step by step, and the difficulty of propagating a Wigner function with negative values is overcome.

We note in passing that in the limit of $\hbar \rightarrow 0$ the dominant contributions in Eq. (4) come from regions of small \mathbf{s} as large \mathbf{s} leads to highly oscillatory contributions with an average contribution of zero. With contributions coming only from small values of \mathbf{s} , Eqs. (10) and (11) approaches the classical equations of motion

$$\frac{\partial \mathbf{R}}{\partial t} = \frac{\mathbf{p}}{m} \quad (12)$$

and

$$\frac{\partial \mathbf{P}}{\partial t} = -\nabla_{\mathbf{R}} V(\mathbf{R}, t). \quad (13)$$

The function $\mathbf{P}(\mathbf{r}_0\mathbf{p}_0\mathbf{s}, t)$ is then independent of \mathbf{s} , and Eq. (4) gives

$$f(\mathbf{r}\mathbf{p}, t) = \int d\mathbf{r}_0 d\mathbf{p}_0 \delta[\mathbf{r} - \mathbf{R}(\mathbf{r}_0\mathbf{p}_0, t)] \delta[\mathbf{p} - \mathbf{P}(\mathbf{r}_0\mathbf{p}_0, t)] f(\mathbf{r}_0\mathbf{p}_0, t_0), \quad (14)$$

which is the solution of the evolution of the classical distribution function, as expected.

3. Implementation of the Explicit Solution

The explicit solution of Eqs. (4), (10) and (11) given in the previous section allows one to propagate the Wigner function from one time to another. One considers a small time increment $\delta t = t - t_0$, and solves Eqs. (10) and (11). One obtains

$$\mathbf{r} = \mathbf{R}(\mathbf{r}_0\mathbf{p}_0\mathbf{s}, t) = \mathbf{r}_0 + \frac{\mathbf{p}}{m}\delta t. \quad (15)$$

and

$$\mathbf{P} = \mathbf{p}_0 + \mathbf{e}_s \frac{V\left(\mathbf{r} - \frac{\mathbf{s}}{2}, t\right) - V\left(\mathbf{r} + \frac{\mathbf{s}}{2}, t\right)}{s} \delta t, \quad (16)$$

where \mathbf{e}_s is the unit vector in the \mathbf{s} direction. After $\mathbf{r}(\mathbf{R})$ and \mathbf{P} for different \mathbf{s} have been obtained, we can substitute them in Eq. (4) and carry out the integration to give the new Wigner function at the next time step. Eqs. (15) and (16) lead to

$$f(\mathbf{r}\mathbf{p}, t) = \int d\mathbf{r}_0 d\mathbf{p}_0 \int \frac{d\mathbf{s}}{(2\pi\hbar)^3} \exp \left[i \left\{ \frac{\mathbf{s} \cdot (\mathbf{p} - \mathbf{p}_0)}{\hbar} - \left(V\left(\mathbf{r} - \frac{\mathbf{s}}{2}, t\right) - V\left(\mathbf{r} + \frac{\mathbf{s}}{2}, t\right) \right) \frac{\delta t}{\hbar} \right\} \right] \\ \times \delta\left(\mathbf{r} - \mathbf{r}_0 - \frac{\mathbf{p}}{m}\delta t\right) f(\mathbf{r}_0, \mathbf{p}_0, t_0). \quad (17)$$

The integration over \mathbf{r}_0 can be easily carried out, and the above equation becomes

$$f(\mathbf{r}\mathbf{p}, t) = \int d\mathbf{p}_0 2 \int_0^\infty \frac{d\mathbf{s}}{(2\pi\hbar)^3} \cos \left[\frac{\mathbf{s} \cdot (\mathbf{p} - \mathbf{p}_0)}{\hbar} - \left(V\left(\mathbf{r} - \frac{\mathbf{s}}{2}, t\right) - V\left(\mathbf{r} + \frac{\mathbf{s}}{2}, t\right) \right) \frac{\delta t}{\hbar} \right] \\ \times f\left(\mathbf{r} - \frac{\mathbf{p}}{m}\delta t, \mathbf{p}_0, t_0\right). \quad (18)$$

This explicit solution of the time evolution of the Wigner function can be written as

$$f(\mathbf{r}\mathbf{p}, t) = \int d\mathbf{p}_0 \left\{ F_c(\mathbf{r}, \mathbf{p} - \mathbf{p}_0) + F_s(\mathbf{r}, \mathbf{p} - \mathbf{p}_0) \right\} f\left(\mathbf{r} - \frac{\mathbf{p}}{m}\delta t, \mathbf{p}_0, t_0\right), \quad (19)$$

where $F_c(\mathbf{r}, \mathbf{p} - \mathbf{p}_0)$ and $F_s(\mathbf{r}, \mathbf{p} - \mathbf{p}_0)$ are cosine and sine transforms given by

$$F_c(\mathbf{r}, \mathbf{p} - \mathbf{p}_0) = 2 \int_0^\infty \frac{d\mathbf{s}}{(2\pi\hbar)^3} \cos \left[\frac{\mathbf{s} \cdot (\mathbf{p} - \mathbf{p}_0)}{\hbar} \right] \cos \left[\left(V\left(\mathbf{r} - \frac{\mathbf{s}}{2}, t\right) - V\left(\mathbf{r} + \frac{\mathbf{s}}{2}, t\right) \right) \frac{\delta t}{\hbar} \right] \quad (20)$$

and

$$F_s(\mathbf{r}, \mathbf{p} - \mathbf{p}_0) = 2 \int_0^\infty \frac{d\mathbf{s}}{(2\pi\hbar)^3} \sin \left[\frac{\mathbf{s} \cdot (\mathbf{p} - \mathbf{p}_0)}{\hbar} \right] \sin \left[\left(V\left(\mathbf{r} - \frac{\mathbf{s}}{2}, t\right) - V\left(\mathbf{r} + \frac{\mathbf{s}}{2}, t\right) \right) \frac{\delta t}{\hbar} \right]. \quad (21)$$

The above set of equations (19)-(21) provide a simple implementation of the explicit solution (4), (11), and (10) of the time evolution of the Wigner function. Using these results one can propagate the Wigner function forward in time to describe the quantum dynamics of the system.

If one keeps only terms up to first order in δt for small values of δt , the Wigner function evolution equation becomes

$$f(\mathbf{r}\mathbf{p}, t) = f\left(\mathbf{r} - \frac{\mathbf{p}}{m}\delta t, \mathbf{p}, t_0\right) + \frac{\delta t}{\hbar} \int \frac{d\mathbf{p}_0}{(2\pi\hbar)^3} V_s(\mathbf{r}, \mathbf{p} - \mathbf{p}_0) f\left(\mathbf{r} - \frac{\mathbf{p}}{m}\delta t, \mathbf{p}_0, t_0\right), \quad (22)$$

where

$$V_s(\mathbf{r}, \mathbf{p} - \mathbf{p}_0) = 2 \int_0^\infty \frac{d\mathbf{s}}{(2\pi\hbar)^3} \sin\left[\frac{\mathbf{s} \cdot (\mathbf{p} - \mathbf{p}_0)}{\hbar}\right] \left\{ V\left(\mathbf{r} - \frac{\mathbf{s}}{2}, t\right) - V\left(\mathbf{r} + \frac{\mathbf{s}}{2}, t\right) \right\} \quad (23)$$

4. An Example of the Evolution of the Wigner Function

It is of interest to consider an explicit example to test whether the solutions in Eqs. (19)-(21) or (22)-(23) leads to the correct results. For this purpose we study the dynamics of the Wigner function for a case that can be easily evaluated and compared with the Wigner function obtained by using the explicit solution.

We examine a particle in a one-dimensional attractive Gaussian potential well. We express physical quantities in dimensionless units, with a Schrödinger equation given by

$$H\Psi(x) = \left\{ -\frac{1}{2} \frac{d^2}{dx^2} - e^{-x^2/2\sigma^2} \right\} \Psi(x). \quad (24)$$

The wave function $\Psi(x)$ can be expanded in terms of a set of non-orthogonal Gaussian wave functions with different widths,

$$\Psi(x) = \sum_{n=1}^{n_{\max}} a_n \psi_n(x), \quad (25)$$

where the normalized basis function $\langle x|n\rangle = \psi_n(x)$ is taken to be

$$\psi_n(x) = \frac{e^{-x^2/2\beta_n^2}}{(\sqrt{\pi}\beta_n)^{1/2}}, \quad (26)$$

and $\beta_n^2 = n\beta_0^2$. The Hamiltonian matrix in this basis set can be easily constructed. Specifically, one calculates the matrix element of the overlap matrix B for this set of basis states

$$B_{nm} = \langle n|m\rangle = \sqrt{\frac{2\beta_n\beta_m}{\beta_n^2 + \beta_m^2}}, \quad (27)$$

the matrix element of the kinetic energy matrix T

$$T_{nm} = \langle n| \left\{ -\frac{1}{2} \frac{d^2}{dx^2} \right\} |m\rangle = \frac{1}{2} \sqrt{\frac{2\beta_n\beta_m}{\beta_n^2 + \beta_m^2}} \frac{1}{\beta_n^2 + \beta_m^2}, \quad (28)$$

and the matrix element for potential energy matrix V

$$V_{nm} = \langle n| (-e^{-x^2/2\sigma^2}) |m\rangle = -\sqrt{\frac{2\beta_n\beta_m}{\beta_n^2 + \beta_m^2}} \frac{\sigma^2}{\beta_{nm}^2 + \sigma^2}, \quad (29)$$

where

$$\beta_{nm}^2 = \frac{\beta_n^2\beta_m^2}{\beta_n^2 + \beta_m^2}. \quad (30)$$

The eigenvalue equation becomes

$$(T + V)a = EBa, \quad (31)$$

where a is the column matrix of the coefficients $\{a_n\}$ of Eq. (25). This eigenvalue equation can be diagonalized to yield the eigenenergies E_λ and eigenfunctions $\Psi_\lambda(x)$ represented by the set of coefficients $\{a_{\lambda n}\}$. We normalize $\Psi_\lambda(x)$ by $\int dx |\Psi_\lambda(x)|^2 = 1$.

A simple non-stationary state $\Phi(x)$ of the system can be constructed as a linear combination of the eigenstates $\Psi_\lambda(x)$ with amplitudes b_λ ,

$$\Phi(x, t = 0) = \sum_\lambda b_\lambda \Psi_\lambda(x). \quad (32)$$

The time dependence of this non-stationary system is

$$\Phi(x, t) = \sum_\lambda b_\lambda e^{-iE_\lambda t} \Psi_\lambda(x). \quad (33)$$

The Wigner function of the system is then given by

$$f(xp, t) = \sum_{nm} c_n(t) c_m^*(t) f_{nm}(xp), \quad (34)$$

where

$$c_n(t) = \sum_\lambda b_\lambda e^{-iE_\lambda t} a_{\lambda n}, \quad (35)$$

$$f_{nm}(xp) = 2\sqrt{\frac{2\beta_n\beta_m}{\beta_n^2 + \beta_m^2}} e^{-\nu_{nm}}, \quad (36)$$

$$\nu_{nm} = \frac{(\beta_n^2 + \beta_m^2)(x^2 - \mu_{nm}^2/4)}{2\beta_n^2\beta_m^2}, \quad (37)$$

and

$$\mu_{nm} = 4\frac{\beta_n^2\beta_m^2}{\beta_n^2 + \beta_m^2} \left[x \left(\frac{1}{2\beta_n^2} - \frac{1}{2\beta_m^2} \right) + ip \right]. \quad (38)$$

In our numerical example, we study the dynamics of a system in a potential with a width parameter $\sigma = 3$. The two lowest energy even-parity eigenstates $\Psi_0(x)$ and $\Psi_1(x)$ have eigenvalues $E_0 = -0.844$ and $E_1 = -0.312$ respectively. As a test, we construct a non-stationary wave function with equal amplitudes in these two eigenstates at $t = 0$,

$$\Phi(x, t = 0) = \frac{1}{\sqrt{2}} \{ \Psi_0(x) + \Psi_1(x) \}. \quad (39)$$

The time dependence of the wave function is then

$$\Phi(x, t) = \frac{1}{\sqrt{2}} \{ e^{-iE_0 t} \Psi_0(x) + e^{-iE_1 t} \Psi_1(x) \}. \quad (40)$$

The time dependence of the Wigner function can be evaluated using Eq. (34). The Wigner functions for different values of p and t are shown in Figs. (1a), (1b), and (1c) on the left panel of Fig. 1. The Wigner function has both positive and negative values in different regions of phase space. The eigenfunctions and eigenvalues give a correct representation of the Wigner function as it depends only on the accuracy of the

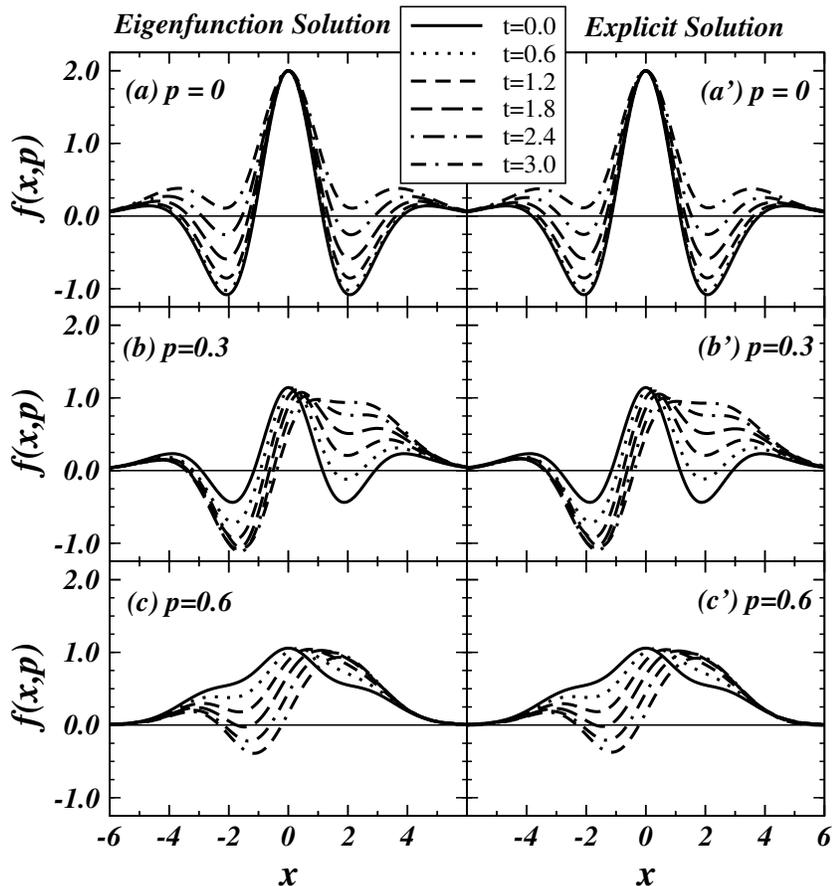


Figure 1. Time dependence of the Wigner function obtained in two different methods. The left panel gives the Wigner function obtained from the eigenvalues and eigenfunctions, and the right panel shows that Wigner function obtained by the explicit solution of Eqs. (19)-(21).

eigenvalues and eigenfunctions, and not on the accuracy of the method of propagating forward in time.

The non-stationary state we have used leads to an initial Wigner function with significant spatial and temporal variation as well as regions of negative values. These properties provide a stringent test of the methods of using Eqs. (19)-(21) or Eqs. (22)-(23) to propagate the Wigner function.

For our tests we take the initial Wigner function for our non-stationary state Eq. (39) at time $t = 0$, and evolve the Wigner function using the explicit solution. In Eqs. (20) and (21), the factor of $(2\pi\hbar)^3$ in the denominator (for a three-dimensional system) is replaced by $2\pi\hbar$ for this one-dimensional example.

We carry out the time evolution using small time increments. One can choose either Eqs. (19)-(21) or Eqs. (22)-(23) to evolve the Wigner function. The former includes higher order effects in δt , and can be used with a larger time increment than the second approach. We choose to use Eqs. (19)-(21), and the results in Fig. 1 from $t = 0$ to $t = 3.0$ were calculated using 30 time steps. The cosine and sine transforms can be

calculated using the method of fast Fourier transforms. The numerical integration over p_0 in Eq. (19) can then be carried out to yield the Wigner function at the next time step. This process is repeated in a stepwise manner to propagate forward in time. The resulting time evolution of the Wigner function is shown in Figs. (1a'), (1b'), and (1c') on the right panel of Fig. 1.

A comparison of the left and the right panels indicates that the explicit solution of Eqs. (19)-(21) gives an excellent reproduction of the time evolution of the Wigner function obtained by using eigenvalues and eigenfunctions. The phases and the negative regions of the Wigner function are correctly reproduced. The difference between the eigenfunction solution and the explicit solution is small. For example, for $p = 0.6$ at $t = 3$, the maximum value of the eigenfunction solution of the Wigner function is 0.9313 at $x = 1.692$, and the explicit solution gives 0.9206 at $x = 1.692$. For this momentum p and $t = 3$, the minimum of the eigenfunction solution of the Wigner function is -0.3888 at $x = -1.1667$, and the the explicit solution gives -0.3735 at $x = -1.1667$. The positions of the maxima and minima in the two methods are the same, and the magnitudes differ by about 1%. The explicit solution of Eqs. (19)-(21) thus leads to an accurate determination of the time evolution of the Wigner function, even if it contains regions of negative or oscillating values.

5. Conclusions

We have reviewed and applied here the explicit solution of the time evolution of the Wigner function obtained previously in 1982 [3]. The basic idea is to represent the Wigner function in terms of auxiliary phase space coordinates, which obey simple equations of motion. These equations are similar to the classical equations of motion, but have important differences. They can be solved easily. The solutions of these equations of motion can then be used to evaluate the time evolution of the Wigner function. We have demonstrated the usefulness of the explicit solution using a numerical example. We find that the explicit solution leads to the correct time evolution of the Wigner function, even for a Wigner function with strong spatial and temporal variations and regions of negative values.

In the final form of Eqs. (19)-(21) or (22)-(23), the results for the time evolution of the Wigner function is quite simple. This simplicity will facilitate its application to problems involving quantum dynamics in phase space. The explicit solution can be applied to study particle dynamics in a time-dependent, multi-dimensional potential. It can also be applied to study the one-body Wigner function of a many-particle system in a time-dependent mean-field potential, as in [3]. With the addition of a collision term, it can be used to describe the dynamics of a quantum Boltzmann equation involving a Wigner function with positive and negative regions in phase space. Future research in these directions will allow us to explore further the richness of quantum dynamics in phase space, which Professor Wigner first opened for us.

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