Numerical Method for the Propagation of Quantum-Mechanical Wave Functions in Phase Space

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A recently proposed phase-space representation for quantum mechanics provides a formal means for investigating the correspondence between classical and quantum mechanics. To explore the implications of this new representation, we introduce a numerical method for propagating an initial wave function directly in phase space. We illustrate the usefulness of the proposed method by analyzing two simple quantum-mechanical systems in phase space.

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Recently, we have introduced a phase-space representation of quantum mechanics which satisfies the mathematical requirements of a quantum-mechanical representation [1,2]. In this representation, the momentum $\hat{P}$ and coordinate $\hat{Q}$ operators take the form $p/2-i\hbar\,\partial/\partial q$ and $q/2+i\hbar\,\partial/\partial p$, respectively. As in the coordinate or momentum representations, the time evolution of an initial wave packet in phase space is governed by the quantum propagation operator, $\exp(-it\hat{H}/\hbar)$, where $\hat{H}$ is the Hamiltonian operator in the phase-space representation,

$$e^{-it\hat{H}/\hbar}\rightarrow\exp\left\{-\frac{i}{\hbar}t\left[\frac{1}{2\mu}\left(\frac{1}{2}p-i\hbar\frac{\partial}{\partial q}\right)^2+V\left(\frac{1}{2}q+i\hbar\frac{\partial}{\partial p}\right)\right]\right\}. \quad (1)$$

Formally, the propagator in Eq. (1) generates the time evolution for an initial wave function $\psi(p,q;0)$ from time $t=0$ to time t directly in phase space; however, it is not clear from Eq. (1) how one might implement this equation practically to study quantum dynamics in phase space. The subject of this Letter is the description of a numerical method that will accomplish this task.

The use of a symmetrically split propagation operator, implemented successfully by Feit, Fleck, and Steiger [3] for the propagation of the Schrödinger equation in the coordinate representation, can be applied to the time propagation of a wave function in phase space as well. In this algorithm, the operator $\exp\{-t[\hat{A}+\hat{B}]\}$ is written in terms of the operators $\exp[-t\hat{A}/2]$ and $\exp[-t\hat{B}]$ as follows:

$$e^{-t[\hat{A}+\hat{B}]}\approx e^{-(t/2)\hat{A}}e^{-t\hat{B}}e^{-(t/2)\hat{A}}, \quad (2)$$

where the difference between the two sides of the above relationship is given by

$$e^{-t[\hat{A}+\hat{B}]}-e^{-(t/2)\hat{A}}e^{-t\hat{B}}e^{-(t/2)\hat{A}}=-\frac{t^3}{24}[(\hat{A}+2\hat{B}),[\hat{A},\hat{B}]]+\mathcal{O}(t^4), \quad (3)$$

and $[\hat{A},\hat{B}]=\hat{A}\hat{B}-\hat{B}\hat{A}$ is the commutator between the operators $\hat{A}$ and $\hat{B}$. By choosing the time interval to be sufficiently small, one can render the terms in Eq. (3) negligible.

When the approximate propagator (2) is adopted, one is actually replacing the evolution equation

$$(\partial/\partial t)\exp[-t(\hat{A}+\hat{B})]=-(\hat{A}+\hat{B})\exp[-t(\hat{A}+\hat{B})]$$

with

$$\frac{\partial}{\partial t}e^{-(t/2)\hat{A}}e^{-t\hat{B}}e^{-(t/2)\hat{A}}=-\left[\tfrac{1}{2}\hat{A}+e^{-(t/2)\hat{A}}\hat{B}e^{+(t/2)\hat{A}}+\tfrac{1}{2}e^{-(t/2)\hat{A}}e^{-t\hat{B}}\hat{A}e^{+t\hat{B}}e^{+(t/2)\hat{A}}\right]e^{-(t/2)\hat{A}}e^{-t\hat{B}}e^{-(t/2)\hat{A}},$$

an equation with time-dependent operators, affecting the phase of the wave function.

In the phase-space representation of quantum mechanics, the split-operator approximation (2), when applied to the quantum propagator (1) for a small time Δt, takes the form

$$\exp\left[-\frac{i\Delta t}{4\hbar\mu}\left(\frac{1}{2}p-i\hbar\frac{\partial}{\partial q}\right)^2\right]\exp\left[-i\frac{\Delta t}{\hbar}V\left(\frac{1}{2}q+i\hbar\frac{\partial}{\partial p}\right)\right]\exp\left[-\frac{i\Delta t}{4\hbar\mu}\left(\frac{1}{2}p-i\hbar\frac{\partial}{\partial q}\right)^2\right].$$

Although seemingly difficult to apply, this is actually a very convenient expression since a fast-Fourier-transform routine can be utilized to evaluate the action of this operator on a function of p and q, as we show below.

The Fourier transform of the application of $p/2-i\hbar\,\partial/\partial q$ to a wave function $\psi(p,q;t)$ is given by (the limits of all in-

tegrals are understood to be $\pm\infty$ unless otherwise noted)

$$\mathcal{F}\left\{\left[\left(\frac{1}{2}p-i\hbar\frac{\partial}{\partial q}\right)\psi(p,q;t)\right]\right\}\equiv\frac{1}{\sqrt{4\pi\hbar}}\int dq\, e^{-ip'q/2\hbar}\left[\frac{1}{2}p-i\hbar\frac{\partial}{\partial q}\right]\psi(p,q;t)$$
$$=\left[\frac{1}{2}(p+p')\right]\frac{1}{\sqrt{4\pi\hbar}}\int dq\, e^{-ip'q/2\hbar}\psi(p,q;t)\,, \tag{4}$$

where we have assumed that boundary terms vanish. Equation (4) suggests that one can calculate the Fourier transform of the wave packet, multiply it by $(p+p')/2$, where p' is the reciprocal variable to q, and invert the Fourier transform to compute the operation of $\hat{P}$ on the wave function $|\psi_t\rangle$ in phase space. This is also true for any function of the momentum operator $\hat{P}$; therefore,

$$\mathcal{F}\{e^{-(it/4\mu\hbar)[p/2-i\hbar(\partial/\partial q)]^2}\psi(p,q;t)\}=e^{-(it/4\mu\hbar)[(p+p')/2]^2}\frac{1}{\sqrt{4\pi\hbar}}\int dq\, e^{-ip'q/2\hbar}\psi(p,q;t)\,.$$

We can repeat the above derivation for the part of the propagator that contains the potential operator, obtaining (note the change in sign in the Fourier kernel and the integration over p)

$$\mathcal{F}^{-1}\{e^{-(it/\hbar)V[q/2+i\hbar(\partial/\partial p)]}\psi(p,q;t)\}=e^{-(it/\hbar)V[(q+q')/2]}\frac{1}{\sqrt{4\pi\hbar}}\int dp\, e^{ipq'/2\hbar}\psi(p,q;t)\,,$$

where q' is the reciprocal variable to p. The above expressions can be evaluated numerically quite efficiently through the use of the fast Fourier transform.

As a simple illustration of the method, we examine the dynamics of the scattering of a Gaussian wave packet from a potential step. This is a textbook example and has been reviewed by Kosloff and Kosloff [4] to illustrate their method for wave-packet propagation in coordinate space (we note that a variation of their coordinate-space propagation algorithm could be applied to phase space equally well by using the results in this paper). In this system, the energy of the wave packet is 1.26 and the barrier height is 1. This model system illustrates the development of nodal structure due to quantum interference between the advancing and reflected parts of the wave packet when it encounters the potential step. By treating the same problem in phase space, we can obtain a more comprehensive picture of the processes involved in the dynamics.

Figure 1(a) shows a phase-space diagram of the square magnitude of the initial Gaussian wave packet, $|\psi(\Gamma;t=0)|^2$, and the energy surface on which it evolves. Below the phase-space diagram, the square magnitude $|\psi(q;t)|^2$ of the projection [1,2] $\psi(q;t)=\int dp\exp(+ipq/2\hbar)\psi(\Gamma;t)$ of the phase-space wave function onto the coordinate representation is shown. The square magnitude $|\psi(p;t)|^2$ of the projection $\psi(p;t)=\int dq\exp(-ipq/2\hbar)\psi(\Gamma;t)$ onto the momentum representation is shown to the right. Figures 1(b) and 1(c) correspond to "snapshots" of the dynamics taken at subsequent times. From these frames, one can see how the wave packet in phase space breaks into three parts as it is evolving in time. First, there is a part whose momentum is near zero and which, consequently, moves very slowly. A second part of the wave packet smoothly changes its direction as it is reflected from the step, and combines with the part that stayed behind. Finally, a third part of the wave packet has enough energy to overcome the barrier and continues moving past the step with smaller momentum.

The analysis in phase space allows us a better under-

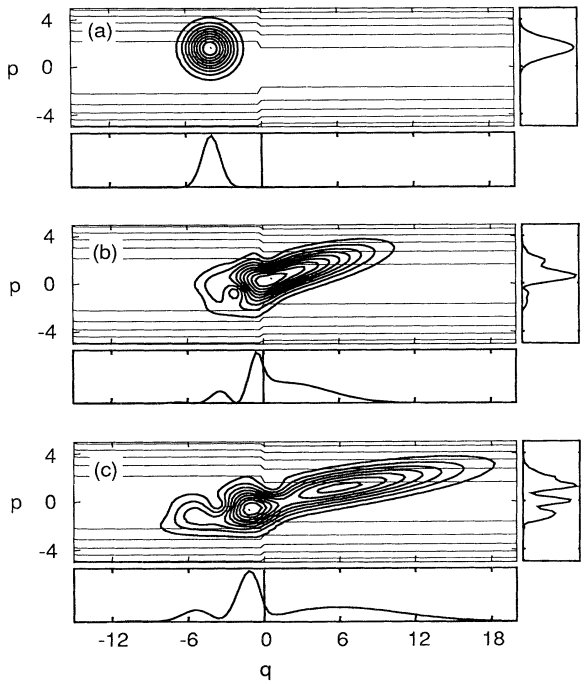

FIG. 1. Snapshots of the evolution of the Gaussian wave packet which is being scattered from a step potential at $q=0$, in a dimensionless phase space. The energy of the wave packet is 1.26 and the height of the barrier is 1. Thin and dark lines correspond to contour plots of the energy surface and the wave packet, respectively. Below and to the right of each diagram is a plot of the projection of the wave function onto the coordinate and momentum spaces (coordinate and momentum wave functions), respectively.

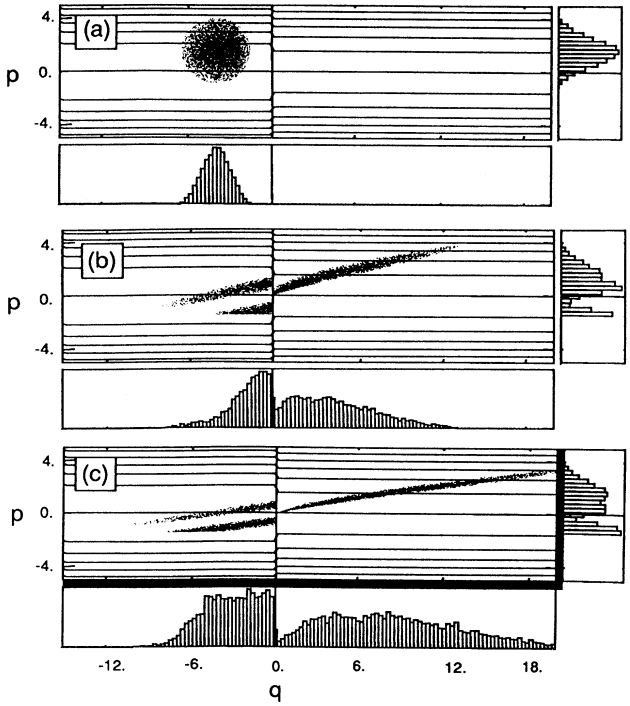

FIG. 2. Snapshots of the evolution of a set of 10000 point particles, with an initial distribution like the one in Fig. 1(a), which are being scattered from a step potential at $q=0$, in a dimensionless phase space. Below and to the right of each diagram there is a histogram indicating the distribution of particles with momentum or coordinate, respectively, lying within a small range of values (coordinate and momentum distributions).

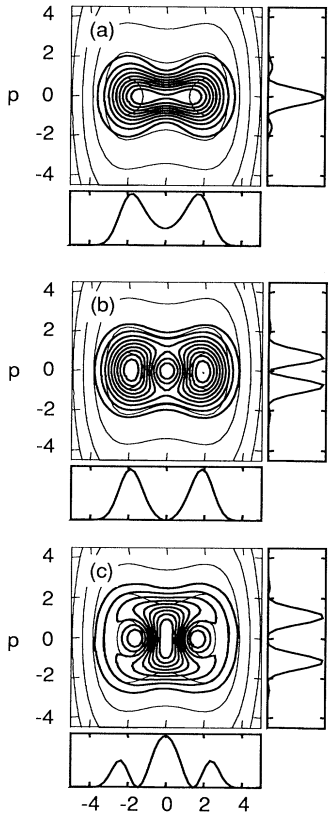

FIG. 3. The three lowest eigenfunctions for the quartic double-well potential in phase space. Below and to the right of each diagram there is a plot of the projection of the wave function onto the coordinate and momentum spaces, respectively (coordinate and momentum eigenfunctions).

standing of the dynamics: Each peak appearing in the coordinate wave function corresponds to a different part of the wave packet in phase space. These pictures suggest that, in this case, "quantum interference" effects may be partly explainable in classical terms. Each piece of the reflecting and transmitting wave packet resides in a different region of phase space and it is only when the wave function is projected onto coordinate or momentum space that one loses this perspective.

In Refs. [1] and [2], we have suggested that a classical analog of the square magnitude of the wave function in phase space is a classical probability density $\rho(\Gamma;t)$, whose time evolution is dictated by the classical Liouville equation of motion. In addition, the classical analog of the square magnitude of the coordinate-space wave function $|\psi(q;t)|^2$ is the average $\int dp\,\rho(\Gamma;t)$ over p of the classical probability density, and, likewise, the classical analog of $|\psi(p;t)|^2$ is the average $\int dq\,\rho(\Gamma;t)$. Because of the different ways in which the quantum and classical projections are done, we should expect the interference pattern observed in $\psi(q;t)$ to be "washed out" in corresponding pictures of $\int dp\,\rho(\Gamma;t)$.

In a classical calculation, we used 10000 trajectories with initial conditions distributed in phase space according to the Gaussian density given by the initial quantum Gaussian probability of Fig. 1 to simulate the dynamics of $\rho(\Gamma;t)$. In Fig. 2, snapshots of this set of points in phase space and of its averages over p and q are shown at the same times as in Fig. 1. By comparing Figs. 1 and 2 we conclude that the classical and quantum behavior are qualitatively the same with some small quantitative differences. Since the classical averaging process is over real-valued functions, only constructive addition of the pieces of the distribution are permitted, thus, "washing out" the interference effects. Clearly, further differences between the classical and quantum dynamics will arise for systems that display purely quantum effects such as tunneling.

The time evolution of a wave function in phase space can also be used to find the energy eigenvalues E_n and eigenfunctions $|\Psi_n\rangle$ via the standard time-dependent formalism which utilizes the Fourier transforms $\lim_{T\to\infty}\int_{-T}^{T} dt\exp(i\omega t)\langle\psi_0|\psi_t\rangle$ and

$$|\Psi_n\rangle \propto \lim_{T\to\infty}(1/2T)\int_{-T}^{T} dt\exp(iE_n t/\hbar)|\psi_t\rangle\,,$$

for a given initial wave packet $|\psi_0\rangle$. In Fig. 3, we show the lowest three eigenfunctions in phase space for the quartic potential $U(q)=\gamma q^4-q^2/2$, with $\gamma=0.06$.

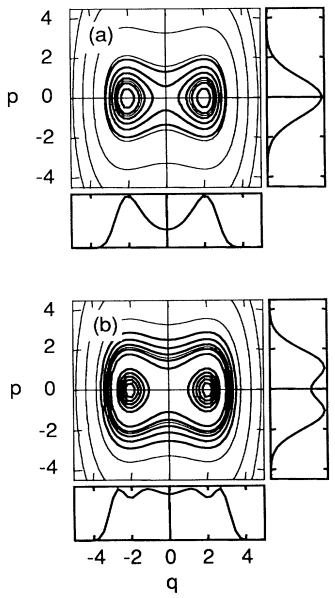

FIG. 4. Classical analogs of the eigenfunctions of Fig. 3. (a) Classical analogs of Figs. 3(a) and 3(b); (b) classical analog of Fig. 3(c). Below and to the right of each diagram there is a plot of the averages over momentum and coordinate, respectively (coordinate and momentum densities).

In our earlier study, the harmonic oscillator in phase space was found to have many eigenfunctions corresponding to a given eigenvalue [1], one of which has the appealing property that the classical analogs are proportional to $[H(\Gamma)]^n \exp[-H(\Gamma)/\hbar\omega]$. In Fig. 4, we show two of these classical densities for $n=0,1$ and for the case of the quartic potential of Fig. 3. The lowest two quantum eigenstates in Fig. 3 correspond to eigenenergies with very close values, forming a pair of eigenstates, and they look very similar to the classical density of Fig. 4(a). The third eigenfunction of Fig. 3(c) is very similar to the classical density of Fig. 4(b). Even the corresponding projections in coordinate and momentum spaces share similar features. Nevertheless, the difference in the projections of classical (real-valued) and quantum (complex-valued) functions onto coordinate and momentum spaces causes the classical distributions in Fig. 4(b) to differ from their quantum counterparts in Fig. 3(c).

The current algorithm provides us, for the first time, with a novel opportunity to generate information about quantum wave-packet dynamics in phase space with the possibility of (i) projecting it onto either position or momentum space, or (ii) comparing it directly to the classical dynamics of the same probability distribution. Time evolution is accomplished within the Schrödinger picture; therefore, unlike the Wigner [5] or Husimi [6] distributions, phase information is preserved during transformations between phase space and position or momentum space. Finally, this algorithm implements a self-consistent theoretical framework for generating quantum dynamics completely in phase space, without recourse to the position or momentum representations, and allows one to contrast this dynamics with the classical dynamics of the same initial distribution in phase space. As a tool for gaining insight into the correspondence between classical and quantum mechanics, it might prove extraordinarily useful.

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