Lanczos method for the numerical propagation of quantum densities in phase space with an application to the kicked harmonic oscillator

Go. TorresVega

Citation: The Journal of Chemical Physics **98**, 7040 (1993); doi: 10.1063/1.464747
View online: http://dx.doi.org/10.1063/1.464747
View Table of Contents: http://scitation.aip.org/content/aip/journal/jcp/98/9?ver=pdfcov
Published by the AIP Publishing

Lanczos method for the numerical propagation of quantum densities in phase space with an application to the kicked harmonic oscillator

Go. Torres-Vega
Departamento de Física, Centro de Investigación y de Estudios Avanzados del IPN, Apartado Postal 14-740, 07000 México D.F.

(Received 18 December 1992; accepted 22 January 1993)

A numerical propagation scheme based on dual Lanczos transformation theory is introduced for the propagation of quantum mechanical wave functions in coordinate and phase spaces. This method is applied to the numerical propagation of the coherent state moving in the kicked harmonic oscillator potential. We also make comparisons with classical analogs and we make some comments regarding the advantage of working directly in phase space.

I. INTRODUCTION

The analysis of the time evolution of quantum mechanical wave functions on phase space is a topic still open to research.[1-4] Many ways for obtaining a two-variable function from a one-variable one have been proposed in order to generate probability densities on phase space from a coordinate quantum mechanical wave function. Since this can be done in a number of ways, these probability densities are not well defined. A more reasonable approach would be to postulate wave functions, operators and a Schrödinger equation, directly in phase space in such a way that all the requirements for a quantum mechanical representation are satisfied, and that the quantities involved are reduced to the corresponding ones in coordinate or momentum spaces by means of appropriate projections onto these spaces.

Recently, we have introduced a phase space representation which satisfies the mathematical requirements for a quantum mechanical representation, including the impossibility to measure coordinate and momentum of a given quantum system with arbitrary precision.[4] In that representation, the momentum $\hat{P}$ and coordinate $\hat{Q}$ operators take the forms $p/2-i\hbar\partial/\partial q$ and $q/2+i\hbar\partial/\partial p$, respectively. As in coordinate or momentum representations, the time evolution of a wave packet in phase space, $\psi(\Gamma;t)$, where Γ denotes a point the phase space (p,q), is governed by a Schrödinger equation,

$$i\hbar\frac{\partial}{\partial t}\psi(\Gamma;t)=\left[\frac{1}{2m}\left(\frac{p}{2}-i\hbar\frac{\partial}{\partial q}\right)^2+V\left(\frac{q}{2}+i\hbar\frac{\partial}{\partial p}\right)\right]\psi(\Gamma;t). \tag{1.1}$$

Therefore, the wave function $\psi(\Gamma;t)$, at a time t, is obtained by the application of the propagator

$$\exp(-it\hat{H}/\hbar)\rightarrow\exp\left\{-\frac{i}{\hbar}t\left[\frac{1}{2m}\left(\frac{p}{2}-i\hbar\frac{\partial}{\partial q}\right)^2+V\left(\frac{q}{2}+i\hbar\frac{\partial}{\partial p}\right)\right]\right\} \tag{1.2}$$

to a given initial wave function $\psi(\Gamma;0)$. The subject of this paper is to develop a numerical method based in dual Lanczos transformation theory, in the form developed by Wassam *et al.*,[5] that will allow us to calculate $\psi(\Gamma;t)$ completely in phase space. We prefer the approach due to Wassam since it is more developed than other methods, allowing an infinite order approximation in time. The implementation of a method similar to the one used in this paper in coordinate space has shown to be a better approximation than the time split method.[6]

In Sec. II, we apply dual Lanczos transformation theory to the determination of the time evolution of an abstract ket, and later on, we particularize to wave functions in coordinate and in phase spaces. In the third section, this method is applied to the determination of the time evolution of an initial wave function for a one and a half-dimensional nonlinear system. Finally, we summarize our findings in Sec. IV.

II. DUAL LANCZOS TRANSFORMATION METHOD

In this paper, we present the application of dual Lanczos transformation theory to the propagation of initial abstract quantum kets, and later on, to the propagation of wave functions in coordinate and phase spaces. The reader interested in the details of this theory is encouraged to read Refs. 5. A convenient way of dealing with the evolution of a given state is to express that state as a linear combination of eigenstates of the Hamiltonian. Unfortunately, in most cases there is no knowledge of eigenvalues and eigenfunctions, rendering this method inapplicable. An alternative method is to generate a set of basis vectors for the same invariant vector subspace in which the system of interest evolves. By extraction the dynamical information from the equations of motion, dual Lanczos transformation theory generates, in a systematic way, an invariant dynamical vector subspace, equivalent to the eigenstate space, in which the dynamical quantities we are interested in evolve in time.

 0021-9606/93/097040-06$06.00

A. Brief summary of the theory

In dual Lanczos transformation theory, the dynamics of a linear system takes place in a dynamical vector space containing two fundamental types of vectors. Right handed vectors, denoted by $|\psi(t)\rangle$, represent quantities that evolve according to the evolution equation

$$\frac{\partial}{\partial t}|\psi(t)\rangle = -\hat{\mathscr{L}}|\psi(t)\rangle. \tag{2.1}$$

In the present work, $|\psi(t)\rangle$ represents a quantum ket, so that $\hat{\mathscr{L}}$, called the transition operator, is given by $\hat{\mathscr{L}} \equiv i\hat{\mathscr{H}}/\hbar$, then, the adjoint operator to $\hat{\mathscr{L}}$ is given by $\hat{\mathscr{L}}^{\dagger} = -\hat{\mathscr{L}}$. There are also left handed vectors $\langle\phi(t)|$ which are just the adjoint vectors to $|\phi(t)\rangle$.

This method generates in a systematic way such a basis set denoted by $\{\langle r_s^{LZ}|\}$, $\{|p_s^{LZ}\rangle\}$ (the superscript LZ is used to indicate that the quantity is a dual Lanczos vector). We can start the process by choosing two of the quantities we are interested in as the initial vectors $\langle r_0^{LZ}|$ and $|p_0^{LZ}\rangle$ of the basis set [in this work the two starting vectors are chosen to be the initial ket we wish to propagate: $|p_0^{LZ}\rangle = |\psi(t=0)\rangle$, and its adjoint $\langle r_0^{LZ}| = \langle\psi(t=0)|$] and then generate the remaining vectors by means of a recursion relationship. These vectors should be normalized with respect to an inner product. The inner product $\langle\psi|\phi\rangle$ between the vectors $\langle\psi|$ and $|\phi\rangle$ is defined in the usual way for quantum systems; in coordinate space $\langle\psi|\phi\rangle \equiv \int_{-\infty}^{+\infty} dq\, \psi^*(q)\phi(q)$, whereas, in phase space, the inner product is defined as $\langle\psi|\phi\rangle \equiv \int_{-\infty}^{+\infty} d\Gamma\, \psi^*(\Gamma)\phi(\Gamma)$.

Once the initial vectors $\langle r_0^{LZ}|$ and $|p_0^{LZ}\rangle$ are chosen, the remaining vectors $\{\langle r_s^{LZ}|\}$ and $\{|p_s^{LZ}\rangle\}$; $s=1,2,3,\cdots$ of the basis set, are generated by means of the recursion relationships

$$\beta_{s+1}|p_{s+1}^{LZ}\rangle = (\hat{\mathscr{L}} - \alpha_s\hat{I})|p_s^{LZ}\rangle - \beta_s|p_{s-1}^{LZ}\rangle, \tag{2.2a}$$

$$\beta_{s+1}\langle r_{s+1}^{LZ}| = \langle r_s^{LZ}|(\hat{\mathscr{L}} - \alpha_s\hat{I}) - \beta_s\langle r_{s-1}^{LZ}|. \tag{2.2b}$$

In Eqs. (2.2a) and (2.2b), $|p_{-1}^{LZ}\rangle$ and $\langle r_{-1}^{LZ}|$ are the null vectors, $\hat{I}$ is the identity operator, and the Lanczos parameters $\{\beta_s\}$; $s=1,2,3,...$, and $\{\alpha_s\}$; $s=0,1,2,3,...$ are the only non-vanishing matrix elements of $\hat{\mathscr{L}}$ in the dual Lanczos representation,

$$\alpha_s = \langle r_s^{LZ}|\hat{\mathscr{L}}|p_s^{LZ}\rangle, \tag{2.3a}$$

$$\beta_{s+1} = \langle r_s^{LZ}|\hat{\mathscr{L}}|p_{s+1}^{LZ}\rangle = \langle r_{s+1}^{LZ}|\hat{\mathscr{L}}|p_s^{LZ}\rangle. \tag{2.3b}$$

Note that, in this representation, the operator $\hat{\mathscr{L}}$ becomes a complex symmetric tridiagonal matrix with diagonal elements α_s and off-diagonal elements β_s. The dual Lanczos space has either an infinite or a finite dimensionality according to the values of β_s. If there exist a finite integer N such that $\beta_N = 0$, then the dimensionality of the dual Lanczos vector space is N. The set of dual Lanczos vectors generated in this way is a biorthonormal one, that is, $\langle r_s^{LZ}|p_{s'}^{LZ}\rangle = \delta_{s,s'}$. Note that, since we have chosen the initial left handed Lanczos vector $\langle r_0^{LZ}| = \langle\psi(t=0)|$ to be the adjoint to the right handed one $|p_0^{LZ}\rangle = |\psi(t=0)\rangle$, then all the left Lanczos vectors $\langle r_s^{LZ}|$ will be the adjoints of the right ones $|p_s^{LZ}\rangle$. An equivalent way to calculate the Lanczos parameter β_{s+1} is given by the relationship

$$\beta_{s+1}^2 = \langle r_s^{LZ}|\hat{\mathscr{L}}^2|p_s^{LZ}\rangle - \alpha_s^2 - \beta_s^2, \tag{2.4}$$

where $\beta_0 = 0$.

The set of vectors generated by relationships (2.2) is a basis set in terms of which we can express any dynamical quantity lying in that vector subspace. Consequently, we can make use of these vectors to describe the time evolution of quantum kets. The closure relation

$$\hat{I}^{LZ} = \sum_s |p_s^{LZ}\rangle\langle r_s^{LZ}|, \tag{2.5}$$

where $\hat{I}^{LZ}$ is the identity operator for the dual Lanczos vector subspace, allows us to write an expression for the time evolution of the Lanczos vectors themselves,

$$\langle r_s^{LZ}(t)| \equiv \langle r_s^{LZ}|\exp(-\hat{\mathscr{L}}t), \tag{2.6a}$$

$$|p_s^{LZ}(t)\rangle \equiv \exp(-\hat{\mathscr{L}}t)|p_s^{LZ}\rangle, \tag{2.6b}$$

in terms of the time correlation functions

$$\begin{aligned} A_{i,j}(t) &\equiv \langle r_i^{LZ}|\exp(-\hat{\mathscr{L}}t)|p_j^{LZ}\rangle \\ &= \langle r_j^{LZ}|\exp(-\hat{\mathscr{L}}t)|p_i^{LZ}\rangle, \end{aligned} \tag{2.7}$$

between Lanczos vectors in the following way:

$$\begin{aligned} \langle r_s^{LZ}(t)| &= \sum_{s'} A_{s,s'}(t)\langle r_{s'}^{LZ}|, \\ |p_s^{LZ}(t)\rangle &= \sum_{s'} A_{s',s}(t)|p_{s'}^{LZ}\rangle. \end{aligned} \tag{2.8}$$

Since we are only interested on the time evolution of the initial ket $|p_0^{LZ}\rangle = |\psi(t=0)\rangle$, only the time correlation functions $\{A_{0,s}(t)\}$ are needed.

After some algebraic manipulation of the Laplace transform of the time correlation functions (2.7), it is found that these functions can be calculated from

$$\begin{aligned} A_{j,k}(t) = (-1)^{j+k}\left[\prod_{m=j}^{k}\frac{\beta_m}{\beta_j}\right]\sum_{l=1}^{N} e^{z_l t}\mathscr{S}_0^{(j)}(z_l)\mathscr{S}_{k+1}^{(N)}(z_l) \\ \times \lim_{z\to z_l}\frac{(z-z_l)}{\mathscr{S}_0^{(N)}(z)}, \end{aligned} \tag{2.9}$$

for $k \geqslant j$, where N is the dimensionality of the Lanczos vector space, z_l are the roots of $\mathscr{S}_0^{(N)}(z)$, and the polynomials $\mathscr{S}_m^{(s)}(z)$ are given by

$$\mathscr{S}_m^{(s)}(z) = \sum_{j=0}^{s-m} d_m^{(s,j)} z^j, \tag{2.10a}$$

and its coefficients can be generated by means of the recursion relationships

$$
\begin{aligned}
d_m^{(s,0)} &= \alpha_m d_{m+1}^{(s,0)} - \beta_{m+1}^2 d_{m+2}^{(s,0)}, \\
d_m^{(s,j)} &= d_{m+1}^{(s,j-1)} + \alpha_m d_{m+1}^{(s,j)} - \beta_{m+1}^2 d_{m+2}^{(s,j)}, \\
d_m^{(s,s-m-1)} &= d_{m+1}^{(s,s-m-2)} + \alpha_m d_{m+1}^{(s,s-m-1)}, \\
d_m^{(s,s-m)} &= 1,
\end{aligned}
\tag{2.10b}
$$

where $s-m-1>j>0$. Note that the characteristic frequencies and time scales are determined by the roots of the polynomial $\mathscr{S}_0^{(N)}(z)$, which are just the negatives of the eigenvalues of $\hat{\mathscr{L}}$. The time correlation functions (2.9) obey the symmetry relations $A_{i,j}(t)=A_{j,i}(t)$ and, therefore, it is enough to calculate only a subset of them [for the propagation of quantum wave functions, we only require $A_{0,j}(t)$]. In case that the dimensionality N of the subspace is too large or infinite, we can make an approximation by taking a finite value of N (which means that we have to propagate the wave function for a small amount of time Δt) for which convergence is ensured. We can also avoid numerical instability due to the dual vectors becoming orthogonal by decreasing the dimensionality of the vector space, which means, again, that Δt should be decreased.

B. Coordinate representation

When dealing with a particular quantum system, we chose a particular representation. In the generation of dual Lanczos vectors in coordinate space from the recursion relationships (2.2), it is necessary to compute the result of the application of the transition operator

$$
\mathscr{L}(q)=\frac{i}{\hbar}\left[\frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial q}\right)^2+V(q)\right], \tag{2.11}
$$

on a function of q. This can be done numerically quite easily with the help of a fast Fourier transform routine (FFT). The Fourier transform, with kernel $(2\pi\hbar)^{-1/2}\times\exp(-ip'q/\hbar)$ and integration over q, of the application of $-i\hbar(\partial/\partial q)$ to a wave function $\psi(q)$, in coordinate space is given by

$$
\begin{aligned}
&\int_{-\infty}^{+\infty} dq \frac{e^{-ip'q/\hbar}}{\sqrt{2\pi\hbar}}\left(-i\hbar\frac{\partial}{\partial q}\right)\psi(q) \\
&\quad = p'\int_{-\infty}^{+\infty} dq \frac{e^{-ip'q/\hbar}}{\sqrt{2\pi\hbar}}\psi(q),
\end{aligned}
\tag{2.12}
$$

where we have assumed that boundary terms vanish. This equation suggests that one can calculate the Fourier transform of the wave packet, multiply it by p', where p' is the reciprocal variable to q, and invert the Fourier transform in order to compute the operation of $\hat{P}$ on the wave function $|\psi\rangle$ in coordinate space. This is also true for any well behaved function of the momentum operator $\hat{P}$, therefore

$$
\begin{aligned}
&\int_{-\infty}^{+\infty} dq \frac{e^{-ip'q/\hbar}}{\sqrt{2\pi\hbar}}\left(-i\hbar\frac{\partial}{\partial q}\right)^2\psi(q) \\
&\quad = (p')^2\int_{-\infty}^{+\infty} dq \frac{e^{-ip'q/\hbar}}{\sqrt{2\pi\hbar}}\psi(q).
\end{aligned}
\tag{2.13}
$$

Then, a numerical propagation, in coordinate space, of an initial wave packet is done as follows: (1) Define a grid in the region of coordinate space q on which the wave function is going to evolve in time, and also the corresponding grid in the reciprocal space p. (2) Define the initial wave function $\psi(q;t=0)$ to be propagated on the grid and take it as the initial Lanczos vectors $p_0^{LZ}(q)=[r_0^{LZ}(q)]^*=\psi(q;t=0)$. (3) Calculate $ip^2/2m\hbar$ and $iV(q)/\hbar$ on their respective grids and store those values for later use. (4) Select the dimensionality N and propagation time Δt and generate the dual Lanczos vector subspace $\{r_s^{LZ}(q)\}$ and $\{p_s^{LZ}(q)\}$; $s=1,2,\ldots,N-1$ by means of Eqs. (2.2)–(2.4), which in coordinate space becomes

$$
\begin{aligned}
&\beta_{s+1}p_{s+1}^{LZ}(q)=[\mathscr{L}(q)-\alpha_s]p_s^{LZ}(q)-\beta_s p_{s-1}^{LZ}(q), \\
&r_s^{LZ}(q)=[p_s^{LZ}(q)]^*, \\
&\alpha_s=\int_{-\infty}^{+\infty} dq[r_s^{LZ}(q)]^*\mathscr{L}(q)p_s^{LZ}(q), \\
&\beta_{s+1}^2=\int_{-\infty}^{+\infty} dq[r_s^{LZ}(q)]^*\mathscr{L}^2(q)p_s^{LZ}(q)-\alpha_s^2-\beta_s^2,
\end{aligned}
\tag{2.14}
$$

where $\mathscr{L}(q)$ is given by Eq. (2.11). (5) Generate the generalized polynomials $\mathscr{S}_0^{(j)}(z)$ by means of Eqs. (2.10) and find the roots of $\mathscr{S}_0^{(N)}(z)$. (6) Calculate the time correlation functions $A_{0,j}(\Delta t)$ by means of Eq. (2.9). (7) Assemble the wave function at time Δt, $\psi(q;\Delta t)$, by making use of Eq. (2.8) for $s=0$, $\psi(q;\Delta t)\equiv p_0^{LZ}(q;\Delta t)=\Sigma_s A_{0,s}(\Delta t)p_s^{LZ}(q)$. (8) Repeat steps (4) to (8), now taking the wave function $\psi(q;\Delta t)$ generated in step (7) as the initial Lanczos vectors $p_0^{LZ}(q)$ and $r_0^{LZ}(q)$ for the next step in the propagation. Repeat this as many times as needed until the desired total time t is reached.

C. Phase space representation

Now, in the generation of dual Lanczos vectors in phase space from the recursion relationships (2.2) it is necessary to compute the result of the application of the transition operator on the right-hand side of Eq. (1.1), times $i/\hbar$, on a function of p and q. This can be done numerically quite easily with the help of a fast Fourier transform routine (FFT). The Fourier transform, with kernel $(4\pi\hbar)^{-1/2}\exp(-ip'q/2\hbar)$ and integration over q, of the application of $p/2-i\hbar(\partial/\partial q)$ to a wave function $\psi(\Gamma;t)$ is given by

$$
\begin{aligned}
&\int_{-\infty}^{+\infty} dq \frac{e^{-ip'q/2\hbar}}{\sqrt{4\pi\hbar}}\left(\frac{p}{2}-i\hbar\frac{\partial}{\partial q}\right)\psi(\Gamma) \\
&\quad = \left[\frac{1}{2}(p+p')\right]\int_{-\infty}^{+\infty} dq \frac{e^{-ip'q/2\hbar}}{\sqrt{4\pi\hbar}}\psi(\Gamma),
\end{aligned}
\tag{2.15}
$$

where we have assumed that boundary terms vanish. Equation (2.15) 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 in order to compute the operation of $\hat{P}$ on the ket $|\psi\rangle$ in phase space. This is also true for any well behaved function of the momentum operator $\hat{P}$, therefore

$$\int_{-\infty}^{+\infty} dq \frac{e^{-ip'q/2\hbar}}{\sqrt{4\pi\hbar}} \left(\frac{p}{2}-i\hbar\frac{\partial}{\partial q}\right)^2 \psi(\Gamma)$$

$$= \left[\frac{1}{2}(p+p')\right]^2 \int_{-\infty}^{+\infty} dq \frac{e^{-ip'q/2\hbar}}{\sqrt{4\pi\hbar}} \psi(\Gamma). \tag{2.16}$$

We can repeat the above derivation for the calculation of the effect that a well behaved function $\hat{V}(\hat{Q})$ of the coordinate operator has on a ket $|\psi\rangle$ on phase space (note the change in sign in the Fourier kernel and the integration over p)

$$\int_{-\infty}^{+\infty} dp \frac{e^{ipq'/2\hbar}}{\sqrt{4\pi\hbar}} V\left(\frac{q}{2}+i\hbar\frac{\partial}{\partial p}\right)\psi(\Gamma)$$

$$= V\left[\frac{1}{2}(q+q')\right] \int_{-\infty}^{+\infty} dp \frac{e^{ipq'/2\hbar}}{\sqrt{4\pi\hbar}} \psi(\Gamma), \tag{2.17}$$

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 (FFT) on an appropriate grid on phase space.

Then, a numerical propagation, in phase space, of an initial wave packet is done as follows: (1) Define a grid on the region of phase space $\Gamma=(p,q)$ on which the wave function is going to evolve in time, and also the corresponding grid in its reciprocal space $\Gamma'=(q',p')$. (2) Define the initial wave function $\psi(\Gamma;0)$ to be propagated on the grid and take it as the initial Lanczos vectors $p_0^{LZ}(\Gamma) = [r_0^{LZ}(\Gamma)]^* = \psi(\Gamma;0)$. (3) Calculate $(i/2m\hbar)[(p+p')/2]^2$ and $iV[(q+q')/2]/\hbar$ on the grid and store those values for later use. (4) Select the dimensionality N and propagation time Δt and generate the dual Lanczos vector subspace $\{r_s^{LZ}(\Gamma)\}$ and $\{p_s^{LZ}(\Gamma)\}$; $s=1,2,\ldots,N-1$ by means of Eqs. (2.2)–(2.4) which in phase space becomes

$$\beta_{s+1}p_{s+1}^{LZ}(\Gamma) = [\mathcal{L}(\Gamma)-\alpha_s]p_s^{LZ}(\Gamma)-\beta_s p_{s-1}^{LZ}(\Gamma),$$

$$r_s^{LZ}(\Gamma) = [p_s^{LZ}(\Gamma)]^*,$$

$$\alpha_s = \int_{-\infty}^{+\infty} d\Gamma [r_s^{LZ}(\Gamma)]^* \mathcal{L}(\Gamma) p_s^{LZ}(\Gamma),$$

$$\beta_{s+1}^2 = \int_{-\infty}^{+\infty} d\Gamma [r_s^{LZ}(\Gamma)]^* \mathcal{L}^2(\Gamma) p_s^{LZ}(\Gamma) - \alpha_s^2 - \beta_s^2, \tag{2.18}$$

where $\mathcal{L}(\Gamma)$ is given by the right-hand side of Eq. (1.1) times $i/\hbar$. (5) Generate the generalized polynomials $\mathcal{L}_0^{(j)}(z)$ by means of Eqs. (2.10) and find the roots of $\mathcal{L}_0^{(N)}(z)$. (6) Calculate the time correlation functions $A_{0,j}(\Delta t)$ by means of Eq. (2.9). (7) Assemble the wave function at time Δt, $\psi(\Gamma;\Delta t)$ by making use of Eq. (2.8) for $s=0$, i.e., $\psi(\Gamma;\Delta t)\equiv p_0^{LZ}(\Gamma;\Delta t) = \Sigma_s A_{0,s}(\Delta t) p_s^{LZ}(\Gamma)$. (8) Repeat steps (4) to (8), now taking the wave function $\psi(\Gamma;\Delta t)$ generated in step (7) as the initial Lanczos vectors $p_0^{LZ}(q)$ and $r_0^{LZ}(q)$ for the next step in the propagation. Repeat this as many times as needed until the desired total time t is reached.

III. THE KICKED HARMONIC OSCILLATOR

As a simple application of the method, we examine the classical and quantum evolution of a Gaussian wave packet moving in the periodically kicked harmonic oscillator with Hamiltonian[7] (in dimensionless units)

$$H(\Gamma) = \frac{p^2}{2}+\frac{q^2}{2}-K\cos q \sum_{n=-\infty}^{+\infty} \delta(t-n\alpha). \tag{3.1}$$

Between kicks, quantum propagation is carried out by means of the schemes outlined in Sec. II. At time $n\alpha$, the effect of the kick is $\exp[iK\cos(q)]$, in coordinate representation, and in phase space is given by

$$\exp\left[iK\cos\left(\frac{q}{2}+i\frac{\partial}{\partial p}\right)\right], \tag{3.2}$$

whose effect on a wave function is calculated following the methods described in Sec. II. In the numerical calculations, $K=1.0$ and $\alpha=2\pi/4$.

Now, for classical systems, we make use of a method for the determination of the evolution of classical densities which operates backwards in time. In order to find the values of the density $\rho(\Gamma;t)$ we recall that the members of this ensemble follow classical trajectories. Then the amount $\rho(\Gamma;t)$ of the members of the ensemble at the phase point Γ, at time t, is the same one as the amount of members $\rho(\Gamma_0;0)$ that were located at the old point Γ_0 at the earlier time $t=0$. Therefore, in order to determine $\rho(\Gamma;t)$, we just propagate backwards in time the phase point Γ by an amount $-t$, leading to Γ_0, and then we assign the value $\rho(\Gamma_0;0)$, of the initial density, to $\rho(\Gamma;t)$. In a numerical calculation we only need to know the values of the classical density $\rho(\Gamma;t)$ at the points of a given grid in phase space, therefore, we only need to calculate the backwards evolution of the points of the grid. Note that the accuracy of this method is limited only by the accuracy in the determination of classical trajectories. For the periodically kicked harmonic oscillator, these densities are determined by backward propagation of phase points by means of the inverse mapping

$$q_{n-1} = q_n\cos\alpha - p_n\sin\alpha,$$

$$p_{n-1} = q_n\sin\alpha + K\sin(q_n\cos\alpha - p_n\sin\alpha) + p_n\cos\alpha. \tag{3.3}$$

Figure 1 shows snapshots of the quantum evolution of the coherent state in phase space

$$\psi(\Gamma;0) = \frac{1}{\sqrt{2\pi}} e^{[-(q-q_0)^2/4-(p-p_0)^2/4+i(qp_0-pq_0)/2]}, \tag{3.4}$$

centered at $(p_0,q_0)=(4,0)$. Figure 1 shows density plots of the square magnitude of the phase space wave function at time $t=0$ as well as just before the kicks 6, 12, and 18. In darker regions the probability density is higher than in lighter ones. In order to get a better understanding of the pattern formation of the wave function in Fig. 1, we can make a similar propagation in the classical domain. We can take, as the classical analog to the initial quantum density, the Gaussian density

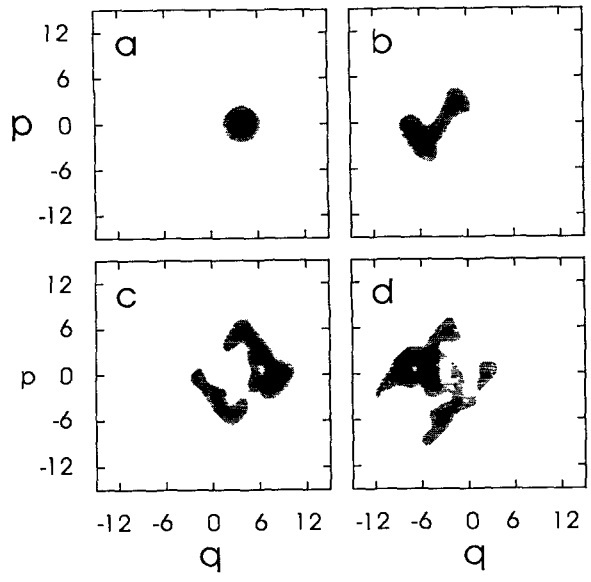

FIG. 1. Snapshots of the quantum dynamics of the coherent state, in phase space, which moves in the periodically kicked harmonic oscillator potential. Probability densities at times (a) 0, and just before the kicks (b) 6, (c) 12, and (d) 18.

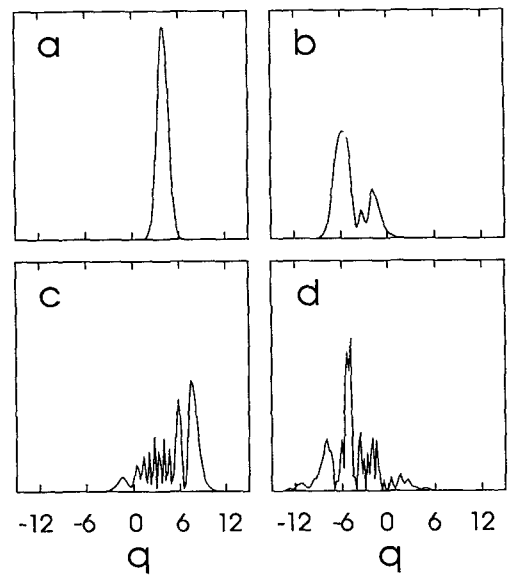

FIG. 3. Snapshots of the quantum dynamics of the coherent state, in coordinate space, which moves in the periodically kicked harmonic oscillator potential. Probability densities at times (a) 0, and just before the kicks (b) 6, (c) 12, and (d) 18.

$$\rho(\Gamma;0)=\frac{1}{2\pi}e^{-(q-q_0)^2/2-(p-p_0)^2/2}, \tag{3.5}$$

also centered at $(p_0,q_0)=(4,0)$ and propagate it in time, which is shown in Fig. 2. Very few of the elements of the classical ensemble lie on the stochastic web compared with the ones that occupy the regions of regular motion, and therefore, stochastic diffusion is very small in the classical system. However, comparison between the densities of Figs. 1 and 2, reveals that the quantum density follows classical motion until stochastic diffusion takes precedence and dominates the dynamics of the system. The quantum density becomes large in regions that will facilitate diffusion.

In Fig. 3 we show snapshots, at the same times as in Figs. 1 and 2, of the quantum evolution of the coherent state in coordinate representation. It was suggested[4] that the classical analog to $|\psi(q;t)|^2$ is the average over p of the classical density $\rho(\Gamma;t)$, i.e., $\rho(q;t)=\int_{-\infty}^{+\infty} dp\ \rho(\Gamma;t)$. This average is shown in Fig. 4. Even though we can observe

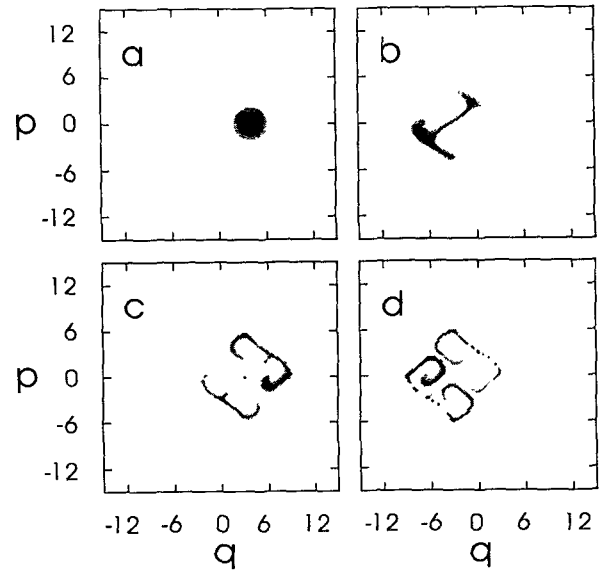

FIG. 2. Snapshots of the classical dynamics of the Gaussian density equivalent to the coherent state of Fig. 1. Probability densities at times (a) 0, and just before the kicks (b) 6, (c) 12, and (d) 18.

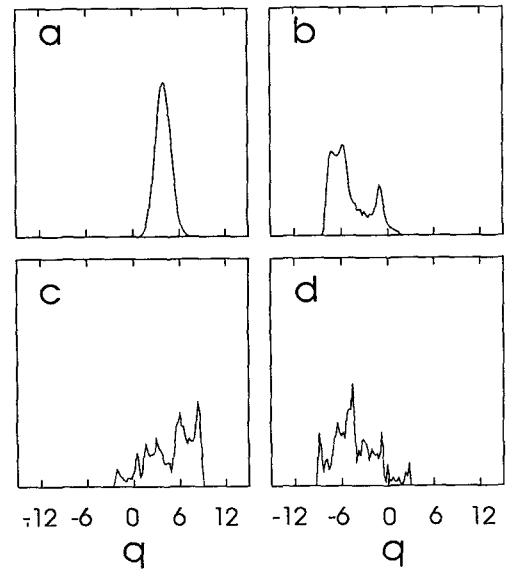

FIG. 4. Snapshots of the average over p of the classical density of Fig. 2. Probability densities at times (a) 0, and just before the kicks (b) 6, (c) 12, and (d) 18.

that the coordinate quantum density follows classical behavior up to some point in time and then departs from it; what happens to the wave packet is better understood if the dynamics is analyzed in phase space.

IV. CONCLUDING REMARKS

This algorithm provides with an accurate way to generate information about quantum wave packet dynamics in phase space with the possibility of (i) projecting it onto either position or momentum space,[4] or (ii) comparing it directly to the classical dynamics of the same probability distribution. Time evolution is accomplished within the Schrödinger picture; therefore, unlike Wigner of Husimi distributions, all of the quantities involved in the calculation have a clear physical meaning, avoiding unnecessary complications. Finally, this phase space representation implements a self-consistent theoretical framework for generating quantum dynamics completely in phase space, without recourse to the position or momentum representations. As a tool for gaining insight into the correspondence between classical and quantum mechanics, it might prove extraordinarily useful.

ACKNOWLEDGMENTS

We would like to acknowledge support from CONACyT and SNI, México.

[1] E. Wigner, Phys. Rev. **40**, 749 (1932); M. Hillery, R. F. O'Connell, M. O. Scully, and E. P. Wigner, Phys. Rep. **106**, 121 (1984), and references therein.

[2] K. Husimi, Proc. Phys. Math. Soc. Jpn. **22**, 264 (1940); *Coherent States*, edited by J. R. Klauder and B. S. Skagerstum (World Scientific, Singapore, 1985), and references therein.

[3] K. Takahashi, J. Phys. Soc. Jpn. **57**, 442 (1988); Prog. Theor. Phys. Supple. No. 98, 109 (1989); Go. Torres-Vega, J. Phys. Soc. Jpn. **60**, 714 (1991).

[4] Go. Torres-Vega and John H. Frederick, J. Chem. Phys. **93**, 8862 (1990); Phys. Rev. Lett. **67**, 2601 (1991).

[5] W. A. Wassam, Jr. and Go. Torres-Vega, Chem. Phys. Lett. **134**, 355 (1987); J. Chem. Phys. **88**, 1837 (1988); W. A. Wassam, Jr., J. Nieto-Frausto, and Go. Torres-Vega, *ibid.* **88**, 1876 (1988); W. A. Wassam, Jr., Go. Torres-Vega, and A. Balderas-López, *ibid.* **90**, 7611 (1989); W. A. Wassam, Jr. and Go. Torres-Vega, Phys. Rev. A **42**, 1693 (1990).

[6] C. Leforestier *et al.*, J. Comput. Phys. **94**, 59 (1991). R. Riedinger and M. Benard, J. Chem. Phys. **94**, 1222 (1991); T. J. Park and J. C. Light, *ibid.* **85**, 5870 (1986).

[7] G. P. Berman, V. Yu. Rubaev, G. M. Zaslavsky, Nonlinearity **4**, 543 (1991); G. M. Zaslavskii, M. Yu. Zakharov, R. Z. Sagdeev, D. A. Usikov, and A. A. Chernikov, Sov. Phys. JETP **64**, 294 (1986).