Gaussian wave-packet dynamics: Semiquantal and semiclassical phase-space formalism

Arjendu K. Pattanayak and William C. Schieve
Department of Physics and Ilya Prigogine Center for Studies in Statistical Mechanics & Complex Systems, The University of Texas, Austin, Texas 78712
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Gaussian wave packets are a popular tool for semiclassical analyses of classically chaotic systems. We demonstrate that they are extremely powerful in the semiquantal analysis of such systems, too, where their dynamics can be recast in an extended potential formulation. We develop Gaussian semiquantal dynamics to provide a phase-space formalism, and construct a propagator with desirable qualities. We qualitatively evaluate the behavior of these semiquantal equations, and show that they reproduce the quantal behavior better than the standard Gaussian semiclassical dynamics. We also show that these semiclassical equations arise as non-self-consistent (in $\hbar$) truncations to semiquantal dynamics. This enables us to introduce an extended semiclassical dynamics that retains the power of the Hamiltonian phase-space formulation. Finally, we show how to obtain approximate eigenvalues and eigenfunctions in this formalism, and demonstrate with an example that this works well even for a classically strongly chaotic Hamiltonian.

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I. INTRODUCTION

There has been a recent renewal of interest in the study of the quantum-classical correspondence problem in many fields of physics, termed "postmodern quantum mechanics," in analogy with the postmodern movements in the humanities [1]. These studies are an attempt to understand the characteristics of quantum systems in terms of the dynamics of associated classical systems [2,3]. If the classical system is obtained in the canonical fashion by replacing operators with c numbers, the approach is the usual semiclassical approach. The association here is straightforward only when the classical system is integrable: the invariant torii of the classical phase space provide the Einstein-Brillouin-Keller (EBK) quantization rules [4]. Matters are substantially more complicated when the classical system is nonintegrable, which is the more general case. It is this $\hbar \to 0$ limit of the quantum mechanics of systems where the classical ($\hbar \equiv 0$) dynamics are chaotic that is not well understood, and where the recent focus has largely centered [5–8]. In particular, there has been work examining the statistical properties of the spectrum of such systems [6] and the remarkable calculation method known as the Gutzwiller trace formula, which says that the eigenvalues of the quantum system arise as poles in a weighted sum over the unstable periodic orbits of the classical system [5].

Chaos in classical mechanics is best observed in phase space, using techniques such as Poincaré sections. Hence, alongside the spectrum, there have been studies which attempt to associate the complex structures of a classically chaotic phase space with the eigenfunctions of the quantum system. These have included the study of "scars," which are the intensity peaks in an eigenfunction along the unstable periodic orbits of the classical system [9,10]. This idea also figures in the association of localized eigenstates with structures such as invariant stable and unstable manifolds [11] and cantori (Birkoff-Gustavson quantization [12]).

Neither quantum mechanics nor semiclassical mechanics has a standard phase space; all the analyses above must, perforce, carry out calculations in Hilbert space and then project onto the classical phase space using "symbols" such as the Wigner distribution function or the Husimi distribution function [13]. This makes a direct interpretation of the results, and the association of quantum properties with classical structures all that more difficult.

There exists, however, another systematic approach to associating quantum mechanics with a classical system. This may be motivated in many ways, the simplest being the time-dependent variational principle (TDVP). This approach starts with the variational restriction of Schrödinger's equation to a subspace of the full Hilbert space. It can be shown that in this approach, one always obtains a "classical" phase space, where the dimensions of the phase space correspond to the wave function parameters. One can then derive and study the approximate (variationally guessed) dynamics of the wave function in a straightforward manner. Since this technique starts from the quantum Hamiltonian, with no reference to the classical system, and can be shown to exist even for systems without a well-defined classical dynamics, it has been termed semiquantal dynamics [14,3]. In this paper we start with this semiquantal approach; we now sketch the motivation for developing it.

Semiquantal dynamics studies a classical system (different from the canonical one) to be able to understand the quantum system. Since these dynamics derive as a variationally restricted form of the Schrödinger equation, it follows that as the size of the Hilbert space accessed is increased, the full quantum dynamics will be more closely approximated by the classical system thus obtained. (We

point out that most numerical work involving "exact" quantum mechanics uses a superficially similar argument, wherein the wave function is expanded in a basis set of finite size. There are fundamental differences between the two approaches; in particular, even when the Hilbert space is inherently noncompact, as in the systems we consider, basis-set truncations are a finite-dimensional restriction to a *compact* subset of the Hilbert space whereas the semiquantal restriction is to a noncompact space.) There is hence intrinsic value in understanding these approximate dynamics. Further, as we will show, classical and semiclassical mechanics can be derived as special limits or truncations of semiquantal mechanics. This route thus provides a smooth transition, in principle, between the two extremes of the classical limit and the fully quantal system. The transition is made without, at any stage, sacrificing the access to the considerable formal power of a classical phase space. It therefore constitutes an alternative way to the understanding of the quantum-classical correspondence question. This provides the formal motivation; since semiclassical dynamics is contained within semiquantal dynamics, the approach supplements the semiclassical procedure without being detached from it. Secondly, recognizing the connection between semiclassical and semiquantal dynamics enables us to propose a Hamiltonian semiclassical dynamics, which combines the advantages of both approaches. All the formalism of semiquantal dynamics carries over to this Hamiltonian semiclassical dynamics; this is our practical motivation.

Our discussion of semiquantal dynamics in this paper will be through the use of coherent states [15–17]. These arise naturally in semiclassical limits and also in the limit $N \to \infty$ where N is the number of degrees of freedom of a quantum system [18,19]. Coherent states come in various flavors, and can be constructed in any quantum system if the dynamical group and the algebra are specified [20–22]. Their simplest version is in ordinary quantum mechanics with a Hamiltonian $\hat{H} = \hat{p}^2/2 + V(\hat{x})$; they are Gaussian wave packets. We work with this particularization; however, most of the ideas are constructively generalizable.

Our presentation is organized as follows: in the next section we review the derivation of the semiquantal dynamics of Gaussian wave packets. In Sec. III, we derive the standard semiclassical dynamics of Gaussians, following the work of Heller [23]. We then show explicitly that those dynamics, derived as consistent truncations in derivatives of the Hamiltonian, are not self-consistent truncations in the moments of the wave packet. We thus propose an extended semiclassical dynamics "midway" between these semiclassical and semiquantal dynamics, which retains the Hamiltonian formulation, and hence constitutes a Hamiltonian semiclassical dynamics. We include a qualitative discussion of the comparative validity of these three dynamics in various regions of a classically chaotic phase space, and argue that the approaches developed in this paper improve upon the dynamics derived by Heller. In Sec. IV we then develop the formalism of the phase-space construction, including the explicit representation of arbitrary wave functions and of the propagator. Finally, we show how to obtain approximate eigenvalues and eigenfunctions in this formalism, and demonstrate with an example that this works well even for a classically strongly chaotic Hamiltonian; we conclude with a short summary.

II. SEMIQUANTAL DYNAMICS OF GAUSSIAN WAVE PACKETS

The basic idea behind the use of Gaussian wave packets relies on the following [24,23,25].

(1) Since Gaussians are their own Fourier transform, they are well behaved in phase space and their dynamics has an invariant meaning; unlike the WKB method and the Van Vleck propagator [5], there are no singularities that have to be dealt with by using "matching formulas," etc.

(2) Their dynamics are simply parametrized by the c-number variables that specify the centroid (average variables) and spread (fluctuation variables).

(3) They form an overcomplete set; an arbitrary wave function can be expanded in terms of Gaussians (albeit an infinite number of them).

This has led to their use in methods known variously as the time-dependent Gaussian variational approximation [26–28], the time-dependent Hartree-Fock-Boguliobov method, or the squeezed coherent state ansatz. The usual derivation considers the time-dependent variational principle formulation [29,30], wherein one posits the action

$$\Gamma = \int dt \left\langle \Psi, t \left| i\hbar \frac{\partial}{\partial t} - \hat{H} \right| \Psi, t \right\rangle . \tag{2.1}$$

The requirement that $\delta\Gamma = 0$ against independent variations of $\langle\Psi, t|$, and $|\Psi, t\rangle$ yields the Schrödinger equation and its complex conjugate (note that a ray rotation, i.e., $|\Psi, t\rangle \to \exp[i\lambda(t)/\hbar]|\Psi, t\rangle$ leaves the variational equations unchanged). The true solution is approximated by restricting the choice of states to a subspace of the full Hilbert space and finding the path along which $\delta\Gamma = 0$ within this subspace.

While the formal derivation of semiquantal dynamics relies on the TDVP, we review here the alternative derivation of semiquantal dynamics via the Ehrenfest theorem [3,31]; we believe that this is a simpler, somewhat more intuitive approach similar to formulations in nonequilibrium statistical mechanics. It also helps us make the connection with the standard semiclassical dynamics of Gaussian wave packets in a straightforward fashion. The dynamics obtained are the same as in the TDVP approach. We work, for simplicity, with a one-dimensional problem. The extension to multiple dimensions is presented in the Appendix.

Consider, therefore, a particle of unit mass moving in a bounded potential with a Hamiltonian $\hat{H} = \frac{\hat{p}^2}{2} + V(\hat{x})$ (V is assumed analytic in $\hat{x}$ and $\hat{O}$ denotes operators). Accordingly, the equations of motion for the centroid of a wave packet are

$$\frac{d}{dt}\langle\hat{x}\rangle = \langle\hat{p}\rangle , \tag{2.2}$$

$$\frac{d}{dt}\langle\hat{p}\rangle = -\left\langle\frac{\partial V(\hat{x})}{\partial x}\right\rangle, \tag{2.3}$$

where the $<>$ indicate expectation values. If V is at most quadratic in $\hat{x}$ then the $<>$ factor;

$$\left\langle\frac{\partial V(\hat{x})}{\partial x}\right\rangle = \left.\frac{\partial V}{\partial x}\right|_{\langle\hat{x}\rangle}, \tag{2.4}$$

and the centroid therefore follows the classical trajectory.

The classical equations of motion do not hold for the centroid in the case of nonlinear gradients, however, and to study such systems we expand in Taylor series around $\langle\hat{x}\rangle$ and $\langle\hat{p}\rangle$. The expansions are of the form

$$\langle F(\hat{u})\rangle = \frac{1}{n!}\langle\Delta u^n\rangle F^{(n)}, \quad n \geq 0 \tag{2.5}$$

where $F^{(n)} = (\partial^n F/\partial u^n)|_{\langle\hat{u}\rangle}, \Delta u = \hat{u} - \langle\hat{u}\rangle$ (we use the repeated index summation convention throughout this section of the paper unless otherwise specified). We note that if all the terms in the expansion are retained, Eq. (2.5) is an identity. Using this expansion and commutation rules of operators, we can generate a series of moment equations. In general these are infinite in number; an arbitrary distribution (wave packet) is completely specified only if all moments are known. We have little interest in the entire wave function and it would suffice to keep track only of $\langle\hat{x}\rangle$ and $\langle\hat{p}\rangle$, thus creating an "Ehrenfest phase space". The convergence properties of the infinite hierarchy are not well understood; it cannot be (or at least has not been) reduced in general.

A possible way [33] of obtaining a finite set of equations is to adopt a Hartree-like approach, requiring that all n-point functions be expressible in terms of the one- and two-point functions. This is equivalent to assuming that the wave packet is a normalized squeezed coherent state [32] of the form

$$\Psi(q,t) = (2\pi\mu)^{-\frac{1}{4}}\exp\left\{i[A(q-x)^2 + p(q-x)]\right\} \tag{2.6}$$

and implies the relations

$$\langle\Delta x^{2m}\rangle = \frac{(2m)!\mu^m}{m!2^m} \text{ (no summation)}, \tag{2.7}$$

$$\langle\Delta x^{2m+1}\rangle = 0, \tag{2.8}$$

$$4\mu\langle\Delta p^2\rangle = \hbar^2 + \alpha^2, \tag{2.9}$$

$$\langle\Delta x\Delta p + \Delta p\Delta x\rangle = \alpha, \tag{2.10}$$

where

$$A = \frac{1}{4\mu}(i+\alpha). \tag{2.11}$$

(This assumption is the same as that of the TDVP: the wave packet is restricted to a given subspace.) This yields the equations

$$\frac{dx}{dt} = p, \tag{2.12}$$

$$\frac{dp}{dt} = -\frac{\mu^m}{m!2^m}V^{(2m+1)}(x), \quad m = 0,1,\ldots \tag{2.13}$$

$$\frac{d\mu}{dt} = \alpha, \tag{2.14}$$

$$\frac{d\alpha}{dt} = \frac{\hbar^2+\alpha^2}{2\mu} - \frac{\mu^m}{(m-1)!2^{m-2}}V^{(2m)}(x), \quad m = 1,2,\ldots . \tag{2.15}$$

The system is now reduced to the dynamics of x, p, μ, and α (where we write x, p for $\langle\hat{x}\rangle, \langle\hat{p}\rangle$) and are exactly those derived from the action principle. To see the equivalence, equate the variables x, p, μ, and α with $q, p, \hbar G$, and $4\hbar G\Pi$, respectively, of Refs. [26,27,34]. (Note that we do not, for the moment, have an equation for the phase of the wave packet — this will be derived later.)

If we now introduce the change of variables $\mu = \rho^2$, and $\alpha = 2\rho\Pi$, Eqs. (2.12)–(2.15) transform to [35]

$$\frac{dx}{dt} = p, \tag{2.16}$$

$$\frac{dp}{dt} = -\frac{\rho^{2m}}{m!2^m}V^{(2m+1)}(x), \quad m = 0,1,\ldots \tag{2.17}$$

$$\frac{d\rho}{dt} = \Pi, \tag{2.18}$$

$$\frac{d\Pi}{dt} = \frac{\hbar^2}{4\rho^3} - \frac{\rho^{2m-1}}{(m-1)!2^{m-1}}V^{(2m)}(x),$$

$$m = 1,2,\ldots . \tag{2.19}$$

Remarkably, these new variables form an explicit gradient system, yielding an *extended potential system* as our approximation to the Hilbert space. The classical degrees of freedom are now the "average" variables x, p and the "fluctuation" variables ρ, Π, respectively; the associated Hamiltonian is

$$H_{\text{ext}} = \frac{p^2}{2} + \frac{\Pi^2}{2} + V_{\text{ext}}(x,\rho)\ , \tag{2.20}$$

$$V_{\text{ext}}(x,\rho) = V(x) + \frac{\hbar^2}{8\rho^2} + \frac{\rho^{2m}}{m!2^m}V^{(2m)}(x)\ ,$$

$$m = 1,2,\ldots \tag{2.21}$$

where the subscript ext indicates the "extended" potential and Hamiltonian.

This formulation is very interesting and possibly quite powerful; the extended potential provides a simple visualization of the geometry of the semiquantal space. We may thus get a qualitative idea of the semiquantal dynamics before proceeding to detailed analysis.

We note here, for instance, the following points.

(1) Both the fluctuation and average variables are treated on the same footing and the phase space is dimensionally consistent: ρ has the dimensions of length and Π that of momentum.

(2) The value of H_{ext} is $< \hat{H} >$ under this approximation, and is conserved.

(3) V_{ext} has an infinite barrier at $\rho = 0$, arising, as appropriate, from the momentum squeezing. Hence "quantum fluctuations" cannot be zero except in the limit $\hbar \to 0$: as stated, there are no caustics in this representation.

(4) V_{ext} is symmetric in ρ corresponding to a choice of sign in $\rho = \sqrt{\mu} = \sqrt{\langle X^2 \rangle}$; the infinite barrier renders the choice one of convenience and of no physical significance.

It is now straightforward to introduce a Poisson bracket on this space:

$$\{f, g\} = \frac{\partial f}{\partial x}\frac{\partial g}{\partial p} + \frac{\partial f}{\partial \rho}\frac{\partial g}{\partial \Pi} - \frac{\partial f}{\partial p}\frac{\partial g}{\partial x} - \frac{\partial f}{\partial \Pi}\frac{\partial g}{\partial \rho}. \quad (2.22)$$

This bracket renders the dynamics into the standard form

$$\dot{y} = \{y, H_{\text{ext}}\} , \quad (2.23)$$

where y represents the phase-space variables x, p, ρ, Π. The rate of change of an arbitrary function $f(y)$ is

$$\frac{df}{dt} = \{f, H_{\text{ext}}\} . \quad (2.24)$$

This Hamiltonian picture for the evolution of the wave-packet parameters is not quite the complete one since, as before, a ray rotation leaves the expectation values unchanged. To determine the overall phase of the wave packet, therefore, consider the Schrödinger equation itself,

$$i\hbar\frac{\partial}{\partial t}|\Phi, t\rangle = \hat{H}|\Phi, t\rangle , \quad (2.25)$$

where

$$|\Phi, t > \equiv \exp[i\lambda(t)/\hbar]|\Psi, t\rangle . \quad (2.26)$$

If we substitute Eq. (2.26) into Eq. (2.25), and take the inner product with $|\Psi, t\rangle$, we get for $\lambda(t)$ the differential equation

$$\frac{d\lambda}{dt} = \left\langle \Psi, t \left| i\hbar\frac{\partial}{\partial t} - \hat{H} \right| \Psi, t \right\rangle . \quad (2.27)$$

The right-hand side of the above equation is the Lagrangian corresponding to the extended Hamiltonian [see (2.1)]. The phase is then just the action function Γ (divided by $\hbar$) and its explicit time derivative is

$$\dot{\lambda} = \frac{\dot{\rho}\Pi - \dot{\Pi}\rho}{2} + p\dot{x} - H_{\text{ext}}. \quad (2.28)$$

It is natural to separate the phase into two parts $\lambda = \lambda_D + \lambda_G$ with the first part

$$\lambda_D = -\int_0^t d\tau \, \langle \hat{H} \rangle = -t \, H_{\text{ext}} \quad (2.29)$$

corresponding to the dynamical phase (i.e., a measure of the time of evolution). The second part is the geometrical phase:

$$\lambda_G = \int_0^t d\tau \left\langle i\hbar\frac{\partial}{\partial \tau} \right\rangle = \int_0^t d\tau \left(\frac{\dot{\rho}\Pi - \dot{\Pi}\rho}{2} + p\dot{x} \right) . \quad (2.30)$$

For the case of cyclic evolution of the wave packet this corresponds to "Berry's phase" [36] of the evolution. It depends only on the geometry of the evolutionary path in phase space since it can be written in the canonical form

$$\lambda_G(C) = \oint_C \mathbf{P} \cdot \mathbf{dQ}, \quad (2.31)$$

where $\mathbf{P} \equiv (p, \Pi)$ and $\mathbf{Q} \equiv (x, \rho)$. Note that the integrand of (2.30) differs from that of (2.31) by a total derivative which vanishes for the closed line integral. The expression for $\lambda_G(C)$ has this simple form because of the Hamiltonian character of semiquantal dynamics. We will use this later for the construction of eigenvalues and eigenfunctions.

The equation for the phase, along with the Hamiltonian equations of motion for the evolution of the wave-packet parameters constitute the semiquantal dynamics of the wave packet. This lies on a space $\mathcal{R}(2N) \times \mathcal{S}(1)$ where $\mathcal{R}(2N)$ is the Cartesian space of dimension $2N$ and $\mathcal{S}(1)$ is the circle. For the case just considered, $N = 2$, the result is completely general, however. Finally, we note that the overall normalization factor for the Gaussian wave function is a trivial function of ρ and does not constitute an independent variable. The normalization is maintained by the evolution.

To summarize, the semiquantal restriction of the dynamics to Gaussian wave packets has taken us from a Hilbert space to an extended phase space and the dynamics are described on this phase space by a generalized Poisson bracket. An arbitrary operator of the Hilbert space may be associated with a function (called its "symbol") through

$$O(y) = \langle y|\hat{O}|y\rangle, \quad (2.32)$$

where $y = (x, p, \rho, \Pi)$ and the $|y\rangle$ are normalized Gaussians serving as the basis set for the association. The dynamics of this symbol are determined by Eq. (2.24): the Heisenberg equations of motion are now represented by Poisson bracket equations. These are not the classical equations of motion, however, since the generator of time translations is not the classical Hamiltonian, but H_{ext}. We emphasize that for the expectation values of operators, the space $\mathcal{R}(2N)$ (the approximation to the projective Hilbert space) suffices for a complete description of the dynamics. The dynamics of the wave function, however, also require the specification of the phase; this is what lives on $\mathcal{R}(2N) \times \mathcal{S}(1)$.

As with any variational principle, these equations are approximations to the same extent as the restriction of the variational space. Similar equations hold for the full space: the actual specification of an appropriate variational wave function may not, of course, be possible.

III. COMPARISON WITH SEMICLASSICAL DYNAMICS

In this section, we first derive the standard semiclassical dynamics of Gaussian wave packets, following Heller [23] (we hence term these dynamics, with apologies to others, Heller's semiclassical dynamics). We demonstrate that though these equations arise as consistent truncations to semiquantal dynamics in derivatives of the Hamiltonian, they are not self-consistent truncations in $\hbar$. We thus are able to introduce an extended semiclassical dynamics; this restores the consistency of the above truncation, and is a Hamiltonian semiclassical dynamics. We finally compare the three approaches — semiquantal dynamics, Heller's semiclassical dynamics, and extended semiclassical dynamics.

We make a preliminary note that any truncation to the sums in Eqs. (2.16)–(2.19) at a specified order in m, say the nth, retains the Hamiltonian structure. Its properties (as developed in the next two sections) thus transfer over to the truncated systems. The only detail that one has to be careful about is the evaluation of the symbols for operators. This consideration and the interpretation of the truncations is simplified by the standard semiclassical ansatz that

$$\langle \hat{x} - \langle \hat{x} \rangle \rangle^2 = \rho^2 = \mathcal{O}(\hbar). \tag{3.1}$$

This implies, therefore, that

$$\langle \hat{p} - \langle \hat{p} \rangle \rangle^2 = \mathcal{O}(\hbar) = \Pi^2. \tag{3.2}$$

The truncations are then to the same order (the nth) in $\hbar$. The calculation of the symbols is straightforward — one proceeds with the computation as if for the full semiquantal dynamics and then retains only terms to the specified order in $\hbar$.

A. Heller's semiclassical dynamics

The semiclassical derivation of the equations of motion for Gaussian wave packets, following Heller [23], makes an expansion around the wave-packet centroid, truncated to second order in derivatives of the Hamiltonian. We make the same simplifications as before; the Hamiltonian is $\frac{\hat{p}^2}{2} + V(\hat{x})$ and we use a one-dimensional wave packet

$$\Psi(q,t) = \exp\left[\frac{i}{\hbar}[(q-x)A(q-x) + p(q-x) + s]\right]. \tag{3.3}$$

The physical meaning of the parameters $p(t), x(t)$ are, as before, $\langle \hat{x}(t) \rangle = x(t), \langle \hat{p}(t) \rangle = p(t)$ and A and s are, in general, complex.

The fundamental approximation is a truncation of the Taylor series expansion of the Hamiltonian as

$$H \approx -\frac{\hbar^2}{2}\frac{\partial^2}{\partial q^2} + V^{(0)} + V^{(1)}(q-x) + \frac{1}{2}V^{(2)}(q-x)^2, \tag{3.4}$$

where $V^{(n)}$ is the nth derivative of $V(\hat{x})$ evaluated at x, as before. This is exact for quadratic potentials, of course. If we insert this, and the wave function above, into Schrödinger's equation, equate coefficients of $(q-x)$, and make the identification $\dot{x} = p$, we recover classical equations of motion for the centroid:

$$\dot{x} = p, \tag{3.5}$$

$$\dot{p} = -V^{(1)}, \tag{3.6}$$

and obtain, for the wave-packet parameters,

$$\dot{A} = -2A^2 - \frac{V^{(2)}}{2}, \tag{3.7}$$

$$\dot{s} = i\hbar A - V(x) - \frac{p^2}{2} + p\dot{x}. \tag{3.8}$$

At this point, using our knowledge of the derivation of semiquantal Gaussian dynamics, we make the transformation

$$s = s_r + is_i, \tag{3.9}$$

$$A = a_r + ia_i = \frac{\Pi}{2\hbar\rho} + i\frac{\hbar}{4\rho^2}. \tag{3.10}$$

These then provide us the equations

$$\dot{s}_r = -\frac{\hbar^2}{4\rho^2} - V(x) - \frac{p^2}{2} + p\dot{x}, \tag{3.11}$$

$$\dot{s}_i = \frac{\Pi}{2\rho}, \tag{3.12}$$

$$\dot{\rho} = \Pi, \tag{3.13}$$

$$\dot{\Pi} = \frac{\hbar^2}{4\rho^3} - \rho V^{(2)}, \tag{3.14}$$

along with

$$\dot{x} = p, \tag{3.15}$$

$$\dot{p} = -V^{(1)} \tag{3.16}$$

as the equations of motion for the wave packet.

It is straightforward to show that s_i is the time-dependent normalization term [23]. The solution for it is $s_i(t) = \frac{1}{2}\ln(\rho)$ modulo a constant; we ignore it hereafter, except to note that it is the same as the semiquantal case. The equation for s_r can be rewritten, using the relationships

$$\rho\dot{\Pi} = \frac{\hbar^2}{4\rho^2} - \rho^2 V^{(2)}, \tag{3.17}$$

$$\dot{\rho}\Pi = \Pi^2, \tag{3.18}$$

as

$$\dot{s}_r = p\dot{x} + \frac{\dot{\rho}\Pi - \dot{\Pi}\rho}{2} - E, \tag{3.19}$$

where

$$E = \frac{p^2}{2} + \frac{\Pi^2}{2} + V(x) + \frac{\hbar^2}{8\rho^2} + \frac{\rho^2}{2}V^{(2)}. \tag{3.20}$$

Note that this equation for the phase is the same as Eq. (2.28) with E replacing $H_{\rm ext}$ and that

$$E = H_{\rm ext}\Big|_{m=1}. \tag{3.21}$$

This system of equations has been used with great success to study semiclassical dynamics by Heller [23] and Littlejohn [25], among others. In particular, it has been used to construct the semiclassical spectra of various sytems, by a method we shall sketch later. Littlejohn has argued [47] that the spectrum thus computed for integrable classical systems is exactly the EBK spectrum. For nonintegrable systems, it provides an alternative to basis-set quantization and the trace formula. The interesting question of the connection between these methods remains an open one.

B. Extended semiclassical dynamics

How does this system compare with the semiquantal system we had derived earlier? It is a simple exercise to show that Eqs. (3.13)–(3.16) above are truncations to $m = 1$ of the semiquantal equations (2.16)–(2.19), *except* for a missing term $\frac{\rho^2}{2}V^{(3)}$ in Eq. (3.16) for $\dot{p}$. The phase, as mentioned, is also a truncation of the semiquantal phase to $m = 1$. The structural correspondence between the two systems is then exact, except that Eq. (3.16) is truncated to $m = 0$ compared to the others.

We have thus demonstrated that the standard equations for the semiclassical dynamics of wave packets correspond to truncations of the semiquantal equations derived earlier. These truncations are to different values in m; there is hence no extended Hamiltonian for these equations and the formalism developed below does not apply. However, it is now easy to construct a semiclassical Hamiltonian.

We restore consistency in the truncation by adding back the "extra" term $\frac{\rho^2}{2}V^{(3)}$, in the equation for $\dot{p}$. This term arises naturally in the expansion around the centroid, but was neglected by the truncation to the second derivative. Hence arguments similar to the above, truncated not in derivatives of the Hamiltonian, but moments of the Gaussian, give us an extended semiclassical Hamiltonian

$$H_{\rm sc} = \frac{p^2}{2} + \frac{\Pi^2}{2} + V(x) + \frac{\hbar^2}{8\rho^2} + \frac{\rho^2}{2}V^{(2)}. \tag{3.22}$$

This Hamiltonian is a truncation of the semiquantal Hamiltonian to $m = 1$ and by the arguments above, to $\mathcal{O}(\hbar)$. This is what we call extended semiclassical dynamics — it lies "midway" between the standard semiclassical dynamics and semiquantal dynamics.

It is now simple to show that these systems contain within themselves the classical limit. If for each system we take the physical limit $\rho, \Pi \to 0$ along with $\hbar \to 0$, we get a Gaussian that corresponds in the limit to a classical point particle, and the dynamics reduce to that of the classical Hamiltonian. Equivalently, we could make the same $\mathcal{O}(\hbar)$ ansatz as before, and take $\hbar \to 0$ to recover the classical equations.

We now compare the three approaches: semiquantal dynamics, Heller's dynamics, and extended semiclassical dynamics, and discuss their validity and utility.

C. Similarity of the three aproaches

We first wish to emphasize that all three approaches are similar in principle. The simplest way of seeing this is to consider their derivation in the Heisenberg picture, which we now sketch. This is a straightforward excercise that we do not belabor here. First rewrite the quantum Hamiltonian as follows:

$$\hat{H} = \frac{\hat{p}^2}{2} + V(\hat{x}) \tag{3.23}$$

$$= \frac{p^2}{2} + p\Delta p + \Delta p^2 + V(x) + \sum_{n=1} \frac{1}{n!}\Delta x^n V^{(n)}, \tag{3.24}$$

where $u = \langle \hat{u} \rangle$, $\Delta u = \hat{u} - u$, and $V^{(n)} = (\partial^n V/\partial x^n)|_{\langle \hat{x} \rangle}$ as usual. Now use this (still exact) form of the Hamiltonian to derive equations of motion for the Heisenberg operators $\hat{x}$, $\hat{p}$, Δx^2, and $\Delta x \Delta p + \Delta p \Delta x$. Having obtained these operator equations turn them into c-number equations by *imposing* a Gaussian ansatz and evaluating the expectation values of these equations in that ansatz. These equations are now the semiquantal equations derived earlier. If, in the above expansion of the potential, we truncate at $n = 2$, and proceed as outlined, again imposing the Gaussian ansatz, we obtain Heller's equations. A truncation at $n = 3$ yields the extended semiclassical dynamics. All three approaches are hence identical in nature. In particular, we note that all three are *local* expansions around the centroid. The global Hamiltonians $H_{\rm ext}$ and $H_{\rm sc}$ are effective Hamiltonians that govern the wave packet motion and are obtained by no more a global approximation than for the standard semiclassical case. The only point to consider is that the Gaussian ansatz seems "natural" in the quadratic approximation; however, as far as the real system is concerned, it is just as valid (or invalid) a constraint for all the approaches.

We also note that both the semiquantal and extended semiclassical dynamics can also be derived as examples of "symbol" dynamics [37]. In this approach, we project out a c-number symbol of the Hamiltonian (or its local quadratic approximation, respectively) in appropriate states (the squeezed coherent states), and treat this as a classical Hamiltonian, with an eye to understanding the quantum behavior. Heller's semiclassical dynamics are similar, but not Hamiltonian because the projection onto the squeezed coherent states is done after the dynamics are derived, instead of before, leading to an inconsistency in the truncation.

For the semiclassical approaches, a time scale of validity [38] for the ansatz may be estimated and is normally

argued to be $\mathcal{O}(\ln(\hbar^{-1}))$, the "log time". Recent work [1], however, argues that this may be unduly pessimistic. Further, as we demonstrate below, many *qualitative* features of quantum behavior can certainly be reproduced by these dynamics.

D. Qualitative behavior in model potentials

We now discuss how the qualitative behavior of these approaches conforms to intuition. We examine these dynamics in a few simple model Hamiltonians corresponding to local neighborhoods of a classically chaotic phase space. We start with the corresponding quantal Hamiltonian and derive from it the various dynamics. We then consider the behavior of wave packets that start centered or slightly displaced from the origin in these model potentials. We will not go into the details; they can be easily worked out from the results of the last two sections.

We first consider the more forgiving case of elliptic regions (equivalently, in general, an anharmonic well) where such a Gaussian ansatz might be expected to work. Our model Hamiltonian is

$$\hat{H} = \frac{\hat{p}^2}{2} + \hat{x}^{2n} \tag{3.25}$$

(where we consider $n > 1$ since all three dynamics are identical and exact in quadratic potentials). The potential is bounded in $\hat{x}$ and its highest nonvanishing even derivative hence is positive. For the semiquantal dynamics, the form of the semiquantal Hamiltonian then guarantees that ρ always remains bounded as well; this is physically reassuring. However, this fails for the two semiclassical systems. In particular, for the simple $\hat{x}^4$ potential, the dynamics for ρ for both semiclassical systems are unphysically unstable. This is easiest seen by considering the wave packet centered at the origin $[x(t) \equiv x(0) = 0]$ where $V^{(2)}$ identically vanishes. The situation improves when the wave packet is displaced from the origin though the dynamics are still asymptotically unstable with the extended semiclassical system performing better than Heller's dynamics due to the coupling between the average and fluctuation variables.

We now look at hyperbolic regions. If the model potential is unbounded, the semiquantal approach *will* always give unstable solutions. This is not a breakdown of the method, but only as appropriate: an unbounded potential *must* give a spreading wave packet. However, note that for the unbounded Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2} + a\hat{x}^2 - \hat{x}^4 \tag{3.26}$$

($a > 0$) both Heller's dynamics and the extended semiclassical dynamics will be deceived into remaining stable with a centered wave packet except in the singular limit $a \equiv 0$. This persists even for small displacements with finite a for Heller's dynamics. For the extended semiclassical system the coupling of the average and fluctuation dynamics kicks in to drive the wave packet away from the origin and give a spreading wave packet.

We turn to the more appropriate case of hyperbolicity embedded in a bounded potential, with a model Hamiltonian hence, say, of the form

$$\hat{H} = \frac{\hat{p}^2}{2} - \hat{x}^2 + \hat{x}^4. \tag{3.27}$$

If we once again start centered at the origin, the semiquantal approach provides for a growing wave packet that is ultimately reigned in by the quartic term, as is the appropriate physical behavior. Both semiclassical systems will again be deceived — in this case into rapidly spreading without a bound. With small displacements, the semiquantal behavior is unaltered. Both semiclassical dynamics improve marginally and can be stabilized, but in general remain unstable.

These discussions demonstrate that in these model potentials, the semiquantal approach improves substantially upon Heller's semiclassical Gaussian ansatz, while the extended semiclassical approach does so at least marginally. The arguments above are not the whole story, of course, since the wave packet will in general be moving through these regions of phase space instead of being statically centered there, but capture the essential features of the expected behavior. It should be clear that the coupling between the fluctuation and average variables is in general not simple to analyze. This is a physically valid coupling and has its advantages, as just argued, but may lead to behavior which has to be interpreted carefully.

E. Interpretation

In a recent paper [3], it was demonstrated that the semiquantal dynamics of the double-well system are chaotic, even though the classical and quantum problem are understood to be regular. This is to be viewed largely as a formal result: the transition between classical and quantum dynamics is not quite as straightforward as is usually understood; quantal effects do *not* always suppress chaotic behavior. Further, an examination of the range of parameters and initial conditions within which chaos appears indicates the following realistic interpretation. The dynamics of the wave packet both deep within either well, and at energies such that the system looks essentially like an anharmonic well, are regular. It is in the transition regime, at energies close to the classical unstable fixed point and separatrix, that the dynamics are complicated. It is the interplay between classically unstable behavior and quantal tunneling effects that are reflected in the observed chaotic tunneling. By the methods outlined below, this would give rise to a rather complicated spectrum in this region — a wholly appropriate result.

We reiterate that uncoupling the variables, thus yielding Heller's semiclassical dynamics, would do worse in reflecting the quantal behavior in this system, as outlined above. Irrespective, it is obvious that this sort of behavior needs to be better understood. The discussion in the rest of the paper leads us towards doing so: matters do

not end at having observed chaos or lack thereof in these classical-like dynamics. This structure is reflected in the spectrum and other pure quantal properties.

Considering all these factors, therefore, we argue for the use of semiquantal and extended semiclassical dynamics in exactly the same situations as Heller's semiclassical Gaussian dynamics. Wave-packet dynamics must ultimately break down in the presence of chaotic classical dynamics; however, the two Hamiltonian approaches should better reproduce the quantal behavior and thus improve upon the already remarkable results of Heller's semiclassical dynamics. The spirit of these approaches, we believe, is truly semiclassical; the Hamiltonian formulations make them particularly powerful. This is developed in the following.

IV. PHASE-SPACE PROPERTIES OF THE REPRESENTATION

To understand formal power and properties of the Hamiltonian formulations constructed above, we briefly discuss the properties of coherent states using the standard notation, simplifying our discussion considerably; we relate the notations later.

If we consider the non-Hermitian operator

$$\hat{a} = \frac{1}{\sqrt{2}}(\hat{x} + i\hat{p}) \ , \tag{4.1}$$

with

$$[\hat{a}, \hat{a}^\dagger] = 1 \tag{4.2}$$

we can construct the states $|\alpha\rangle$ defined as the eigenstates of $\hat{a}$,

$$\hat{a}|\alpha\rangle = \alpha|\alpha\rangle \ . \tag{4.3}$$

These states are minimum uncertainty Gaussians, known as coherent states. Due to the non-Hermiticity of $\hat{a}$, they are not orthonormal, nor are their eigenvalues real. The properties of coherent states [20,39] are well known; we mention two we use later. Coherent states have the following representation in terms of the number states, the energy eigenstates of the harmonic oscillator (in this case with $m = \hbar = \omega = 1$):

$$|\alpha\rangle = \sum e^{(-\frac{1}{2}|\alpha|^2)} \frac{\alpha^n}{\sqrt{n!}} |n\rangle \tag{4.4}$$

and they form an overcomplete basis set.

The coherent states do not include all Gaussians: we parametrize the space of all Gaussians (for a one-dimensional system) using four real parameters x, p, ρ, Π whereas the coherent states use just two real parameters,

$$\alpha = \alpha_1 + i\alpha_2. \tag{4.5}$$

To understand the extra parameters, we consider squeezed coherent states. We follow Yuen [40] in introducing an operator $\hat{b}$,

$$\hat{b} \equiv \mu\hat{a} + \nu\hat{a}^\dagger \ , \tag{4.6}$$

with the c numbers μ, ν satisfying

$$|\mu|^2 - |\nu|^2 = 1. \tag{4.7}$$

The real and imaginary parts of this equation imply that μ and ν correspond to two independent real parameters. It can be shown that

$$[\hat{b}, \hat{b}^\dagger] = 1, \tag{4.8}$$

and therefore that the transformation (4.6) is a linear canonical transformation. This provides $\hat{b}$ with properties identical to those of $\hat{a}$. In particular, there exist a set of eigenstates of $\hat{b}$ (which we denote $|\beta\rangle_q \equiv |\alpha_1, \alpha_2, \mu, \nu\rangle$) equivalent to the states $|\alpha\rangle$: these are the squeezed coherent states. These states include the coherent states as a particular case, where $\mu = 1$ and $\nu = 0$, and in general include all Gaussian wave functions. The independent parameters $\alpha_1, \alpha_2, \mu, \nu$ provide us with our four-parameter representation.

If we consider the self-adjoint operators $\hat{a}_1, \hat{a}_2$ defined through $\hat{a} = \hat{a}_1 + i\hat{a}_2$ (corresponding to the quadrature components) we see that

$$\langle \Delta a_1^2 \rangle = \langle \Delta a_2^2 \rangle = \frac{1}{4} \tag{4.9}$$

$(\Delta m = \hat{m} - \langle \hat{m} \rangle$) where all expectation values are taken with respect to the states $|\alpha\rangle$. Since $[\hat{a}_1, \hat{a}_2] = \frac{i}{2}$, the uncertainty principle constraint on $\hat{a}_1, \hat{a}_2$ is

$$\langle \Delta a_1^2 \rangle \langle \Delta a_2^2 \rangle \ \geq \frac{1}{16}. \tag{4.10}$$

The minimum uncertainty states $|\alpha\rangle$ have equal uncertainty in the two quadrature components; their correlation is minimal:

$$\langle \Delta a_1 \Delta a_2 \rangle = \frac{i}{4}. \tag{4.11}$$

If we evaluate the same quantities in the states $|\beta\rangle_q$, we get

$$\langle \Delta a_1^2 \rangle_q = \frac{1}{4}|\mu - \nu|^2, \tag{4.12}$$

$$\langle \Delta a_2^2 \rangle_q = \frac{1}{4}|\mu + \nu|^2, \tag{4.13}$$

$$\langle \Delta a_1 \Delta a_2 \rangle_q = \frac{1}{4} i(\mu^* \nu - \nu^* \mu + 1). \tag{4.14}$$

The squeezed states, therefore, "squeeze" one quadrature component at the expense of the other, and in general have correlations between the two components. However, there is a linear canonical transformation of variables ($\hat{a} \rightarrow \hat{b}$) such that the new quadrature components $\hat{b}_1, \hat{b}_2$ satisfy the minimum uncertainty equation in these states. We use here Eqs. (4.12) – (4.14) to make the connection with our previous notation. x and p are the same as above, and

$$\rho^2 = \frac{1}{2}|\mu - \nu|^2, \tag{4.15}$$

$$\rho\Pi = \frac{1}{2}i(\mu^*\nu - \nu^*\mu). \tag{4.16}$$

We now use these properties for the representation of arbitrary wave functions.

We have so far considered the dynamics of a wave packet that is constrained to remain Gaussian: this yields trajectories in a generalized phase space. However, it is also possible to construct propagators for arbitrary wave functions. In this case we have to consider functions on this phase space. We use the fact that it is possible to associate with every operator a symbol as in Eq. (2.32) and choose $\hat{O}$ to be the density matrix (or projection operator) $\hat{P} = |\Psi\rangle\langle\Psi|$. We now associate with every wave function (up to an arbitrary global phase) a real positive function

$$\mathcal{P}(y) = \langle y|\Psi\rangle\langle\Psi|y\rangle \ . \tag{4.17}$$

This function is an extended Q representation (or extended Husimi function): we now demonstrate this, and touch upon its relevant properties.

With the coherent states as defined above, the Q function corresponding to a projection operator $\hat{P}$ is defined as [39]

$$Q(\alpha,\alpha^*) \equiv \frac{1}{\pi}\langle\alpha|\hat{P}|\alpha\rangle \ . \tag{4.18}$$

The Husimi function is defined in almost the same way, up to the normalization of the coherent states. Since the normalization of the coherent states is well defined, we use the terms interchangeably.

The Q function is essentially a probability distribution function, with useful properties for the computation of expectation values of operators, etc. [39]. We do not use it directly, however, since the dynamics we have derived do not leave coherent states invariant. Hence the dynamics in the Q representation are awkward and the Hamiltonian formulation cannot be used to advantage. However, the space of squeezed coherent states is invariant under the derived dynamics. We take advantage of this by defining, as an intermediate tool, an extended Q function over the space of squeezed coherent states. The semiquantal dynamics of this can be easily handled — we detail this below. The Q function (and the projection operator itself) can also be extracted from the extended Q function in a straightforward fashion — we first take care of this.

We define the extended Q function $Q_{\rm ext}(\alpha,\mu,\nu)$ as

$$Q_{\rm ext}(\alpha,\mu,\nu) = \langle\alpha,\mu,\nu|\hat{P}|\alpha,\mu,\nu\rangle \ , \tag{4.19}$$

where we absorb normalization constants into the definition of the states. We have also suppressed the dependence of $Q_{\rm ext}$ on the complex conjugates of α,μ,ν. This function is precisely the representation we have derived through semiquantal dynamics: $Q_{\rm ext} \equiv \mathcal{P}$. It is defined over a four-parameter space $\alpha_1,\alpha_2,\mu,\nu$ and has the obvious and convenient property that a slice [41] of it, taken at $\mu = 1, \nu = 0$, reduces to the Q function:

$$Q_{ext}(\alpha,\mu,\nu)\Big|_{\mu=1,\nu=0} = Q(\alpha,\alpha^*). \tag{4.20}$$

This, and other expressions involving μ,ν, should be regarded as essentially formal ones indicating the various properties of the representation, rather than to be used for computational purposes. For that, we work directly in the x,p,ρ,Π representation.

We now come to the physical meaning of the extended Q function: it is a generalized probability distribution function defined on this semiquantal phase space. To see this, we consider the properties of the Q function, which we can obtain as a slice of $Q_{\rm ext}$. In particular, the definition Eq. (4.18) can be used to show that

$$\int d^2\alpha\, Q(\alpha,\alpha^*) = 1 \tag{4.21}$$

and that the average of *antinormally* ordered products of the creation and destruction operators is

$$\langle\hat{a}^r(\hat{a}^\dagger)^s\rangle = \int d^2\alpha\, \alpha^r(\alpha^*)^s Q(\alpha,\alpha^*). \tag{4.22}$$

These are properties similar to those of classical probability distribution functions. There are many discussions [13,39,14] on the merits of the Q representation versus those of others like the Wigner function and the P representation. Each has been critically examined for its merits and demerits. We confine ourselves to the observation that in most cases it can be easily shown that one can move between the various representations with the help of well-defined transformations, and that the representations have properties which render each convenient for different calculations. We do, however, want to address the popular misconception that the Q function (or the Husimi function) is an inadequate representation in that it cannot be used to reconstruct the original projection operator. As is known in the quantum optics literature, $Q(\alpha,\alpha^*)$ can be expressed as an absolutely convergent power series in α and α^*. To wit, since $Q(\alpha,\alpha^*)$ can be written as

$$Q(\alpha,\alpha^*) = e^{(-\alpha\alpha^*)}\sum_{n,m}\frac{\langle n|\hat{P}|m\rangle}{\pi\sqrt{n!m!}}\alpha^m(\alpha^*)^n, \tag{4.23}$$

we can use the fact that for any projection operator $\hat{P}$, the number state matrix elements satisfy

$$|\langle n|\hat{P}|m\rangle| \le 1 \tag{4.24}$$

to show that the double power series for $Q(\alpha,\alpha^*)$ is absolutely convergent (see Gardiner [39] for details).

If we write this power series as

$$Q(\alpha,\alpha^*) = \sum_{n,m} Q_{n,m}\alpha^m(\alpha^*)^n, \tag{4.25}$$

the number state matrix elements of $\hat{P}$ can be explicitly written as

$$\langle n|\hat{P}|m\rangle = \pi\sqrt{n!m!}\sum_r Q_{n-r,m-r}. \tag{4.26}$$

Alternatively, $\hat{P}$ may be written as a *normally ordered*

power series

$$\hat{P} = \pi \sum Q_{n,m}(\hat{a}^\dagger)^n \hat{a}^m. \tag{4.27}$$

Thus the projection operator is obtained by replacing $\alpha^m(\alpha^*)^n$ in the power series for $Q(\alpha,\alpha^*)$ by the corresponding *normally ordered* product of the operators $\hat{a}$ and $\hat{a}^\dagger$.

This discussion therefore provides us with a way of constructing an extended Q function for any wave function. We have also shown how to reconstruct the corresponding density matrix (or projection operator) from $Q_{\rm ext}$: first project down onto $Q(\alpha,\alpha^*)$, and then use the power series expansion mentioned above. It should be pointed out that this is a consequence of the overcompleteness of Gaussians. A representation in a basis set with the usual properties of orthonormality would not permit this reconstruction.

We also note that the eigenstates of x and p are contained as asymptotic limits of the squeezed coherent states, hence the reduced position and momentum distribution functions of the wave function $|\Psi\rangle$ may be obtained directly from $Q_{\rm ext}$. To get this, we evaluate $Q_{\rm ext}$ along $\mu = \delta\nu$ with δ real. The limit $\mu \to \infty$ and $\delta \to 1$ is $|\Psi(x)|^2$ and $\mu \to \infty$, and $\delta \to -1$ yields $|\Psi(p)|^2$ (see Yuen [40] for details). This is simpler in the ρ,Π representation. The two limits are now taken with $\Pi = 0$ and $\rho \to 0$ and $\rho \to \infty$, respectively. In essence, since $Q_{\rm ext}$ is defined on the space of all Gaussians, we have taken advantage of the fact that the δ function can be obtained as an infinitely squeezed Gaussian [42].

The extended Q representation is hence a valid representation. Moreover, the the dynamics of arbitrary wave functions in this representation are very simple. The von Neumann equation for the evolution of the density matrix is replaced by a Liouville equation, by *exactly* the same route that led to the Heisenberg equations of motion for arbitrary operators being replaced by Poisson bracket equations:

$$\frac{\partial Q_{\rm ext}}{\partial t} = \{H, Q_{\rm ext}\}, \tag{4.28}$$

where H is either $H_{\rm ext}$ or $H_{\rm sc}$, the expectation value of $\hat{H}$ taken with regard to the squeezed states. The Poisson bracket is defined by Eq. (2.22). Thus we have constructed a semiquantal and a semiclassical propagator: it is just the classical propagator for an arbitrary distribution function

$$U(t) = \exp(t\{H\}), \tag{4.29}$$

the exponentiation of the Liouvillian for the extended Hamiltonian system. This propagator, by virtue of this construction, is well behaved and has nice properties — in particular, it satisfies the composition property

$$U(t_1)U(t_2) = U(t_1 + t_2). \tag{4.30}$$

This is the primary formal result of this section. It is not quite a computational tool, however, since it corresponds to the calculation of an infinite number of trajectories.

This discussion of phase-space properties demonstrates the formal power of this Hamiltonian approach: In particular, the construction of a propagator with desirable properties. In the following section, we show how the Hamiltonian properties help us to obtain eigenfunctions and eigenvalues.

V. QUANTIZATION

We now sketch how to use these dynamics for requantization [43] in two different ways. The first, which uses the Fourier transform (FT) of the survival probability $[S(t) \equiv \langle\Psi(0)|\Psi(t)\rangle]$ is a computational method in that it is geared towards the numerical computation of eigenfunctions and eigenvalues, directly using the dynamics of the wave function. The second is a more formal consideration of the invariance properties of periodic orbits and invariant torii, which enables the construction of a quantization rule associated with these structures. These separate considerations help us bring out different properties of these dynamics. In particular, they help understand the spectrum obtained in terms of the phase-space structures.

A. Quantization using the survival probability

As has been pointed out [23], any approximate method of computing the time-dependent behavior of a wave packet can be used to construct a spectrum. The argument goes as follows. Note that an expansion of the wave packet (at any time t) in terms of the eigenfunctions of the Hamiltonian exists, since they form a complete set:

$$|\Psi(t)\rangle = \sum c_n(t)|\phi_n\rangle \ . \tag{5.1}$$

All the time dependence is in the complex coefficients, since the states $|\phi_n\rangle$ are stationary states and the above can be written as

$$|\Psi(t)\rangle = \sum c_n(0)e^{-iE_nt/\hbar}|\phi_n\rangle \ . \tag{5.2}$$

E_n is the eigenvalue of the appropriate eigenfunction:

$$\langle\phi_n|\hat{H}|\phi_n\rangle = E_n \ . \tag{5.3}$$

This implies that the survival probability can be written as

$$S(t) = \langle\Psi(0)|\Psi(t)\rangle = \sum |c_n(0)|^2 e^{-iE_nt/\hbar} \tag{5.4}$$

by orthonormality:

$$\langle\phi_n|\phi_m\rangle = \delta_{nm}. \tag{5.5}$$

It is now straightforward that the Fourier transform of $S(t)$ yields the spectrum of the Hamiltonian. Extracting the eigenfunctions is equally straightforward; the Fourier integral of the wave function provides these:

$$\int_{-\infty}^{\infty} e^{iE_mt/\hbar}|\Psi(t)\rangle = c_m|\phi_m\rangle, \tag{5.6}$$

where we use the spectrum obtained from above to project out the mth state.

The exact spectrum is available only when $|\Psi(t)\rangle$ can be exactly computed. Any approximation can be used to generate a spectrum, however, which is in some sense as good (or as bad) as the approximate dynamics itself. When we use any of the extended dynamics above for the case of the harmonic oscillator, since these approximations are exact, it is easy to show that this yields the exact spectrum and eigenfunctions [23,31]. For this case, the (x,p) variables decouple from the (ρ,Π) variables, and all initial conditions give us periodic orbits (POs). We take advantage of these POs to evaluate (in this case, analytically) the infinite Fourier integrals above. [Note that this is already better than the WKB method, which does get the spectrum right (with a little bit of work to evaluate the Maslov indices), but does *not* yield the correct eigenfunctions.] In general, for Heller's semiclassical dynamics, one has to work harder to get wave-packet quantization, even if one does find POs. This is because these POs are in the classical phase space and do *not* yield periodic behavior in the fluctation variables. This is true even when they are stable POs.

However, for the Hamiltonian constructions, even for general systems, if a PO can be found in the extended phase space (irrespective of stability), the Fourier integrals for the spectrum and eigenfunctions can then be done exactly. This is a remarkable point: in principle, a *single* periodic orbit can be used to extract the entire spectrum of the system. There are some caveats, of course (a) Most POs are found through symmetry considerations; they cannot then provide the full spectrum and will only reflect the appropriate symmetry. (b) The weight factors c_m for most eigenfunctions will be small, for a general PO. Hence it will not be practically possible to extract these eigenvalues and their eigenfunctions. In practice, therefore, several POs will be needed. There has been a lot of effort in recent years to find POs in Hamiltonian systems, directed primarily at trace formula work [44]. This method is thus fortuitously situated.

The features of the spectra obtained through the survival probability method (working with Heller's semiclassical dynamics) are not fully explained, however [45]. A primary problem is that there has not been, so far, any means of verifying these calculations. The only comparisons one could make are with spectra obtained through different methods (basis-set quantization, for example). The discrepancies could then be put down to the differing nature of the approximations. Working within the Hamiltonian formulations of wave-packet dynamics, however, enables us to construct another quantization procedure: a *different* approach within the *same* approximation. This second method is what we might term invariance quantization. The mathematical arguments are essentially the same as those for Bohr-Sommerfeld quantization and are detailed elsewhere [31,46]; we provide here a simple constructive version.

B. Berry's phase and quantization

Consider the phase-space trajectories obtained by solving the ordinary differential equations (obtained above) for the parameters of the wave function. We can see readily that a periodic orbit solution to Hamilton's equations is *invariant* [on the $\mathcal{R}(2N)$ subspace] under the action of the Hamiltonian. Thus a wave function constructed as a sum over all the points of the PO (each point corresponding to a Gaussian wave packet) is a candidate to be an approximate eigenfunction for the system. This ignores the role of the phase factor: each point along the orbit acquires a phase factor during the evolution. The dynamical phase is no problem, since it is the same for all points along the orbit and can thus be factored as a global phase. The geometrical part λ_G for an arbitrary PO, however, destroys the invariance in the full semiquantal space $\mathcal{R}(2N)\times\mathcal{S}(1)$. We must therefore consider the evolution of λ_G as well. We now note that a PO $\times\ \lambda_G$ such that the periodic evolution of λ_G on $\mathcal{S}(1)$ is *commensurate* with that of the PO on $\mathcal{R}(2N)$ constitutes a function invariant on $\mathcal{R}(2N)\times\mathcal{S}(1)$. This, then, is our eigenfunction. The requirement of the commensurate evolution of the phase translates simply to the relation

$$\lambda_G(\mathrm{PO}) = \oint_{\mathrm{PO}} \mathbf{P}\cdot\mathbf{dQ} = nh, \tag{5.7}$$

where we have used Eq. (2.31) and $\mathbf{P} = (p,\Pi)$ and $\mathbf{Q} = (x,\rho)$ as before. This consideration of POs such that the point orbit acquires a Berry's phase equal to integer multiples of Planck's constant h has precisely the same form as the "old" quantization rule of Bohr and Sommerfeld. However, since the rule applies in the *extended* phase space, as opposed to the classical phase space, it does not have the same meaning. In particular, there are no Maslov-Morse corrections [4] to this rule, since there are no singularities in the Gaussian representation. It can be shown [31], however, that the "spread" variables ρ,Π explicitly take care of these corrections. This had earlier been demonstrated through elegant group theoretical arguments by Littlejohn [47] for the case of Heller's dynamics. In general, the quantization condition above will give us results different from the EBK rule (the POs are in the extended space) but will always incorporate the Maslov correction.

We can thus see how to quantize using these POs in the Hamiltonian approaches: the eigenfunction is constructed as a weighted sum over the commensurate periodic orbit. The weight factor for each point along the orbit is precisely the appropriate geometrical phase. The eigenvalue is H_{ext} for that orbit (or H_{sc} if we are using the truncated form). It is interesting to note that this quantization condition arises *entirely* from a consideration of Berry's phase for the dynamics.

The extension of this argument from POs to invariant torii goes through easily [31,46] and leads to a general quantization rule:

$$\oint_{C_i} \mathbf{P}\cdot\mathbf{dQ} = n_i h, \tag{5.8}$$

where the closed integral is now taken over the ith irreducible contour around the torus and the quantum numbers n_i are labeled accordingly. This is exactly Einstein's generalization [48] of the Bohr-Sommerfeld rule to invari-

ant torii. It has been shown [46,49,31] that the eigenfunctions (or rather their Q functions) are, by the construction above, peaked around these invariant torii [50].

We emphasize that this method can be used in either of the Hamiltonian formulations constructed above. We now outline an example; the details are the subject of a forthcoming paper [31].

C. Quantization of a chaotic Hamiltonian

As an example of the methods formulated above, we have studied the Hamiltonian

$$\hat{H} = \frac{\hat{p}_x^2 + \hat{p}_y^2}{2} + \frac{1}{2}\hat{x}^2\hat{y}^2 + \beta(\hat{x}^4 + \hat{y}^4). \tag{5.9}$$

This Hamiltonian has recently been the subject of some large-scale numerical work [51]. These indicate that the classical version ($\hat{O} \to O$ for all operators) is a very strongly chaotic system, with few, if any, stable periodic orbits in the limit $\beta \to 0$. The quantal Hamiltonian with $\beta = 0$ also resists numerical analysis: basis-set quantization with matrices of dimension 3240 does not provide converging eigenvalues (see the paper by Eckhardt *et al.* [51] for details). They have hence used $\beta = 0.01$ for their analysis. As they point out, the eigenfunctions of this Hamiltonian belong to the symmetry classes of the C_{4v} symmetry group which has eight elements (four reflections in the axes and diagonals and four rotations by $\pi/2$). The irreducible representations of this group split into four one-dimensional representations and one two-dimensional representation. They have restricted themselves to the four one-dimensional representations and used harmonic oscillator basis sets to obtain low-lying eigenvalues and eigenstates for this system. We have applied the semiquantal method detailed above to this system. It works very well; in particular it does excellently for $\beta = 0$. The extended Hamiltonian in that case is

$$H_{\text{ext}} = \frac{1}{2}(p_x^2 + p_y^2 + \Pi_x^2 + \Pi_y^2) + \frac{1}{8\rho_x^2} + \frac{1}{8\rho_y^2} + \frac{1}{2}(x^2 + \rho_x^2)(y^2 + \rho_y^2). \tag{5.10}$$

If we consider the same one-dimensional representations as Eckhardt *et al.* corresponding to wave functions which are (A) symmetric under $x \to y, x \to -x$, (B) antisymmetric, symmetric, (C) symmetric, antisymmetric, and (D) antisymmetric, antisymmetric, respectively, we find that the first and third subspaces can be studied by the symmetry reduced version of H_{ext} above:

$$H = \frac{1}{2}(p^2 + \Pi^2) + \frac{1}{8\rho^2} + \frac{1}{4}(z^2 + \rho^2)^2\ , \tag{5.11}$$

where (z,p) and (ρ,Π) are the canonically conjugate pairs. This new Hamiltonian is explicitly integrable: it has two isolating integrals of motion, the total energy, and an invariant obtained by construction,

$$I = (\rho p - z\Pi)^2 + \frac{z^2}{4\rho^2}. \tag{5.12}$$

This fact enables us to find the invariant torii needed for the invariance quantization detailed above, and evaluate the eigenvalues in a straightforward fashion. The details are provided in Ref. [31]; however, we note here that the ground state energy we obtain analytically is $E_0 = 0.5953$. This is substantially lower than the value obtained by Eckhardt *et al.* of $E_0^{\text{num}} = 1.093$. The semiquantal method is based on a time-dependent variational principle; it is easy to show that for the ground state it reduces to the time-independent (Rayleigh-Ritz) variational principle. The semiquantal result thus provides an upper bound to the exact result and hence improves upon the numerical results. This is true even when we use $\beta = 0.01$ in the semiquantal method. The ground state energy in that case is $E_0^{\beta} = 0.6012$, only marginally different from the $\beta = 0$ case, and still better than the numerical result.

This example shows that the semiquantal method can be used to advantage to obtain eigenvalues and eigenfunctions for classically chaotic systems and at least in some cases gives excellent results. It also tells us what the role of semiquantal dynamics is in the agenda of postmodern quantum mechanics: it is the search for a variational space such that the dynamics on this space are explicitly integrable. We then apply the rule (5.8) to quantize the system, hence fulfilling the program of the extension of the "old" quantization rule, and advancing the comprehension of the quantum-classical correspondence limit.

VI. SUMMARY

In this paper, we have developed Gaussian semiquantal dynamics to provide a phase-space formalism. We have thus been able to construct a propagator with desirable qualities. We have compared these equations to the standard semiclassical Gaussian dynamics and have shown that the latter arise as truncations to the semiquantal equations *not self-consistent* in $\hbar$, though consistent in derivatives of the Hamiltonian. This has enabled us to extend the usual treatment and introduce a Hamiltonian semiclassical dynamics that retains the power of the phase-space formulation. We have then qualitatively evaluated the behavior of these three different approaches in various situations and have shown that the semiquantal dynamics substantially improve upon the standard semiclassical equations in reproducing the expected quantal behavior and the extended semiclassical dynamics do so marginally. Finally, we have shown how to obtain approximate eigenvalues and eigenfunctions in this formalism, and have demonstrated with the help of an example that it works well even for a classically chaotic Hamiltonian.

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APPENDIX: GENERALIZATION TO N DIMENSIONS

In this appendix, we discuss the generalization of the Hamiltonian formulation of semiquantal and semiclassical dynamics to N dimensions. The simplest way of doing this is to use product spaces for the variational subspace, for example,

$$\Psi(x,y) = \Psi_x(x)\Psi_y(y). \tag{A1}$$

With this factorization, all the one-dimensional arguments carry through exactly to N dimensions, and an extended potential formulation (with a semiquantal phase space of $4N$) can be shown to exist [31].

If we allow for correlations between the various degrees of freedom, however, this is no longer possible. The Hamiltonian formulation still exists [30], but the extended potential cannot be extracted. The best way to derive the equations of motion in this case is to use the TDVP and a wave packet $\langle \mathbf{x}|\Psi,t\rangle$ of the form

$$\Psi(\mathbf{x},t) = \exp\left[\frac{i}{\hbar}[(\mathbf{x}-\mathbf{q})\cdot\mathbf{A}\cdot(\mathbf{x}-\mathbf{q}) + \mathbf{p}\cdot(\mathbf{x}-\mathbf{q})]\right], \tag{A2}$$

where now $\mathbf{x},\mathbf{p},\mathbf{q}$ are vectors and $\mathbf{A}$ a symmetric $N\times N$ matrix. If we continue to assume a classical Hamiltonian of the form

$$H_{\text{classical}} = \frac{1}{2}\mathbf{p}^2 + V(\mathbf{x}) \tag{A3}$$

and rewrite $\mathbf{A}$ as

$$\mathbf{A} = i\frac{1}{4}\mathbf{G}^{-1} + \mathbf{K}, \tag{A4}$$

with $\mathbf{G},\mathbf{K}$ real symmetric matrices, we can obtain the extended Hamiltonian

$$H_{\text{ext}} = H_{\text{classical}} + \text{Tr}(\tfrac{1}{8}\mathbf{G}^{-1} + \mathbf{K}^2\mathbf{G} + \mathbf{G}\mathbf{K}^2) + \langle V(\hat{\mathbf{x}})\rangle, \tag{A5}$$

where Tr indicates the trace operation on the matrices. The only calculation of any subtlety is the evaluation of $\langle V(\hat{\mathbf{x}})\rangle$, since $\Psi(\mathbf{x})$ is a multivariate Gaussian distribution. The result is a series, as for the one-dimensional case, in even derivatives of V. The coefficients of these terms are found by the standard prescription:

$$\langle X_iX_jX_k\cdots\rangle = \sum\langle X_aX_b\rangle\langle X_cX_d\rangle\cdots, \tag{A6}$$

where the subscripts $a,b,c,d,\ldots$ are the same as $i,j,k,\ldots$ taken two by two. The summation extends over all the ways in which $i,j,k,\ldots$ can be subdivided in pairs. The terms on the right-hand side of this equation are just the $\frac{N^2+N}{2}$ elements of $\mathbf{G}$, which is the covariance matrix of the multivariate distribution. These elements constitute the canonical coordinates (along with the vector $\mathbf{x}$) of the extended Hamiltonian; the corresponding canonical momenta are the elements of $\mathbf{K}$ (and the vector $\mathbf{p}$). If the two matrices are chosen diagonal, the system reduces to the product space discussed above, and the extended potential exists. It is the presence of the cross terms in $\mathbf{K}^2\mathbf{G}+\mathbf{G}\mathbf{K}^2$ that prevents this in the general case. All arguments of the Hamiltonian formulation, including those about truncations and reduction to semiclassical dynamics carry through, irrespective: there are a few more equations, and they do not have as simple a form, however. We also note that the global phase of the wave function is, exactly as before, the extended action evaluated along the trajectory in the extended space.

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