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Effective potentials and chaos in quantum systems

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The dynamic usage of the technique of effective potentials is motivated and established. The one-loop effective potential and the Gaussian effective potential are derived from Ehrenfrest's theorem by using adiabatic elimination. An application is made to the Hénon-Heiles problem, and comparison is made with previous results; it is shown that quantum effects destroy chaos in two ways: (a) quantum fluctuations make the curvature more positive and (b) tunneling dominates the dynamics.

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I. INTRODUCTION

Effective potentials are used to assess the impact of quantum effects such as zero-point fluctuations and tunneling on the magnitude and the geometry of classical potentials; they are a popular field-theoretic tool, used to investigate vacuum exchanges, "quantum resuscitation" (the creation of a finite-energy bound state in unbounded potentials through fluctuation effects) rollover, and other phenomena [1]. The philosophy being valid in ordinary quantum mechanics ($0+1$ dimensions in the field-theoretic nomenclature), we consider here the dynamic use of effective potentials—with reference to "quantum chaos" [2].

We use the term quantum chaos in the conservative way: to refer to the study of the quantum mechanics of a classically chaotic system (restricting ourselves to Hamiltonian systems $H=T+V$). Most such studies have used various properties of the classical systems as windows into the quantum mechanics. For instance, Birkoff-Gustavson quantization [3] is based on the existence of invariant torii (even if fragmented) in the classical phase space. There is the idea of searching for "scars" [4], intensity peaks of highly excited wave functions along the periodic orbits of the classical system, while the technique of trace formulas [5] estimates eigenvalues of the quantum system from a weighted sum over these periodic orbits. The study of spectral statistics [6], however, is based on assumptions about the random distribution of the matrix elements of the Hamiltonian. Gutzwiller's work [5] provides a fine review and exposition of these techniques.

This variety of techniques comes about because the measures (such as K entropy [7], Liapunov numbers [8]), diagnostics (such as the Melnikov function [9], the tests of Zaslavsky and Chirikov, Greene, and Mo [10], Toda, Brumer and Duff (TBD) [11], and Pattanayak and Schieve (PS) [12]) and signatures of chaos lie, in general, in phase space, are dynamical and have no direct interpretation in quantum mechanics. It is in this context that we consider a parallel approach, that of using classical techniques of analysis by reducing the problem to that of an effective classical problem, i.e., instead of considering Schrödinger's equation in a given potential, we look at Hamilton's equations in a modified potential. This approach is local in the sense that quantum-mechanical effects provide local corrections to the dynamics rather than global, static characterizations. The approach is valid for small values of Planck's constant h (caveat: this not in the sense of a tunable parameter but depending on the characteristics of the problem) and is, in fact, in the ground-state regime (the techniques mentioned previously are of the highly excited-state regime). Some of the diagnostics [11,12] for chaos are based on the geometry of the potential; the effective potential technique is especially powerful in combination with such methods. In the region, therefore, of semiclassical dynamics, where quantum effects may be said to provide corrections (a convenient mathematical fiction) this method holds. It must also be emphasized that it is very simple and computationally cheap; yet it provides us with powerful insight that we may use before more complicated methods of analysis.

In Secs. II we derive the one-loop effective potential (1LEP) and the Gaussian effective potential (GEP) from Ehrenfrest's theorem by using the technique of adiabatic elimination and thus establish a dynamical justification for their usage. In Sec. III we apply the GEP (with an exposition, for pedagogical purposes, of the method) to the Hénon-Heiles problem. Comparison and contrast with other studies is made. We finish with some observations regarding this technique and in Sec. IV state two conjectures about quantum (or at least semiclassical) effects on all potentials of this form.

II. DERIVATION OF THE GEP

A. Ehrenfrest's theorem and the hierarchy

Consider, then, Ehrenfrest's theorem; this is the most direct way of seeing quantum corrections. We restrict all arguments in the next two sections to particles of unit mass moving in a one-dimensional potential, i.e., Hamiltonians of the form $H=p^2/2+V(x)$. Generalization of this to higher dimensions is straightforward. Accordingly the equations of motion for the centroid of a wave packet are

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$$\frac{d}{dt}\langle \hat{x}\rangle = \langle \hat{p}\rangle \tag{1a}$$

and

$$\frac{d}{dt}\langle \hat{p}\rangle = -\left\langle \frac{\partial V(\hat{x})}{\partial x}\right\rangle , \tag{1b}$$

where the $\langle\ \rangle$ indicate expectation values. If V (assumed analytic) is at most quadratic in x then the $\langle\ \rangle$ factor,

$$\left\langle \frac{\partial V(\hat{x})}{\partial x}\right\rangle = \left.\frac{\partial V}{\partial x}\right|_{\langle \hat{x}\rangle} , \tag{2}$$

and the centroid therefore follows the classical trajectory.

We, of course, are interested in nonlinear gradients, so that we can study chaos. The classical equation of motion does not hold then for the centroid and to study "corrections" we expand in Taylor series around $\langle \hat{x}\rangle$ and $\langle \hat{p}\rangle$. The expansions are of the form

$$\langle F(\hat{u})\rangle = \frac{1}{n!}\langle \hat{U}^n\rangle F^{(n)} n \geq 0 , \tag{3}$$

where $F^{(n)} = \partial^n F/\partial u^n|_{\langle \hat{u}\rangle}$, $U = \hat{u} - \langle \hat{u}\rangle$. We use the summation convention here and throughout the rest of this paper. Using these 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 "Ehrenfrest phase space." The infinite hierarchy, however, cannot be (or at least has not been) reduced in general.

To proceed with the analysis, therefore, we might truncate at a given order [13] (the mth). The truncation may be justified if the potential (or the mth derivative) varies slowly over the characteristic width of the wave packet; all higher moments are assumed negligible. At that order, then, one gets a closed set of equations. The truncation assumption may always be checked for self-consistency by carrying an extra order along in the equations and ensuring that it does, indeed, stay small. The equations thus generated with $m=2$ are five in number and are analyzed at length in Ref. [13]. With $m=4$, they are 14 in number (see the Appendix).

Another possible technique for reducing the number 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. We can achieve this by requiring that the wave packet be always Gaussian. We then get the following equations:

$$\frac{d}{dt}\langle \hat{x}\rangle = \langle \hat{p}\rangle , \tag{4a}$$

$$\frac{d}{dt}\langle \hat{p}\rangle = -\left\langle \frac{\partial V(\hat{x})}{\partial x}\right\rangle = -\frac{1}{\Omega^m m!2^m}V^{(2m+1)} , \tag{4b}$$

$$\frac{d}{dt}\langle \hat{X}^2\rangle = \langle \hat{X}\hat{P} + \hat{P}\hat{X}\rangle , \tag{4c}$$

$$\begin{aligned}\frac{d}{dt}\langle \hat{X}\hat{P} + \hat{P}\hat{X}\rangle &= 2\Omega(\hbar^2 + \langle \hat{X}\hat{P} + \hat{P}\hat{X}\rangle) - 2\left\langle \hat{X}\frac{\partial V(\langle \hat{x}\rangle)}{\partial x}\right\rangle \\ &= 2\Omega(\hbar^2 + \langle \hat{X}\hat{P} + \hat{P}\hat{X}\rangle) \\ &\quad - \frac{1}{\Omega^m(m-1)!2^{m-2}}V^{(2m)} ,\end{aligned} \tag{4d}$$

where we have used the standard relationships for a Gaussian function, with $\langle \hat{X}^2\rangle = \Omega^{-1}$, $\langle \hat{X}^{2m}\rangle = (2m)!(1/m!2^m)(1/\Omega^m)$, $\langle \hat{X}^{2m+1}\rangle = 0$, and $4\langle \hat{P}^2\rangle\langle \hat{X}^2\rangle = \hbar^2 + \langle \hat{X}\hat{P} + \hat{P}\hat{X}\rangle$.

It is interesting to compare this set of equations (4) with those obtained from Dirac's variational technique [14]. There we apply the principle that

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

be stationary against the variation of $|\Psi,t\rangle$. An arbitrary $|\Psi,t\rangle$ yields Schrödinger's time-dependent equation. Cooper, Pi, and Stancioff [15] chose $|\Psi,t\rangle$ to be the most general Gaussian function. Their Eqs. (2.7) are the same [16] as Eqs. (4) above.

In both the above approaches we get a finite set of equations being carried along with the equations for evolution of $\langle \hat{x}\rangle$ and $\langle \hat{p}\rangle$. In Sec. II B we derive from these effective potentials.

B. Effective potentials by adiabatic elimination

One well-recognized method used in other fields is of adiabatic elimination or slaving [17]. We assume that the time scales of the system are such that at each point in $\langle x\rangle$ space the system is effectively at a steady state. We solve for these values of the moments and substitute them in the Taylor expansion, which then gives us an effective potential $V_{\text{eff}} \equiv \langle V\rangle = 1/n!\langle X^n\rangle V^{(n)}$.

Asking that the odd moments be zero, thus mimicking a particle, for instance, gives useful results. An iterative solution [see the Appendix] at $m=4$ and with odd moments zero is

$$\langle X^2\rangle = \frac{\hbar}{2}\left[\frac{\partial^2 V(\langle \hat{x}\rangle}{\partial x^2}\right]^{-1/2} - \frac{\hbar^2 V^{(3)}V^{(3)}}{4V^{(1)}V^{(1)}V^{(4)} - 8V^{(1)}V^{(2)}V^{(3)}} , \tag{5a}$$

$$\langle X^4\rangle = \frac{\hbar^2 V^{(1)}V^{(3)}}{2V^{(1)}V^{(1)}V^{(4)} - 4V^{(1)}V^{(2)}V^{(3)}} , \tag{5b}$$

$$\langle P^2\rangle = \frac{\hbar}{2}\left[\frac{\partial^2 V(\langle \hat{x}\rangle)}{\partial x^2}\right]^{1/2} + \frac{\hbar^2 V^{(3)}(V^{(1)}V^{(4)} - V^{(2)}V^{(3)})}{12V^{(1)}V^{(1)}V^{(4)} - 24V^{(1)}V^{(2)}V^{(3)}} . \tag{5c}$$

The first order in $\hbar$ gives

$$\langle X^2\rangle = \frac{\hbar}{2}\left[\frac{\partial^2 V(\langle \hat{x}\rangle)}{\partial x^2}\right]^{-1/2} . \tag{6a}$$

This would suggest that

$$V_{\rm eff}=V_{\rm class}+\frac{\hbar}{4}\left[\frac{\partial^2 V(\langle \hat{x}\rangle)}{\partial x^2}\right]^{1/2} . \tag{6b}$$

Let us compare this with the one-loop-effective potential (1LEP) [18]. It is explicitly constructed to incorporate only the lowest-order corrections in $\hbar$ arising from vacuum fluctuations and does not seem to agree with our expression in Eq. (6b) until we remember to include the contribution from the $\langle P^2\rangle$ term [19], i.e., set $V_{\rm eff}\equiv\langle \hat{H}\rangle$,

$$V_{\rm eff}=V_{\rm class}+\frac{\hbar}{2}\left[\frac{\partial^2 V(\langle \hat{x}\rangle)}{\partial x^2}\right]^{1/2}=V_{\rm 1LEP} . \tag{6c}$$

Stevenson has criticized the 1LEP at length [20]. We note that it breaks down for concave potential surfaces. Concavity (in two or more dimensions) is, in fact, a diagnostic for chaos [11,12]. The problem of breakdown is vitiated by considering higher-order corrections in $\hbar$ but is not necessarily removed.

We therefore consider Eqs. (4). Using adiabatic elimination there, we set the left-hand side of Eqs. (4c) and (4d) equal to zero. From (4c) we get $\langle \hat{X}\hat{P}+\hat{P}\hat{X}\rangle=0$ and substituting that in Eq. (4d) we get

$$\begin{aligned} 0&=2\Omega\hbar^2-\frac{1}{\Omega^m(m-1)!2^{m-2}}V^{(2m)}\\ &=4\Omega\frac{\partial}{\partial\Omega}\left\langle \tfrac{1}{2}\hat{p}^2+\frac{1}{\Omega^m m!2^m}V^{(2m)}\right\rangle\\ &=4\Omega\frac{\partial}{\partial\Omega}\langle \tfrac{1}{2}\hat{p}^2+\hat{V}\rangle\\ &=4\Omega\frac{\partial}{\partial\Omega}\langle \hat{H}\rangle . \end{aligned} \tag{7}$$

Therefore, $V_{\rm eff}(x,\Omega)=\langle \hat{H}\rangle$, where Ω minimizes $\langle \hat{H}\rangle$. This is the Gaussian effective Potential (GEP) [20] which normally obtains directly from a static variational approach.

Thus, we have derived the GEP from Ehrenfrest's theorem and established a dynamical justification for it. It is a well-studied potential and the equations derived from it have been shown to give to a very good approximation the same dynamics as Eqs. (4) [15]. To see the use of the GEP in quantum chaos, we study as an example the well-known chaotic Hamiltonian: the Hénon-Heiles problem. In Sec. III we use directly the static approach and make the following changes to conform with convention:

$$\langle \hat{X}^2\rangle=\hbar(2\Omega)^{-1} \tag{8a}$$

and

$$\langle \hat{p}^2\rangle=\tfrac{1}{2}\hbar\Omega , \tag{8b}$$

with $\langle \hat{p}\rangle=0$.

III. APPLICATION OF THE GEP

A. Chaos in the Hénon-Heiles potential

This potential has been a well-studied problem since it was proposed in 1964 [21]. Both analytical and numerical [22] techniques have been used to demonstrate and analyze the existence of classical dynamical chaos in this problem. It has proved particularly of interest as a molecular model and therefore the quantum mechanics of the system has attracted the attention of many researchers [23–26]. The primary attempt has been to find the energy spectrum of the problem. This potential is unbounded from below, however, and does not have a well-defined spectrum, except in a metastable sense; Waite and Miller [24] considered that in their study of the lifetimes of these metastable states.

Originally the problem of a star in an axis-symmetric galactic potential, it is modeled by a two-dimensional polynomial for a particle with unit mass and in Cartesian coordinates is

$$V(x,y)=\tfrac{1}{2}(x^2+y^2)+\tfrac{1}{3}(x^3-3xy^2) . \tag{9}$$

This is a shallow two-dimensional false well with threefold rotational symmetry, as shown in Fig. 1. As the radius increases, the initial harmonic well shape changes gradually in the presence of the cubic term. This has been treated as a perturbation of the two-dimensional harmonic oscillator, as we argue later, to the detriment of the analysis.

The cubic term provides three "mountains" alternating with three narrow "passes" to the unbounded "valleys" beyond. These ionization cusps are at a value of $V_c=0.1667$, and studies of the classical system have been restricted to bound particles, $E<V_c$. The simplest approach used is to numerically integrate Hamilton's equations through the four-dimensional phase space and then examine Poincaré sections in the (x,p_x) plane. Trajectories are termed regular or chaotic depending on whether they form closed curves in the Poincaré plane or not, respectively; this criterion indicates a conserved quantity (an isolating integral of motion) other than the total energy, for the regular motion. As the total energy of the system is increased (as we climb upwards for the well) there is generally agreed to be a transition to chaos, at $E=0.0833$ [27], in exact accordance with TBD and PS geometric criteria [11,12]. This being a Hamiltonian system, the above integral cannot then be global; numerically unobservable chaos may exist at all energies.

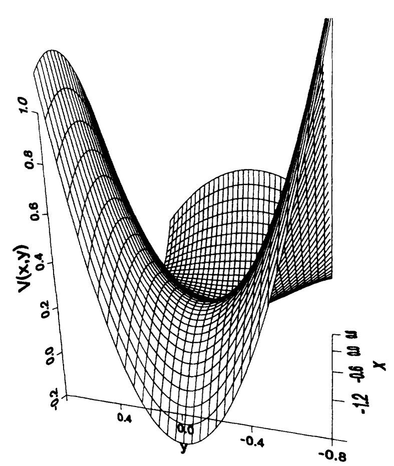

FIG. 1. The Hénon-Heiles potential.

B. Computation of the $V_{\rm GEP}$

We proceed as follows: given a two-dimensional Hamiltonian H, we compute the expectation value of the energy $\langle\Psi|\hat{H}|\Psi\rangle$, where Ψ is a two-dimensional normalized Gaussian function of the form $\exp[-(1/2\hbar)r_i\Omega_{ij}r_j]$ ($r_i=x_i'-x_i$, and $i,j=1,2$), Ω_{ij} being a symmetric 2×2 matrix that depends in general on the position variables x_i. The elements of the matrix can be defined completely in terms of two frequencies Ω and ω (in the principal directions of the Gaussian function) and an angle β that specifies the orientation of these axes with respect to the x and y axes of the potential (see Fig. 2). We then minimize the computed matrix element with respect to all three parameters at each $\hat{\mathbf{x}}$: $V_{\rm GEP}=\min_{\Omega,\omega,\beta}V_g$, where $V_g=\langle\Psi|\hat{H}|\Psi\rangle$, $\Omega\equiv\Omega(\hat{\mathbf{x}})$, $\omega\equiv\omega(\hat{\mathbf{x}})$, and $\beta\equiv\beta(\hat{\mathbf{x}})$.

The Hénon-Heiles potential being polynomial in x and p, the calculation of the matrix element is simplified by using the number representation

$$\begin{bmatrix}\hat{x}\\ \hat{y}\end{bmatrix}=\begin{bmatrix}x\\ y\end{bmatrix}+\begin{bmatrix}\cos\beta & -\sin\beta\\ \sin\beta & \cos\beta\end{bmatrix}\begin{bmatrix}(2\Omega)^{-1/2}(a_\Omega+a_\Omega^\dagger)\\ (2\omega)^{-1/2}(a_\omega+a_\omega^\dagger)\end{bmatrix}, \tag{10a}$$

$$\begin{bmatrix}p_x\\ p_y\end{bmatrix}=\begin{bmatrix}\cos\beta & -\sin\beta\\ \sin\beta & \cos\beta\end{bmatrix}\begin{bmatrix}-i\left[\dfrac{2}{\Omega}\right]^{1/2}(a_\Omega+a_\Omega^\dagger)\\ -i\left[\dfrac{2}{\omega}\right]^{1/2}(a_\omega+a_\omega^\dagger)\end{bmatrix}, \tag{10b}$$

with $[a_\alpha,a_\gamma^\dagger]=\delta_{\alpha\gamma}$, i.e., they are the canonical creation ($a^\dagger$) and annihilations (a) operators; the trial function is the ground state for these operators, i.e., $a_\Omega|\Psi\rangle=0=a_\omega|\Psi\rangle$. We have set $\hbar=1$; it is reinstated using dimensional considerations later.

For $H=\frac{1}{2}p^2+V(x,y)$ as in Eq. (9), we have, for example, for the cubic part,

$$\begin{aligned}\langle\Psi|\hat{x}\hat{y}^2|\Psi\rangle=&\,xy^2+2y(2\Omega)^{-1}\sin\beta\cos\beta\\ &-2y(2\omega)^{-1}\sin\beta\cos\beta\\ &+y(2\Omega)^{-1}\sin^2\beta+x(2\omega)^{-1}\cos^2\beta,\end{aligned} \tag{11a}$$

and further

$$\langle\Psi|\hat{x}^3|\Psi\rangle=x^3+3x\{(2\Omega)^{-1}\cos^2\beta+(2w)^{-1}\sin^2\beta\}. \tag{11b}$$

Proceeding in this manner we get

$$\begin{aligned}V_g=&\,\langle\Psi|\hat{H}|\Psi\rangle\\ =&\,\tfrac{1}{4}(\Omega+\omega)+\tfrac{1}{2}(x^2+y^2)+\tfrac{1}{3}(x^3-3xy^2)+\frac{1}{4}\left[\frac{1}{\Omega}+\frac{1}{\omega}\right]\\ &+\frac{1}{2}\left[\frac{1}{\Omega}-\frac{1}{\omega}\right](x\cos 2\beta-y\sin 2\beta).\end{aligned} \tag{12}$$

The minimization conditions are

$$\frac{\partial V_g}{\partial\beta}=0=\left[\frac{1}{\Omega}-\frac{1}{\omega}\right](-y\cos 2\beta-x\sin 2\beta), \tag{13a}$$

$$\frac{\partial V_g}{\partial\Omega}=\tfrac{1}{4}-\tfrac{1}{4}\Omega^{-2}-\tfrac{1}{2}\Omega^{-2}(x\cos 2\beta-y\sin 2\beta), \tag{13b}$$

and

$$\frac{\partial V_g}{\partial\omega}=0=\tfrac{1}{4}-\tfrac{1}{4}\omega^{-2}+\tfrac{1}{2}\omega^{-2}(x\cos 2\beta-y\sin 2\beta). \tag{13c}$$

The first of these three equations gives

$$\beta=\tfrac{1}{2}\arctan(-y/x) \tag{14}$$

and when we substitute that in the other two, we obtain

$$V_{\rm GEP}=\tfrac{1}{2}(x^2+y^2)+\tfrac{1}{3}(x^3-3xy^2)+\frac{\hbar}{2}(\Omega+\omega), \tag{15a}$$

where

$$\Omega=(1+2r)^{1/2} \tag{15b}$$

and

$$\omega=(1-2r)^{1/2}. \tag{15c}$$

Looking at Eqs. (14) and (15) we note the following.

(1) The terms due to quantum mechanics (the terms with $\hbar$ multiplying them) are purely radial [28]. A quantum-mechanical particle responds to a modified shape of the potential. It avoids the narrow areas (termed quantum claustrophobia [20]) and this, along with fluctuations and the orientation, smooths the potential. We postpone a full discussion to Sec. III C.

(2) Further, the angle β that indicates the orientation of the particle's principal axes shows that the wave packet tends to align with its narrower profiles lined up with the valleys. The angle follows the original $2\pi/3$ symmetry of the well.

(3) However, we see from Eqs. (15) that at values of the radius greater than 0.5 the frequency ω (and hence $V_{\rm GEP}$)

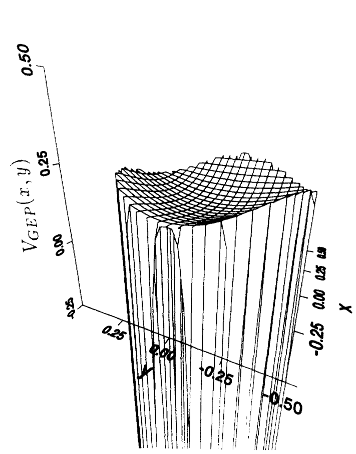

FIG. 2. $V_{\rm GEP}$ for the Hénon-Heiles potential. $\hbar=0.05$ and $\varepsilon=10^{-5}$.

is not real and positive semidefinite. As with the 1LEP earlier (Sec. II), there is not a well-defined effective potential in this instance, not because of transitional concavity but due to the unboundedness of the potential.

For the GEP this problem is not unresolvable, however. If we realize that this technique relies on evaluating the reaction of a bound or at least quasibound state in a given potential, we can extend the analysis for this and other such problems in a simple physical way by closing the potential at infinity. In this instance we do so by embedding the unbounded cubic in a weak quartic (εr^4); the physical problem is unaltered on time scales of interest, since the attraction is to a global minimum at very large values of r (for ε vanishingly small) but the mathematical realization of bound states is achieved.

Consider, therefore,the potential

$$V(x,y)=\tfrac{1}{2}(x^2+y^2)+\tfrac{1}{3}(x^3-3xy)^2+\varepsilon[(x^2+y^2)^2] . \tag{16}$$

A calculation similar to the one above gives

$$V_g=\tfrac{1}{2}(x^2+y^2)+\tfrac{1}{3}(x^3-3xy^2)+\varepsilon[(x^2+y^2)^2]+\tfrac{1}{4}(\Omega+\omega)+\frac{1}{4}\left[\frac{1}{\Omega}+\frac{1}{\omega}\right]+\frac{1}{2}\left[\frac{1}{\Omega}-\frac{1}{\omega}\right](x\cos2\beta-y\sin2\beta)$$
$$+\varepsilon\left[3\{(2\Omega)^{-2}+(2\omega)^{-2}\}+\tfrac{1}{2}\Omega\omega+(x^2+y^2)\left[\frac{1}{\Omega}+\frac{1}{\omega}\right]+\frac{2}{\Omega}(x\cos\beta+y\sin\beta)^2+\frac{2}{\omega}(y\cos\beta-x\sin\beta)^2\right] . \tag{17}$$

On applying the minimization conditions

$$\frac{\partial V_g}{\partial\beta}=0=\left[\frac{1}{\Omega}-\frac{1}{\omega}\right]\{\sin2\beta[2\varepsilon(y^2-x^2)-x] + \cos2\beta(4\varepsilon xy-y)\} , \tag{18a}$$

we get

$$\beta=\tfrac{1}{2}\arctan\left[\frac{4\varepsilon xy-y}{x-2\varepsilon(y^2-x^2)}\right] . \tag{18b}$$

Further,

$$\frac{\partial V_g}{\partial\Omega}=0$$

gives

$$\Omega^3-\Omega\left[a+\frac{2\varepsilon}{\omega}\right]-6\varepsilon=0 , \tag{18c}$$

where

$$a=1+2(x\cos2\beta-y\sin2\beta)+4\varepsilon(x^2+y^2) + 8\varepsilon(x\cos\beta+y\sin\beta)^2 . \tag{18d}$$

Also

$$\frac{\partial V_g}{\partial\omega}=0$$

gives

$$\omega^3-\omega\left[\beta+\frac{2\varepsilon}{\Omega}\right]-6\varepsilon=0 , \tag{18e}$$

where

$$b=1-2(x\cos2\beta-y\sin2\beta)+4\varepsilon(x^2+y^2) + 8\varepsilon(y\cos\beta-x\sin\beta)^2 . \tag{18f}$$

In Eqs. (18c) and (18e) we have two coupled cubic equations which in general may not have real positive semidefinite solutions. However,a systematic evaluation of the equations [29] shows that physical solutions always exist for this particular case. The problem is solved; we have computed an effective quantum-mechanical potential in the Hénon-Heiles problem.

C. Interpretation, comparison, and contrast

The fact that the $\hbar$ terms are radial [Eqs. (15), valid within the false well] can be used to show, as follows, that the Gaussian [30] curvature K of the potential is made more positive by quantum fluctuations,

$$K\propto V_{xx}V_{yy}-V_{xy}^2$$
$$=1-4r^2+\hbar\left[1+2x\frac{(3y^2-x^2)}{r^2}\right]\left[\frac{1}{\omega^3}-\frac{1}{\Omega^3}\right] . \tag{19}$$

The $\hbar$ terms are always positive for $r<0.5$. This implies, then, that quantum effects tend to delay or reduce the effects of chaos.

This compares favorably with previous findings. Within the well, Hutchinson and Wyatt in their investigations [25] of the dynamics of the Wigner distribution function have argued that the classically stochastic behavior is delayed and reduced quantum mechanically. Other studies [23], especially that of Noid *et al.* [26], have found that the quantum spectrum has no signature of the classical chaos. Carlson and Schieve [2] had, with this same technique, analytically predicted that the rounded-off potential reduces chaos.

Let us now look at Eqs. (17) and (18) [31]. The effective potential is evaluated numerically and may be seen in Fig. 2. We see that though the effective quantum-mechanical terms are initially additive, clearly, after a critical distance from the origin, the particle tunnels out. This happens as soon as the larger valley (the global minimum at $\sim r=\varepsilon^{-1}$) begins to dominate. It looks abrupt, but interpreted semiclassically, means that there is a transition energy after which the particle is effectively free on the time scale of the classical dynamics. The seemingly fully radial nature of this tunneling may

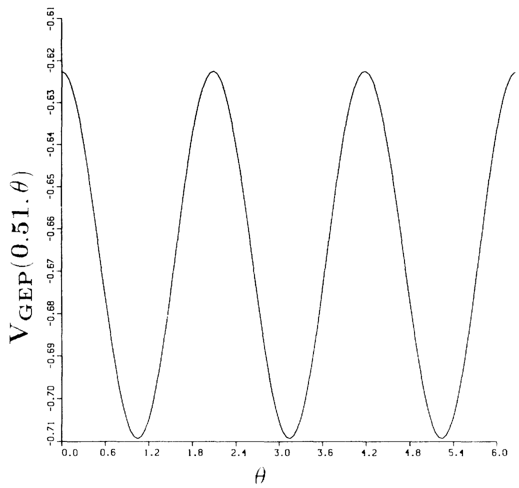

FIG. 3. $V_{\rm GEP}$ as a function of θ, $\hbar=0.05$, $\varepsilon=10^{-5}$, and $r=0.51$.

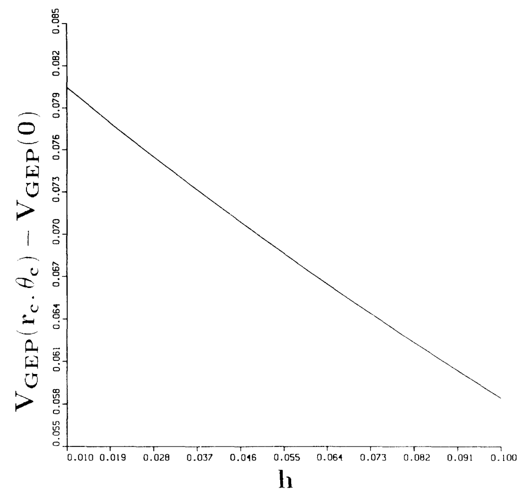

FIG. 5. Barrier height $V_{\rm GEP}(r_c,\theta_c)-V_{\rm GEP}(0)$, i.e., relative height of ionization cusps, as a function of $\hbar$ as it is scaled.

seem puzzling since one intuitively expects that the particle tunnels out along one of the valleys but not along the erstwhile mountains. However, the particle can and does tunnel transversely between the valleys, thus lowering the effective height of the mountain; secondly, a closer inspection of the potential as a function of the angle θ (Fig. 3) reveals the same $2\pi/3$ symmetry as the original problem. On the scale of Fig. 2, tunneling effects so dominate as to mask this.

The energy dependence of the tunneling is qualitatively quite independent of the (rescaled) value of $\hbar$, provided it is small (but nonzero) compared to the classical energy. In a molecular problem, rescaling by the system parameters yields an order of magnitude estimate of $\hbar=0.05$ [32]. Figures 4 and 5 show, respectively, the dependence of the critical barrier energy and its location (distance measured along a classical valley, i.e., along $\theta=\pi$) on the value of $\hbar$. It is necessary to consider relative energies for comparison at differing values of $\hbar$; not subtracting the zero-point energy gives confusing results [24].

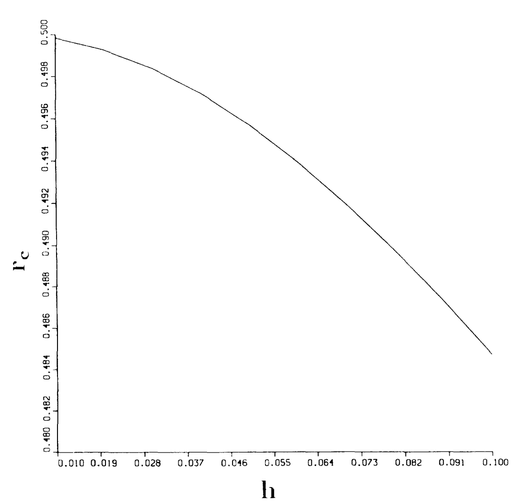

FIG. 4. Barrier distance r_c, i.e., radial distance of ionization cusps at $\theta_c=\pi/3,\pi,6\pi/3$, as a function of $\hbar$ as it is scaled.

Most of the previous studies used large basis sets, both for the spectrum and the dynamical study of quantum ergodicity. This suffers from the difficulty that by treating the problem as a perturbation of the sample harmonic oscillator, one cannot see the tunneling effects clearly.

The study that did investigate the metastability [24] agrees with our results. Firstly, we both see the marked transition from a strong to a weak dependence of the lifetime of a state on its energy. Secondly, a rescaling of their values of this critical energy agrees well with ours [33].

To summarize, the above discussion demonstrates that in the Hénon-Heiles potential (1) quantum-mechanical fluctuations tend to smooth out the irregular behavior, and (2) more dominantly, the unboundedness causes a particle placed within the potential well to tunnel out at energies associated with the classically chaotic regime of this potential. It may, in fact, be appropriate to say that quantum effects destroy chaos.

For this particular case, then, we have remarkably good results. This simple and largely analytical method looks at both the chaotic dynamics and the metastability associated with the potential and agrees well with previous results on both. Within the framework of this technique, results have a straightforward physical interpretation. We account for the disagreements with other studies through the argument that this study brings together both aspects of the problem, whereas other studies treated one or the other.

IV. CONCLUSION

Finally, we make the following two generalizations for all similar potentials.

(1) "Quantum claustrophobia" and the fact that a semiclassical particle samples and responds to the geometry of a neighborhood rather than a point will tend to add radial terms to the effective potential which make the curvature positive. Hence, *quantum effects delay chaos.*

(2) The tunneling commences at the geometrically pre-

dicted onset for stochasticity, i.e., where the potential becomes concave. Hence, through tunneling, *quantum effects remove chaos.*

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APPENDIX

At $m=4$, the equations generated from Ehrenfrest's theorem are as follows:

$$\frac{d\langle \hat{x}\rangle}{dt}=\langle \hat{p}\rangle\ , \tag{A1a}$$

$$\frac{d}{dt}\langle \hat{p}\rangle=-V^{(1)}-\tfrac{1}{2}\langle \hat{x}^2\rangle V^{(3)}-\tfrac{1}{6}\langle \hat{X}^3\rangle V^{(4)}-\tfrac{1}{24}\langle \hat{X}^4\rangle V^{(5)} \tag{A1b}$$

$$\frac{d}{dt}\langle \hat{X}^2\rangle=\langle \hat{X}\hat{P}+\hat{P}\hat{X}\rangle\ , \tag{A1c}$$

$$\frac{d}{dt}\langle \hat{P}^2\rangle=\langle \hat{X}\hat{P}+\hat{P}\hat{X}\rangle V^{(2)}-\langle \hat{X}\hat{P}\hat{X}\rangle V^{(3)} -\tfrac{1}{6}\langle \hat{X}^3\hat{P}+\hat{P}\hat{X}^3\rangle V^{(4)}\ , \tag{A1d}$$

$$\frac{d}{dt}\langle \hat{P}\hat{X}+\hat{X}\hat{P}\rangle=2(\langle \hat{P}^2\rangle-\langle \hat{X}^2\rangle V^{(2)}-\tfrac{1}{2}\langle \hat{X}^3\rangle V^{(3)} -\tfrac{1}{6}\langle \hat{X}^4\rangle V^{(4)})\ , \tag{A1e}$$

$$\frac{d}{dt}\langle \hat{X}^3\rangle=3\langle \hat{X}\hat{P}\hat{X}\rangle+3\langle \hat{X}^2\rangle\langle \hat{p}\rangle\ , \tag{A1f}$$

$$\frac{d}{dt}\langle \hat{P}^3\rangle=-3\langle \hat{P}^2\rangle V^{(1)}-3\langle \hat{P}\hat{X}\hat{P}\rangle V^{(2)}-\tfrac{3}{2}\langle \hat{X}\hat{P}^2\hat{X}\rangle V^{(3)} +\hbar^2 V^{(3)}\ , \tag{A1g}$$

$$\frac{d}{dt}\langle \hat{X}\hat{P}\hat{X}\rangle=2\langle \hat{P}\hat{X}\hat{P}\rangle-\langle \hat{X}^2\rangle V^{(1)}-\langle \hat{X}^3\rangle V^{(2)} -\tfrac{1}{2}\langle \hat{X}^4\rangle V^{(3)}+\langle \hat{X}\hat{P}+\hat{P}\hat{X}\rangle\langle \hat{p}\rangle\ , \tag{A1h}$$

$$\frac{d}{dt}\langle \hat{P}\hat{X}\hat{P}\rangle=\langle \hat{P}^3\rangle+\langle \hat{P}^2\rangle\langle \hat{p}\rangle-\langle \hat{X}\hat{P}+\hat{P}\hat{X}\rangle V^{(1)} -2\langle \hat{X}\hat{P}\hat{X}\rangle V^{(2)}-\langle \hat{X}^3\hat{P}+\hat{P}\hat{X}^3\rangle V^{(3)}\ , \tag{A1i}$$

$$\frac{d}{dt}\langle \hat{X}^4\rangle=2\langle \hat{X}^3\hat{P}+\hat{P}\hat{X}^3\rangle+4\langle \hat{X}^3\rangle\langle \hat{p}\rangle\ , \tag{A1j}$$

$$\frac{d}{dt}\langle \hat{P}^4\rangle=-4\langle \hat{P}^3\rangle V^{(1)}-2\langle \hat{X}^3\hat{P}+\hat{P}\hat{X}^3\rangle V^{(2)}\ , \tag{A1k}$$

$$\frac{d}{dt}\langle \hat{X}^3\hat{P}+\hat{P}\hat{X}^3\rangle=-2\langle \hat{X}^3\rangle V^{(1)}-2\langle \hat{X}^4\rangle V^{(2)}+6\langle \hat{X}\hat{P}^2\hat{X}\rangle +6\langle \hat{X}\hat{P}\hat{X}\rangle\langle \hat{p}\rangle-3\hbar^2\ , \tag{A1l}$$

$$\frac{d}{dt}\langle \hat{P}^3\hat{X}+\hat{X}\hat{P}^3\rangle=2\langle \hat{P}^4\rangle+\langle \hat{P}^3\rangle\langle \hat{p}\rangle-6\langle \hat{X}\hat{P}\hat{X}\rangle V^{(1)} -6\langle \hat{X}\hat{P}^2\hat{X}\rangle V^{(2)}+3\hbar^2 V^{(2)}\ , \tag{A1m}$$

$$\frac{d}{dt}\langle \hat{X}\hat{P}^2\hat{X}\rangle=\langle \hat{P}^3\hat{X}+\hat{P}^3\rangle+\langle \hat{X}\hat{P}\hat{X}\rangle\langle \hat{p}\rangle-2\langle \hat{X}\hat{P}\hat{X}\rangle V^{(1)} -2\langle \hat{P}\hat{X}^3+\hat{X}\hat{P}^3\rangle V^{(2)}\ . \tag{A1n}$$

To solve iteratively (this gives consistent results) we first consider only the first five equations. We set all moments of order greater than 2 to zero, and use the approximation of a minimum uncertainty state: $4\langle \hat{P}^2\rangle\langle \hat{X}^2\rangle=\hbar^2+\langle \hat{X}\hat{P}+\hat{P}\hat{X}\rangle$. We then impose the steady-state condition to obtain

$$\langle \hat{X}^2\rangle=\frac{\hbar}{2}\left[\frac{\partial^2 V(\langle \hat{x}\rangle)}{\partial x^2}\right]^{-1/2} \tag{A2a}$$

and

$$\langle \hat{P}^2\rangle=\frac{\hbar}{2}\left[\frac{\partial^2 V(\langle \hat{x}\rangle)}{\partial x^2}\right]^{1/2}\ . \tag{A2b}$$

We now consider Eqs. (A1a)–(A1n). Substituting the solutions (A2a) and (A2b) gives us the same equations back; they are now all of second order in $\hbar$. We set all odd moments to zero, and impose the steady-state condition. We are left with the equations

$$0=\langle \hat{P}^2\rangle-\langle \hat{X}^2\rangle V^{(2)}V^{(3)}-\tfrac{1}{6}\langle \hat{X}^4\rangle V^{(4)}\ , \tag{A3a}$$

$$0=-3\langle \hat{P}^2\rangle V^{(1)}-\tfrac{3}{2}\langle \hat{X}\hat{P}^2\hat{X}\rangle V^{(3)}+\hbar^2 V^{(3)}\ , \tag{A3b}$$

$$0=-\langle \hat{X}^2\rangle V^{(1)}-\tfrac{1}{2}\langle \hat{X}^4\rangle V^{(3)}\ , \tag{A3c}$$

$$0=-2\langle \hat{X}^4\rangle V^{(2)}+6\langle \hat{X}\hat{P}^2\hat{X}\rangle-3\hbar^2\ , \tag{A3d}$$

$$0=2\langle \hat{P}^4\rangle-6\langle \hat{X}\hat{P}^2\hat{X}\rangle V^{(2)}+3\hbar^2 V^{(2)}\ . \tag{A3e}$$

The solutions to these equations added to the solutions (A2) give us the solutions cited in Eqs. (5) above.

[1] The papers of Stevenson (Ref. [20]) and that of Cooper, Pi, and Stancioff (Ref. [15]) provide detailed references and studies of these phenomena.

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[18] This form of the 1LEP is given in Stevenson's paper (Ref. [20]).

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[31] The potential segues smoothly in using the two sets of equations as we move from the inside to the outside of the well. We use the first set only for computational convenience inside the well, whence it can be analytically shown that the $\hbar$ terms add to the curvature.

[32] Distances of the oder of 10^{-10} m, energies of the order of 10^{-19} J, and a reduced mass of the order of 10^{-27} kg were used. The resultant estimate is consistent with Refs. [25] and [26].

[33] The rescaling is required for consistency in the definition of the ground-state energy, as has been argued already. The comparison is couched in qualitative terms since the rescaling was done off plots from the paper in question, not a recommended procedure for accuracy.