Level-density fluctuations at the bottom of a potential

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We evaluate trace formulas for various perturbations of two-dimensional harmonic oscillators. Such systems arise naturally in the expansion of generic potentials about local minima. For large enough perturbations, the usual theory for isolated orbits applies and we can reproduce the long and medium-range oscillations in the density of states in terms of the shortest periodic orbits. For small perturbations, or low energies, the Gutzwiller amplitudes diverge due to the approaching degeneracy of the harmonic oscillator. We employ a perturbative analysis of the classical dynamics to give a treatment of the trace formula that is valid near the degenerate harmonic regime. First-order perturbation theory works for generic cases. For certain potentials, such as Hénon-Heiles, discrete symmetries lead to a null result at first order and second-order calculations are necessary to capture the dominant features. [S1050-2947(98)06002-8]

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I. INTRODUCTION

Local harmonic approximation near the minima of potentials is a first step in many physical calculations. In this paper we address some fundamental qualitative changes that can occur in quantum fluctuations of such problems when anharmonic corrections are included. These changes arise whenever the starting harmonic approximation has degenerate frequencies, and are due to breaking of the continuous symmetries that characterize such problems. Such symmetry breaking has a strong effect on the behavior of the trace formula [1,2], which relates fluctuations in the density of states to periodic orbits in the corresponding classical system.

Suppose we start with a harmonic Hamiltonian that has a set of frequencies $(\omega_1, \ldots, \omega_r)$ with respective degeneracies $(k_1, \ldots, k_r)$, so that the frequency ω_1 occurs with multiplicity k_1 and so on. Such might be the case for the vibrational spectrum of a molecule, for example. Trace formulas relate spectral oscillations to the classical periodic orbits of this system which, if we assume the frequencies $(\omega_1, \ldots, \omega_r)$ to be mutually nonresonant, consist of trajectories in which motion is confined to the k_j degrees of freedom corresponding to a single frequency ω_j, all other coordinates being fixed. In this way the problem decouples naturally into consideration of isotropic harmonic oscillators. The orbits for each one occur in $(2k_j-1)$-fold degenerate families, filling each energy shell in the restricted phase space corresponding to ω_j. The effect of anharmonicity is to break the degeneracy of these families, so that generically each one is replaced by a discrete set of isolated periodic orbits.

In the trace formula, the large spectral fluctuations produced by the degenerate family are replaced by the much smaller fluctuations associated with isolated orbits. While any slight anharmonicity breaks the classical structure immediately, the effect is visible in quantal properties only as soon as classical action shifts are of the order of $\hbar$ or bigger. Typically, this means that the lowest levels remain harmonic in character and spectral fluctuations are then progressively suppressed as energy increases. In this paper we offer an analysis of this transition and investigate in detail its behavior for the Hénon-Heiles potential [3] and some variants of it.

Calculation of the effect on the trace formula of the breaking of continuous symmetries was first performed in [4], where the perturbation of generically integrable systems is treated. Related results have been applied to the calculation of magnetic susceptibilities of two-dimensional electron gases in [5], where a small magnetic field breaks the integrability of certain billiard potentials. The breaking of arbitrarily degenerate symmetry, of which the harmonic oscillator is an example, was treated in [6]. Applications of this general calculation to the shell structure in metal clusters and in semiconductor quantum dots in external magnetic fields can be found in [7,8]. The underlying idea in all of these calculations is that a calculation to first order in perturbation theory of the actions entering in the trace formula should be sufficiently accurate to capture the transition to a regime where the periodic orbits are effectively isolated and the standard trace formula for isolated orbits can take over. As pointed out in [9], it is often of great value in practical situations to use a uniform calculation that is valid for arbitrarily large values of the perturbation parameter. In that calculation, a resonance in a two-degree-of-freedom near-integrable sys-

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tem is treated in such a way that the usual Gutzwiller expression is recovered exactly in the limit of moderate to large perturbations. Related calculations in the uniform treatment of bifurcations can be found in [10]. A different extension is considered here—to cases where perturbation theory yields a null result at first order. It is then necessary at least to pass to second order in order to capture the essential features of the transition. The second-order calculation is considerably more complex, but can be shown in the case where the first-order result is systematically zero to result in an explicit, canonically invariant expression for the action shifts relevant to the trace formula.

We concentrate on the problem of a single isotropic harmonic oscillator in two degrees of freedom—higher-dimensional systems bring increased complexity of notation but are not fundamentally different. It is also not difficult to include later the effect of decoupled degrees of freedom. Explicit exact trace formulas for two- and three-dimensional harmonic oscillators have been given in [11]. The treatment of anharmonic deformations in the two-dimensional case within the first order of classical perturbation theory has been explicitly discussed in [6]. We review that calculation in Sec. II and in Sec. III we examine in detail the application of this treatment to a problem in which there is a quartic anharmonicity resulting in a potential that is a fourfold analog of the Hénon-Heiles potential. We find that the analysis successfully predicts the level density oscillations up to energies where orbits are effectively isolated and the usual trace formulas for generic systems works.

For many problems, symmetry considerations lead to a null result at first order in perturbation theory and it is necessary to pass to higher order. Such is the case for the Hénon-Heiles potential, for example, where the anharmonic part of the potential is odd under spatial inversion. We offer in Sec. IV a calculation of action perturbations to second order. For systems in which a systematic symmetry is responsible for a vanishing first-order effect, the second-order shift can be put in a form that is explicitly canonically invariant and derives from a calculation in which perturbations of the trajectories themselves are needed only to first order. In Sec. V we apply this calculation to the case of the original Hénon-Heiles potential, finding good agreement up to a regime where the shortest periodic orbits are sufficiently isolated and the Gutzwiller trace formula reproduces the coarse-grained level density very well [12].

II. TRACES FOR PERTURBED HARMONIC OSCILLATORS

The trace formula for a two-dimensional isotropic harmonic oscillator $H=(p_x^2+p_y^2)/2+\omega^2(x^2+y^2)/2$ can be written as a simple modification of a one-dimensional version as follows:

$$\rho(E)=\frac{E}{(\hbar\omega)^2}\left\{1+2\,\mathrm{Re}\sum_{r=1}^{\infty}e^{2\pi irE/\hbar\omega}\right\}. \tag{1}$$

The term in brackets is proportional to the decomposition of the density of states for a one-dimensional oscillator with energies $E_n=(n+1)\hbar\omega$. The energy factor outside reflects the degeneracy of levels of the two-dimensional system, which grows with energy according to $d_n=n+1\sim E/\hbar\omega$.

Similar trace formulas are available for arbitrary oscillators with distinct frequencies ω_j with respective degeneracies k_j. Explicit examples in two and three dimensions with various symmetries are given in [11]. Some elements of the calculation are described in Appendix A. In addition to the Thomas-Fermi density of states, there is a contribution coming from each orbit family, labeled by the frequency ω_i at which motion takes place. Each additional degree of degeneracy leads to a factor of $E/\hbar\omega_i$, resulting eventually in a term proportional to $E^{k_i-1}/(\hbar\omega_i)^{k_i}$ in the amplitude. The transverse degrees of freedom are accounted for by a monodromy matrix term $\sqrt{-\det(M^r-I)}=\Pi_{j\neq i}[2i\sin r\pi\omega_j/\omega_i]^{k_j}$ in the denominator for the rth repetition of the primitive orbit. It just remains to clear up numerical factors and phases, and this is done in Appendix A. In the following, the effect of perturbation on each orbit contribution in this most general case is similar to the calculation for an isotropic harmonic oscillator of the same degeneracy, except that the monodromy terms must be carried along and expressions for phase shifts must be extended somewhat. Little is lost, therefore, in restricting the discussion to the isotropic case, as we do in the main text. Furthermore, degeneracies greater than two are different only in the degree of complexity of orbit labeling and the essential idea is captured by the two-dimensional calculation, so that we may concentrate on that case particularly.

A semiclassical calculation of Eq. (1) from first principles is complicated [13] due to the fact that periodic orbits are highly degenerate in the harmonic oscillator, filling all of phase space. An evaluation of the trace of the Green's function using the stationary phase approximation leads to a sum over orbit repetitions as above. Each contributes an integral over the degenerate orbit family filling the energy shell $H=E$ [6,14], resulting in the amplitude proportional to E seen in Eq. (1). Despite the comparative complexity of this calculation, however, it is necessary to keep it in mind if we wish to treat symmetry breaking perturbations. This is because every orbit is affected differently by the perturbation and the manner in which each contributes individually is of relevance, not just the collective final result.

In order to proceed, we will discuss in detail the labeling of individual orbits in the harmonic oscillator and its relevance for constructing the trace formula. This labeling is achieved using the symmetry group U(n) of the isotropic harmonic oscillator in n dimensions. Assume that a canonical change of coordinates has been performed so that the Hamiltonian is $\Sigma_l\omega(Q_l^2+P_l^2)/2$. Then the symmetry is simply understood if we identify each point in phase space with an n-dimensional complex vector $|\psi\rangle$ whose lth component is Q_l+iP_l. The Hamiltonian is then

$$H=\frac{\omega}{2}\langle\psi|\psi\rangle, \tag{2}$$

which is clearly invariant under unitary rotations of $|\psi\rangle$—hence the U(n) symmetry. Under time evolution, the vector $|\psi\rangle$ is simply multiplied by the phase factor $e^{-i\omega t}$. If we fix the energy, we can therefore make a one-to-one correspondence between orbits in phase space and rays $|\psi\rangle\langle\psi|$

in the projective vector space. Points in the projective space are conveniently labeled by elements $u \in \mathrm{U}(n)$—we fix some reference state $|\psi_0\rangle$ and define $|\psi(u)\rangle = u|\psi_0\rangle$. The only problem with this is that the labeling is not unique since if we precede u with any unitary matrix v such that $v|\psi_0\rangle = e^{i\alpha}|\psi_0\rangle$, then uv defines the same orbit as u. Therefore, for a one-to-one labeling of periodic orbits of fixed energy, we use the space $\mathrm{U}(n)/\mathrm{Fix}(\psi_0)$ of left cosets of the subgroup $\mathrm{Fix}(\psi_0)$ of transformations leaving $|\psi_0\rangle$ invariant up to a phase. This subgroup has the structure $\mathrm{U}(1)\times\mathrm{U}(n-1)$—the first component corresponding to multiplication of $|\psi_0\rangle$ by a phase and the second to unitary rotation in the space orthogonal to $|\psi_0\rangle$.

In two degrees of freedom, this procedure results in the construction of the Poincaré sphere. Phase-space points are identified with two-component spinors in this case. Choosing for a reference spinor the spin-up state $|+\rangle$, we find that the corresponding reference orbit is invariant under the application of unitary matrices of the form $e^{i\alpha+i\beta\sigma_3}$ (we denote by $(\sigma_1,\sigma_2,\sigma_3)$ the Pauli sigma matrices). Removing this degeneracy, distinct orbits are obtained from transformations of the form $|\hat{n}\rangle = e^{-i(\phi/2)\sigma_3}e^{-i(\theta/2)\sigma_2}|+\rangle$. In this way every orbit of a given energy is uniquely labeled by a vector $\hat{n}$ on the unit sphere, for which (θ,ϕ) are the polar coordinates. For concrete calculations, we will take the initial conditions of the orbit from the real and imaginary parts of the components of $|\hat{n}\rangle$. This convention is discontinuous along the meridian $\phi=0$ because the initial coordinates depend on half-angle trigonometric functions. However, when we deal with quantities that depend only on the orbits themselves, this discontinuity disappears and we will be left with whole-angle trigonometric functions defining single-valued functions on the sphere.

In the trace formula, summation over the degenerate family of orbits at each energy E is achieved by integrating over this sphere of orbits with a solid angle as a measure. For the unperturbed system, this integration is done trivially and is no longer evident in the result quoted in Eq. (1). However, this aspect of the calculation is important for the treatment of systems with a symmetry-breaking perturbation. Then the contributing orbits violate the condition of periodicity to some small degree and as a result a slight action variation $\Delta S(\hat{n})$ is introduced in the integration over the orbit family. This is taken approximately into account by including a modulation factor

$$\mathcal{M} = \frac{1}{4\pi}\int d\Omega\, e^{i\Delta S(\hat{n})/\hbar}, \tag{3}$$

with the unperturbed phase of the contribution of each orbit family, as described fully in [6]. The strict definition of the action variation ΔS depends on the representation in which one computes the trace. We will give a more complete discussion of this in Sec. IV. For the moment, we will just state that a simple calculation to first order in classical perturbation theory gives the following approximation:

$$\Delta S(\hat{n}) = \alpha \oint_{\gamma(\hat{n})} -H_1 dt + O(\alpha^2), \tag{4}$$

where the perturbed Hamiltonian is $H = H_0 + \alpha H_1$ and $\gamma(\hat{n})$ is the orbit defined by the unit vector $\hat{n}$. This expression is independent of the choice of initial condition along the orbit, and of the representation in which the trace is computed. We always expect the dominant contribution to the trace formula to be a canonical invariant in this way, but with higher-order corrections, this situation might change.

In generic perturbations of the harmonic oscillator, use of Eq. (4) should capture the essential behavior of the trace until the perturbation is large enough that any surviving isolated periodic orbits can be successfully treated by the usual Gutzwiller formula. There are cases, however, the Hénon-Heiles potential among them, where some discrete symmetry of the perturbation results in a vanishing first-order perturbation. In such cases, it is necessary to use second-order perturbation theory to predict the leading behavior of ΔS. This calculation is considerably more complex because trajectories in the perturbed system must be calculated explicitly and the representation in which the action is defined plays a more prevalent role. We defer this discussion to a later section and instead illustrate the generic first-order calculation with a Hénon-Heiles-type perturbation for which this complication is unnecessary.

Finally, we note that if the dimension of the isotropic oscillator is greater, one still modulates the contribution of an orbit family with a function of the form given in Eq. (3), except that now the integration measure is that of the larger projective space $\mathrm{U}(n)/\mathrm{Fix}(\psi_0)$ discussed earlier. The presence of other frequencies is accounted for by including the monodromy terms of Appendix A.

III. A FOURFOLD HÉNON-HEILES DEFORMATION

We illustrate the general discussion of the previous section with an application to a harmonic oscillator perturbed by adding a potential $\alpha V(x,y)$, where

$$V(x,y) = \frac{3}{2}x^2y^2 - \frac{1}{4}(x^4+y^4) = -\frac{1}{4}r^4\cos 4\theta. \tag{5}$$

In Fig. 1 we show a contour plot in the (x,y) plane for $\alpha = 1$. The potential resembles that of Hénon-Heiles, but with a fourfold instead of a threefold symmetry. Before applying the perturbative analysis, we describe the isolated periodic orbits that dominate spectral fluctuations at larger energies. They are shown in Fig. 1 for the energy at the saddle points of the potential, which equals $E^* = \omega^4/(4\alpha)$. A_1 denotes a straight-line oscillation along a symmetry axis connecting two saddle points. It is stable up to energy $E \simeq 0.85E^*$ and then undergoes a sequence of increasingly frequent bifurcations, alternating between being stable and unstable, until it vanishes at $E = E^*$. A_2 is another straight-line oscillation, this time along the diagonals; this orbit is stable up to energies above $E = 2E^*$. The third orbit C is a rotation and is always unstable. Each of these three orbits has a twofold degeneracy: the straight-line librations because of the choice of their orientation in the (x,y) plane, and orbit C because of its two distinct versions connected by time reversal. When these isolated orbits are sufficiently separated from each other in phase space, the standard Gutzwiller trace formula [1] for the oscillating part of the level density applies:

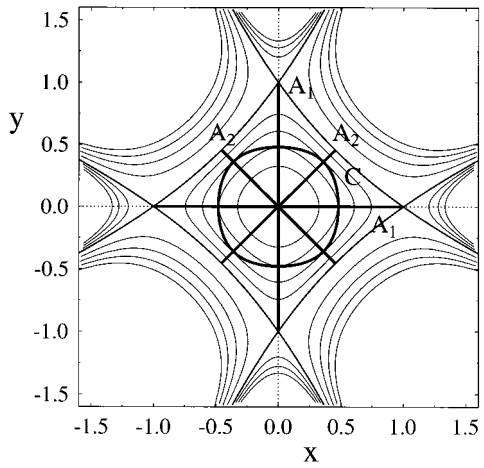

FIG. 1. Equipotential contours of the quartic HH potential (5) for $\alpha=1$. Also shown (by heavy lines) are the three shortest types of periodic orbits in this potential: A_1, A_2, and C (evaluated at the saddle-point energy $E=E^*$).

$$\delta\rho(E)=\sum_{\rm po}\ \mathcal{A}_{\rm po}\cos\left[\frac{S_{\rm po}}{\hbar}-\sigma_{\rm po}\frac{\pi}{2}\right]. \tag{6}$$

The amplitudes $\mathcal{A}_{\rm po}$ and the actions $S_{\rm po}$ of the periodic orbits must be evaluated numerically at each energy E; the Maslov indices have been found to be $\sigma_{A_1}=5$ (below the bifurcations), $\sigma_{A_2}=3$, and $\sigma_C=4$.

The dynamics of this system has a significant chaotic component near the saddle point energy E^*. Figure 2 shows some trajectories in a surface of section for this energy. Regular and chaotic domains coexist; the circles in the middle of the regular regions are elliptic fixed points and the crosses are hyperbolic fixed points. Most of phase space is chaotic at this critical energy, though to a lesser extent than in the equivalent picture for the regular Hénon-Heiles potential. For such moderate to large energies, the dynamics is generic and the trace formula involves summation over isolated orbits and narrow resonances corresponding to rational tori. At lower energies, however, the approximate symmetry

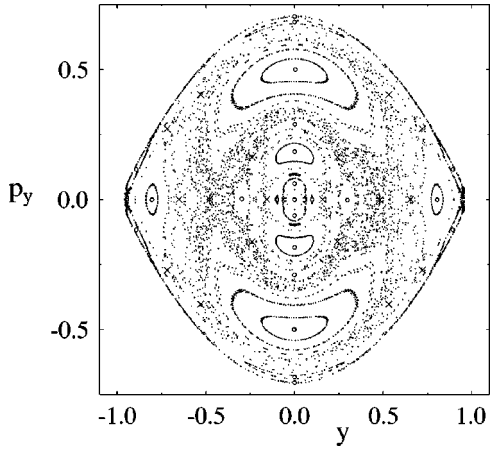

FIG. 2. Poincaré surface of section of the quartic HH potential at the saddle-point energy E^*. The small circles and crosses indicate elliptic and hyperbolic fix points, respectively, corresponding to periodic orbits.

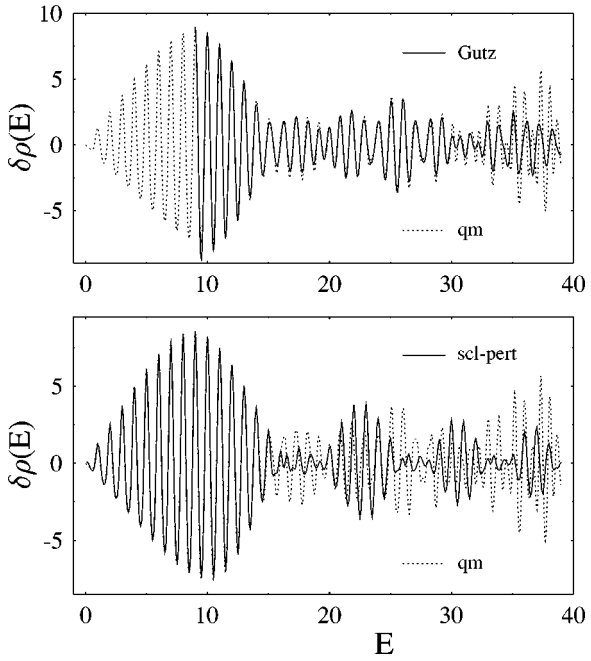

FIG. 3. Oscillating part of level density of the quartic HH potential with $\alpha=0.0064$, Gaussian averaged with $\gamma=0.25\hbar\omega$. Energy units are $\hbar\omega$. Top: semiclassical result of the Gutzwiller trace formula for isolated orbits (solid line), compared to the quantum result (dotted line); the semiclassical result diverges for small energies and is not shown below $E=9\hbar\omega$. Bottom: semiclassical first-order perturbative result (11) (solid line), compared to the quantum result (dotted line).

of the harmonic oscillator will play an important role and it will be necessary to apply the analysis of the previous section.

The quantum-mechanical eigenvalue spectrum was calculated, as in [12], by diagonalization of Eq. (5) in the basis of the unperturbed harmonic oscillator. Some typical results for the level density are shown in Fig. 3 for $\alpha=0.0064$ where the critical energy is $E^*=39\hbar\omega$. Since our focus is not on the semiclassical quantization nor on the short-range correlations in the quantum spectrum, but on the long-range fluctuations of the coarse-grained spectrum, we have averaged the level density by convoluting it with a Gaussian over the energy range $\gamma=0.25\hbar\omega$. In the top part of the figure, the result of the Gutzwiller trace formula (6), using only the lowest harmonics ($r=1$) of the orbits A_1, A_2, and C, is shown as a solid line. The quantum-mechanical result is shown as a dotted line. In the region $10\hbar\omega<E<30\hbar\omega$, the agreement is very good, including details of the beating pattern that comes about through the interference of the three periodic orbits.[1] The growing discrepancies when $E>30\hbar\omega$ arise because some other orbits with comparable actions arise above $E\simeq 0.85E^*=33\hbar\omega$, which are not taken into account. For low energies, the Gutzwiller result diverges (it

[1]We should point out that the amplitude of orbit A_1 formally diverges at the bifurcations points of orbit A_1 at $E>0.85E^*$. It was simply smoothly interpolated through these points, as shown in Fig. 4 below. Errors introduced by skipping over the singularities are not evident after the energy averaging used to obtain the figure.

is not shown in the figure for $E<9\hbar\omega$) as a result of the approaching symmetry of the unperturbed harmonic oscillator.

Here we must apply the perturbative analysis described in the previous section. It is a straightforward matter to evaluate the action shift in Eq. (4) for the rth repetition of an orbit with initial conditions defined by the spinor $|\hat{n}\rangle$. One gets

$$\Delta S=\alpha\left(\frac{2\pi r}{\omega}\right)\frac{3E^2}{8\omega^4}(n_1^2-n_3^2). \tag{7}$$

Now define the dimensionless variable x by

$$x=\frac{3\pi r\alpha E^2}{4\hbar\omega^5}=\frac{3\pi r}{16}\left(\frac{E^2}{\hbar\omega E^*}\right). \tag{8}$$

The resulting modulation factor is

$$\mathcal{M}(x)=\frac{1}{4\pi}\int d\Omega e^{ix(n_1^2-n_3^2)}. \tag{9}$$

It is a real function since the integration measure is symmetric with respect to interchange of n_1 and n_3 while the phase is odd. The harmonic case is recovered in the limit $x\to 0$, which gives $\mathcal{M}(0)=1$. This limit corresponds to $\alpha\to 0$ *or* $E\to 0$ (or both). As x increases, $\mathcal{M}(x)$ decreases and decays to zero in an oscillating manner as $x\to\infty$. When x is large the formula for isolated orbits should be recovered in an approximate way, but for moderate values of x it is necessary to use Eq. (9) fully. In evaluating this integral, we are free to rotate the coordinate system on the sphere at will. If we rotate $n_1^2-n_3^2$ into $2n_1n_3$, the integral can be evaluated as follows:

$$\mathcal{M}(x)=\frac{1}{4\pi}\int d\Omega e^{2ixn_1n_3}=\frac{1}{2}\int_0^\pi \sin\theta\, J_0(x\,\sin 2\theta)d\theta$$

$$=\frac{\pi}{2\sqrt{2}}J_{-1/4}\left(\frac{x}{2}\right)J_{1/4}\left(\frac{x}{2}\right). \tag{10}$$

The last line is obtained from an identity on p. 150 of [15] following a rescaling of the integration variable and some cancellation.

Modifying Eq. (1) by including this modulation factor, we obtain the perturbative trace formula for the oscillating part of the level density:

$$\delta\rho(E)=\frac{2E}{(\hbar\omega)^2}\sum_{r=1}^{r_{\max}}\mathcal{M}(x)\cos(2\pi rE/\hbar\omega). \tag{11}$$

Note that since x must be of order unity or less for the perturbation theory to apply, the sum over the repetition index r has to be cut at a maximum value $r_{\max}$, which is not too large.

The numerical result obtained from Eq. (11) is shown as a solid line in the bottom part of Fig. 3. It is compared with the the quantum-mechanical result shown as a dotted line (both averaged over the same energy range $\gamma=0.25\hbar\omega$). The agreement in the low-energy limit is very good. Note that both of the two lowest harmonics ($r=1$ and $r=2$) had to be used to reproduce correctly the asymmetry of the quantum result below $E\sim 12\hbar\omega$. (For larger energies, the contributions from $r=2$ are negligible.) Above $E\simeq 14\hbar\omega$, the perturbative result starts differing from the exact one; it reproduces some of the beat structure but with incorrect amplitudes ($E\simeq 14\hbar\omega$ corresponds to $x\simeq 3.0$ for the lowest harmonic).

It is instructive to investigate the asymptotic behavior of the modulation factor as $x\to\infty$. This is done by evaluating the solid angle integration using the stationary phase approximation. The three isolated orbit-types A_1, A_2, and C then emerge as critical points of the phase $n_1^2-n_3^2$. The harmonic orbits labeled by these critical points on the sphere approximate the isolated orbits in the perturbed system. For example, the pair of saddle points $(n_1,n_2,n_3)=(0,\pm 1,0)$ label circular orbits with maximal angular momentum and correspond to the orbit-type C. Similarly, the two saddle points at $(n_1,n_2,n_3)=(0,0,\pm 1)$ correspond to the two librating orbits A_1 and those at $(n_1,n_2,n_3)=(\pm 1,0,0)$ to the orbits A_2. The asymptotic amplitudes for $r=1$ are predicted from the stationary phase evaluation to vary as

$$\mathcal{A}_C(E)\sim\frac{E}{(\hbar\omega)^2}\frac{1}{2x}=\frac{8}{3\pi(\hbar\omega)}\frac{E^*}{E},$$

$$\mathcal{A}_{A_1}(E)\sim\mathcal{A}_{A_2}(E)\sim\frac{E}{(\hbar\omega)^2}\frac{1}{2\sqrt{2}x}=\frac{8}{3\sqrt{2}\pi(\hbar\omega)}\frac{E^*}{E}. \tag{12}$$

The resulting oscillations are valid only when x is neither too small (so that the underlying stationary phase approximation is valid) nor too large (so that the perturbative procedure is still good). In this intermediate regime the results are close to those of the usual Gutzwiller formula. When x is small and the perturbative expansion valid, the expressions (12) correctly reproduce the diverging Gutzwiller amplitudes of Eq. (6) determined numerically, as shown in Fig. 4.

IV. HIGHER-ORDER THEORY

For the standard Hénon-Heiles potential (treated in the following section), the basic first-order calculation used in the previous section gives a null result and it is necessary to pass to second order to calculate the dominant effect. In this section, we outline the calculation of action perturbations at higher order. Much of this discussion applies to problems other than the harmonic oscillator, so we will keep the notation general as long as there is no additional cost.

For first-order shifts of the action, it was sufficient to evaluate a simple integral around the unperturbed orbit. At higher orders, it is necessary to evaluate perturbations of the orbit itself. Therefore, let us develop a perturbation expansion

$$\gamma(t;\alpha)=\gamma_0(t)+\alpha\gamma_1(t)+\alpha^2\gamma_2(t)+\cdots \tag{13}$$

for the orbit γ that replaces the periodic orbit γ_0 in the perturbed system. For an arbitrary function $F(q,p)$ on phase space, it is convenient to denote by $X_F=(\partial F/\partial p,-\partial F/\partial q)$

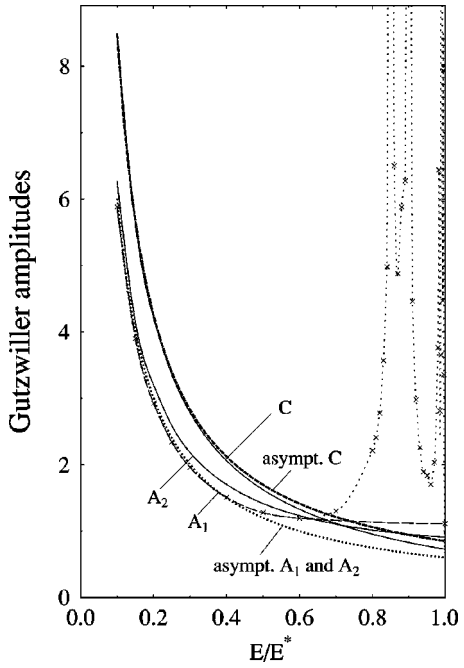

FIG. 4. Amplitudes in the trace formula of the three leading classical orbits A_1, A_2, and C in the quartic HH potential. The thin lines are the numerical result using the Gutzwiller trace formula for isolated orbits. (The values for the orbit A_1 are given by crosses; they diverge at the bifurcation points for $E>0.85E^*$ and have been smoothly interpolated by the long-dashed thin line.) The heavy dashed and dotted lines are the asymptotic predictions (12) for the C orbit (dashed) and the A_1 and A_2 orbits (dotted).

the corresponding Hamiltonian flow vector in phase space. Then, insertion of the expansion for γ in the equations of motion

$$\dot{\gamma}_0(t)+\alpha\dot{\gamma}_1(t)+\alpha^2\dot{\gamma}_2(t)+\cdots = X_{H_0}(\gamma_0+\alpha\gamma_1+\alpha^2\gamma_2+\cdots) + \alpha X_{H_1}(\gamma_0+\alpha\gamma_1+\cdots) \tag{14}$$

yields, at first order in α,

$$\dot{\gamma}_1(t)=\gamma_1(t)\cdot\nabla X_{H_0}(t)+X_{H_1}(t). \tag{15}$$

Here, and in the future, we use the notation that when phase-space functions are to be evaluated at $\gamma_0(t)$, we simply use t as an argument. At higher orders, we obtain identical equations of motion for $\gamma_n(t)$, except that the inhomogeneous term X_{H_1} is replaced by more complicated expressions depending on the solutions at lower orders. A good geometrical account of the systematic expansion is given in [16]. We will concentrate on the first-order calculation.

The homogeneous part of Eq. (15) is the usual linearized equation of motion for unperturbed dynamics around the periodic orbit $\gamma_0(t)$. This fact explains the first term in the solution,

$$\gamma_1(t)=M(t,0)\gamma_1(0)+\Xi(t). \tag{16}$$

We denote by $M(t,t')$ the symplectic matrix linearizing motion from a neighborhood of $\gamma_0(t')$ to one of $\gamma_0(t)$ in unperturbed dynamics. For the harmonic oscillator it is simply $M(t,t')=e^{-\omega J(t-t')}$, where J is the unit symplectic matrix. The second part of the solution is

$$\Xi(t)=\int_0^t dt' M(t,t')X_{H_1}(t'), \tag{17}$$

which is likewise a vector in the tangent space at $\gamma_0(t)$. This contribution reflects the fact that $M(t,t')$ acts as a Green's function for the linearized equations of motion. This second part is independent of the boundary conditions placed on $\gamma(t)$ and will turn out to dominate the second-order action perturbations for the Hénon-Heiles potential.

Before we proceed, it is necessary to specify the boundary conditions placed on the orbits so that $\gamma_1(0)$ may be computed. These boundary conditions arise from the stationary phase calculation of the trace of the Green's function and depend on the representation used for that purpose, so we must examine that calculation more carefully. In a system such as the harmonic oscillator where periodic orbits are very degenerate, one must be careful with the choice of representation so that the Green's function is well defined. An acceptable choice is to evaluate the trace in a mixed representation, using $\mathrm{Tr}\hat{G}(E)=\int dpdx' e^{ipx'/\hbar}\langle p|\hat{G}(E)|x'\rangle$. This leads to an integration over coordinates $\overline{z}=(x',p)$ of orbits at energy E that start at position x' and end with momentum p. [We will keep the initial coordinates $z'=(x',p')$ primed and the final coordinates $z=(x,p)$ unprimed.] These contribute with a phase dominated by the action $S(p,x',E)=(p-p')x'-\int x dp$ whose derivative $\nabla_{\overline{z}}S(\overline{z},E)=J(z-z')$ results in the stationary phase condition selecting periodic orbits $z=z'$. For the unperturbed harmonic oscillator, one integration can be done using stationary phase and the remaining $2n-1$ result in the integration over the orbit family with the measure discussed in the previous section. In the perturbed system, we retain this sequence, the difference being that the integration over the orbit family is nontrivial, leading to a modulation factor of the type shown in Eq. (3).

The boundary conditions for $\gamma(t)$ arise from a choice of integration direction in the first stationary phase integral. This amounts to making a choice, for each point z_0 on the orbit manifold, of a vector ζ along which we require that S be stationary. It leads to the condition

$$0=\zeta\cdot\nabla_{\overline{z}}S(\overline{z},E)=\zeta\cdot J(z-z')=\Omega(\zeta,z-z'), \tag{18}$$

where $\Omega(\xi,\eta)=\xi^T J\eta$ is the symplectic form (T denotes transpose). For systems other than the harmonic oscillator, we would choose a set of vectors ζ_a whose number is the codimension of the orbit family in phase space. It is reasonable to impose the condition that these vectors transform under the symmetry group according to $\zeta(g\cdot z_0)=g\cdot\zeta(z_0)$—for example, $\zeta(z_0)=z_0$ is a sensible choice for the harmonic oscillator. The resulting equations define a surface in phase space of the same dimension as the periodic orbit family and coinciding with it when $\alpha=0$. Stationary phase integration of the trace along the direction defined by ζ leaves an integral over this surface, which we choose to

evaluate using the measure defined by the group as in Eq. (3). It should be noted, however, that the surface is not invariant under the symmetry of H_0, and so there is some ambiguity in labeling points on it with elements of the symmetry group. This will present itself in our calculation as a freedom in the choice of $\gamma_1(0)$ after the condition in Eq. (18) has been imposed. This freedom can be removed by explicit reference to the representation used for the calculation, but the dominant contributions to which we confine our attention, being independent of representation, should ultimately not depend on this choice. Finally, we point out that variation in amplitude is ignored here, but should be included for a consistent treatment of corrections beyond the dominant term (see [9], for example).

Let us now return to the imposition of boundary conditions on $\gamma_1(t)$, for which we once again confine our attention to the harmonic oscillator. It is necessary to take into account the fact that the time of the contributing orbit might also vary with α. So let us develop a perturbation expansion for it:

$$T(\alpha)=T_0+\alpha T_1+\alpha^2 T_2+\cdots. \tag{19}$$

The first-order estimate for $z-z'$ is then given by

$$\gamma_1(T_0)+T_1 X_{H_0}(0)-\gamma_1(0)=\Xi_0+T_1 X_{H_0}(0), \tag{20}$$

where we used the fact that $M(T_0,0)=I$ for the harmonic oscillator. With this, and making use of the identity $\Omega(X_{H_0},\zeta)=dH_0(\zeta)$ $(\equiv\zeta\cdot\nabla H_0)$, the stationary phase condition in Eq. (18) becomes

$$T_1 dH_0(\zeta)=\Omega(\zeta,\Xi_0), \tag{21}$$

where $\Xi_0=\Xi(T_0)$. This determines T_1 uniquely.

We are now ready to develop the expansion for action. Equation (4) results in an expression $\partial S/\partial\alpha=\oint -H_1 dt$ for the first derivative of the action that is valid for any value of α as long as we deal with boundary conditions correctly (and we will). Taking one further derivative we then get

$$\frac{\partial^2 S}{\partial\alpha^2}=-H_1(0)T_1+\oint -dH_1(\gamma_1(t))dt. \tag{22}$$

As suspected, there is some ambiguity in this result corresponding to the choice of $\gamma_1(0)$. In any case the second-order action shift in the expansion $\Delta S=\alpha S_1+\alpha^2(S_2+R_2)+\cdots$ can be written as the sum of a representation-independent part,

$$S_2=\frac{1}{2}\oint -dH_1(\Xi(t))dt, \tag{23}$$

and a possibly representation-dependent part,

$$R_2=-\frac{1}{2}H_1(0)T_1+\frac{1}{2}\oint -dH_1(M(t,0)\gamma_1(0))dt. \tag{24}$$

A significant simplification occurs for systems, such as the standard Hénon-Heiles potential, for which the first-order action shift vanishes systematically due to some discrete symmetry. One finds in such cases that the same symmetry considerations result in $\Xi_0=0$ and Eq. (21) then gives $T_1=0$. Furthermore, $\Xi_0=0$ is equivalent to the fact that $\oint -dH_1(M(t,0)\xi)dt=0$ for arbitrary constant vectors ξ. Therefore we find that $R_2=0$ and the second-order action shift is given by the representation-independent expression for S_2 in Eq. (23). This confirms our expectation that the dominant action shift should never depend on representation.

We also note that there is a straightforward generalization to the case where there are additional degrees of freedom uncoupled to the harmonic oscillator before perturbation. The problem of finding $\gamma_1(t)$ decouples into the one above for the central harmonic degrees of freedom and a separate calculation in the remaining degrees of freedom for which the corresponding components of $\gamma_1(0)$ vanish. The action shift is then accounted for simply by including the additional components of $\Xi(t)$ in Eq. (23).

V. THE STANDARD HÉNON-HEILES POTENTIAL

We will now apply the second-order theory developed in the previous section to the standard Hénon-Heiles potential. At low energies this is a perturbation of the harmonic oscillator by the potential $\alpha V(x,y)$, where

$$V(x,y)=x^2y-\tfrac{1}{3}y^3=-\tfrac{1}{3}r^3\cos 3\theta. \tag{25}$$

As mentioned before, the average of this potential around any orbit of the harmonic oscillator is zero and as a result there are no first-order action shifts according to Eq. (4). We will therefore apply the analysis of the previous section to calculate action shifts at second order.

Let us write the phase-space gradient of this potential as the column vector

$$\nabla H_1=\begin{pmatrix}\nabla V\\0\end{pmatrix}=\begin{pmatrix}2xy\\x^2-y^2\\0\\0\end{pmatrix}. \tag{26}$$

Then the second-order action shift in Eq. (23) is given in coordinates by

$$S_2=-\frac{1}{2}\oint dt\int_0^t dt'[e^{-\omega J t}\nabla H_1(t)]^T\cdot J\cdot[e^{-\omega J t'}\nabla H_1(t')], \tag{27}$$

where T denotes transpose here. Evaluation of these integrals is tedious but straightforward. The result for an orbit whose initial conditions are defined by $|\hat{n}\rangle$ is

$$S_2=\frac{\pi r}{6\omega^7}(5E^2-7\omega^2L^2)=\frac{\pi r E^2}{6\omega^7}(5-7n_2^2), \tag{28}$$

where L is the angular momentum of the unperturbed orbit. We denote

$$x=\frac{\pi r\alpha^2E^2}{\hbar\omega^7}=\frac{\pi r}{6}\left(\frac{E^2}{\hbar\omega E*}\right), \tag{29}$$

where in this section $E^*=\omega^6/(6\alpha^2)$ is the saddle energy for the potential in Eq. (25). The modulation factor is then integrated in terms of Fresnel functions as follows:

$$\mathcal{M}(x)=\frac{1}{4\pi}\int d\Omega e^{ix(5-7n_2^2)/6}=\int_0^1 du e^{ix(5-7u^2)/6}$$

$$=e^{5ix/6}\frac{1}{\xi}[C(\xi)-iS(\xi)],\quad \xi=\sqrt{\frac{7x}{3\pi}}. \tag{30}$$

Since this modulation factor is complex, we have to write the perturbed trace formula for the oscillating part of the level density as

$$\delta\rho(E)=\frac{2E}{(\hbar\omega)^2}\mathrm{Re}\sum_{r=1}^{\infty}\mathcal{M}(x)e^{2\pi irE/\hbar\omega}. \tag{31}$$

A striking feature of the phase function in Eq. (28) is that, depending only on the energy and angular momentum, it is invariant with respect to spatial rotations. This continuous symmetry is not shared by the potential itself. It is an approximate symmetry that emerges in the first few terms of the perturbation expansion but which will disappear at higher order. In fact, an examination of the terms following suggests that the third-order action shift S_3 retains circular symmetry before it is finally broken at fourth order in S_4 (which is proportional to E^3). Here we will satisfy ourselves with a truncation at second order, for which the symmetry remains.

As for the first-order calculation considered in Sec. III, critical points of the phase function on the sphere should correspond to the isolated periodic orbits that replace the orbit family under perturbation. For the Hénon-Heiles potential (25) the shortest isolated orbits can be labeled by A, B, and C; a detailed description of these orbits is given in [12]. As in Sec. III, C is a rotation and is twofold degenerate, corresponding to the two senses of rotation. In the phase function these orbits correspond to the minima at $(n_1,n_2,n_3)=(0,\pm1,0)$. Orbits A and B are each threefold degenerate librations. In the limit $E\to0$, they approach linear orbits with zero angular momentum passing through the origin. In the phase function S_2 there is actually a continuous circle of critical points on the two meridians defined by $n_2=0$. The isolated orbits A and B approach orbits that lie on this circle. When the higher-order correction S_4 is included, this circle will be replaced by an alternating sequence of 3 maxima and 3 saddles corresponding to these isolated orbits.

In Fig. 5 we compare the result of the perturbative trace formula (31) with exact quantum-mechanical results and with those obtained from the Gutzwiller trace formula (6) including orbits A, B, and C [12]. The agreement of the present perturbative treatment with the exact quantum calculation is good at low energies, where the Gutzwiller formula fails, successfully capturing the suppression of shell oscillations for the first couple of beats. Before the perturbative treatment starts to fail, it has reached the Gutzwiller result; there is a reasonable overlap of both semiclassical results in the range $E\sim(35-40)\hbar\omega$. (Note that the critical energy in this example is at $E^*=104\hbar\omega$.)

The stationary phase integration of the modulation factor (30) around $(n_1,n_2,n_3)=(0,\pm1,0)$ predicts the amplitude of the orbit C contribution to the trace formula to go like

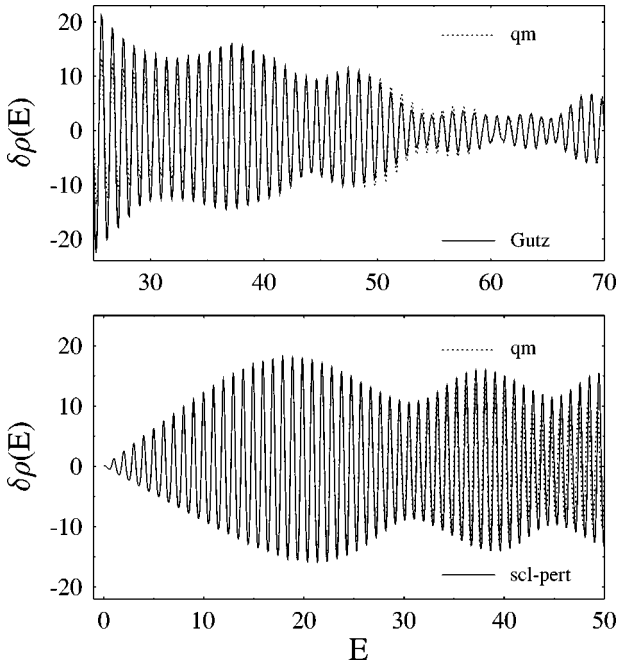

FIG. 5. Same as Fig. 3 for the standard cubic HH potential (25) with $\alpha=0.04$. In the lower part, we show the semiclassical second-order perturbative result of Eq. (31).

$$\mathcal{A}_C(E)\sim\frac{3E}{(\hbar\omega)^2}\frac{1}{7x}=\frac{18}{7\pi(\hbar\omega)}\frac{E^*}{E}. \tag{32}$$

As shown in Fig. 6, this prediction agrees with the numerically evaluated Gutzwiller amplitudes from Ref. [12] extremely well, even up to the critical energy $E=E^*$. This

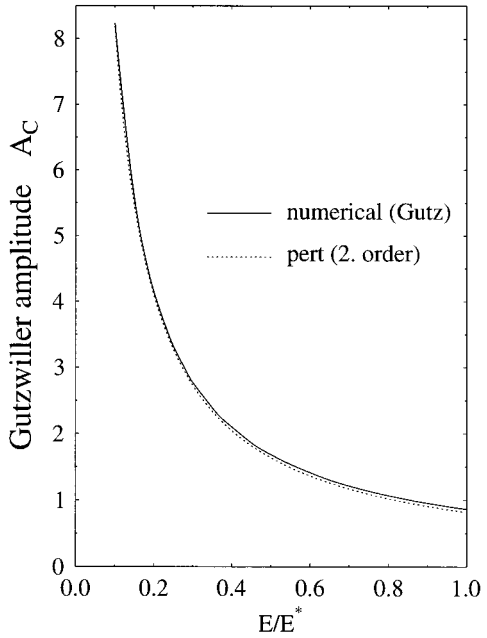

FIG. 6. Amplitude of the circulating orbit C in the trace formula for the standard HH potential. Solid line: numerical result using the Gutzwiller trace formula; dashed line: asymptotic prediction (32) in the present second-order perturbation theory by stationary phase integration of the modulation factor.

shows us that the breakdown of the present second-order perturbation treatment found already at lower energies in Fig. 5 is mainly due to the fact that it does not yield the isolated orbits A and B.

VI. CONCLUSION

We have shown that the suppression of level density fluctuations as energy increases from the bottom of potential wells can be modeled by perturbative treatment of harmonic potentials. This suppression arises from the breaking of SU(n) symmetries characterizing multidimensional harmonic oscillators, which appears because of the increased importance of anharmonicities at higher energies.

For most systems a perturbative analysis of the classical dynamics to first order is sufficient to capture the essential behavior. This has been demonstrated by explicit calculation for a fourfold version of the Hénon-Heiles potential. In certain problems with a discrete symmetry, such as the usual Hénon-Heiles potential, it is necessary to compute perturbations of the classical action to second order. This is considerably more complex but was seen to yield a straightforward canonically invariant result. Explicit comparison with numerical calculations for the Hénon-Heiles potential has shown that the second-order calculation captures the most important features in such cases.

We finally note that the Hénon-Heiles potential (25) and potentials of the form (5) or similar were originally used in an astrophysical context as simple models for flat galaxies [3,17]. But there may actually also be use for this type of potential for modeling the confinement potential in a semiconductor quantum dot of appropriate shape [8,18].

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APPENDIX: ARBITRARY HARMONIC OSCILLATORS

In this Appendix we give the leading-order terms in the semiclassical trace formula for an arbitrary harmonic oscillator in which several nonresonant (i.e., incommensurate) frequencies ω_j occur with the degeneracies k_j. The periodic orbits are labeled by the index i of the frequency to which their motion is constrained, and the number r of repetitions of the primitive orbit. Summing over repetitions of a primitive orbit family i, we obtain the following contribution at lowest order[2] in $\hbar$ to the density of states:

$$\rho_i(E)=\frac{2}{\hbar\omega_i}d_i(E)\mathrm{Re}\sum_{r=1}^{\infty}\mathcal{A}_{ir}e^{2\pi riE/\hbar\omega_i}. \tag{A1}$$

Here,

$$d_i(E)=\frac{1}{(k_i-1)!}\left[\frac{E}{\hbar\omega_i}\right]^{k_i-1} \tag{A2}$$

is a classical approximation to the quantum mechanical degeneracy $(n+k-1)!/n!(k-1)!$ of a state with energy $E=(n+k/2)\hbar\omega_i$ in a k-fold degenerate harmonic oscillator. We note in passing that $d_i(E)/\hbar\omega_i$ is the Thomas-Fermi density of states [2] for an isotropic harmonic oscillator of dimension k_i and frequency ω_i. The amplitudes $\mathcal{A}_{ir}$ in Eq. (A1) are given by

$$\mathcal{A}_{ir}=(-1)^{rk_i}\prod_{j\neq i}[2i\sin(r\pi\omega_j/\omega_i)]^{-k_j}; \tag{A3}$$

they come from the amplitude terms $\sqrt{-\det(M_j^r-I)}$ associated with the monodromy matrices M_j for the motion in the degrees of freedom transverse to the orbit family [11].

To account for perturbations of this system, each such contribution is multiplied by a modulation factor obtained by averaging the phase shift over the corresponding orbit family in phase space, as described in the main text.

[2]Correction terms of higher order in $\hbar$, both to the Thomas-Fermi level density and its oscillating part, may be found in some examples given in [2,11].

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