Near-integrable systems: Resonances and semiclassical trace formulas

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Trace formulas relate the quantum density of states to the properties of the periodic orbits of the underlying classical system. The resulting expressions depend critically on the nature of the dynamics and whether the orbits are stable or unstable. Several open questions exist for the class of classical systems that are near integrability. The most important consequence of a generic perturbation to an integrable system is the creation of resonances. We derive generalized expressions appropriate for resonances and apply them to a system that can be taken as a paradigm for the transition from regular to chaotic dynamics. [S1063-651X(96)06506-3]

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I. INTRODUCTION

Twenty-five years ago, Gutzwiller derived a remarkable semiclassical relationship between the density of states in a quantum system and the properties of the periodic orbits in the underlying classical mechanical system [1]. Known as the ''trace formula,'' it has the form of an oscillatory sum of weighted exponentials, each term corresponding to a unique periodic orbit or one of its forward (backward) multiple retracings. The phases are specified by Hamilton's characteristic function calculated along the periodic orbits with the inclusion of topological phases. Although the phase varies from orbit to orbit, the nature of the dynamics, be it integrable or chaotic, does not specifically enter into its definition. On the other hand, the weighting of each term or prefactor carries information about the local flow of the trajectories neighboring the periodic orbit and thus is sensitive to the structure of the dynamics. As a result, a great deal of effort is typically required to derive the prefactors under the various circumstances that arise.

In Gutzwiller's derivation of the trace formula, he generates the expressions for well isolated orbits whose local dynamics are captured by linearization as corresponds to the method of stationary phase. In two degrees of freedom ($N=2$) there exist two possibilities; the orbits are either stable or unstable and both expressions were given. For $N>2$, various combinations of the simple stable and unstable motions are possible still within the assumption of the orbits being isolated.

When discussing the various possible system dynamics, it is advantageous to take a more global viewpoint than just classifying every periodic orbit with regard to its stability analysis. For our purposes, systems may be thought of as belonging to one of a few classes: integrable, near-integrable, mixed phase space, and fully chaotic. The extreme limits of integrable or fully chaotic motion pose the fewest complications. For integrable systems where there exist as many constants of the motion as degrees of freedom, the trajectories lie on N-dimensional tori in the $2N$-dimensional phase space. In action-angle coordinates, the trajectories have fixed actions and ''wind around'' in the angle coordinates that monotonically increase with time. The periodic orbits can mainly be expected to fall into the category of being nonisolated since they lie on tori with rational ratios of their winding numbers (otherwise they would only be quasiperiodic). To fill out a rational torus typically requires an $N-1$ parameter continuous family of neighboring periodic orbits. Therefore, with the exception of a few central orbits (a torus of zero extent in all but one action coordinate), the Gutzwiller amplitude for stable orbits is insufficient to treat integrable systems. Expressions such as the ones derived by Balian and Bloch [2] and later in a general action-angle formalism by Berry and Tabor [3] are then needed. We will return to that subject later.

It is in the context of the correspondence principle for chaotic systems, about which almost nothing was known prior, that the majority of the work and greatest interest in the trace formula has been focused. The fully chaotic system has only unstable motion, no tori exist, and the majority of the shorter and medium length periodic orbits would typically be isolated and sufficiently linearizable to satisfy the conditions of Gutzwiller's derivation. A number of successes have been achieved whereby an evaluation of the trace formula correctly predicts the lowest-lying energy levels in a ''chaotic'' spectrum [4]. Perhaps more importantly, working in a reverse fashion, oscillations in physical observables or densities of states were associated with underlying classical periodic orbits [5]. The trace formula furthermore played an essential role, along with the Hannay-Ozorio sum rule [6], in Berry's derivation of the connection between long periodic orbits uniformly wandering in phase space and spectral rigidity [7] as found in random matrix theories [8].

The level of difficulty that the dynamics presents in finding an appropriate trace formula tremendously increases away from these two extremes. The near-integrable regime is characterized by imagining a weak generic perturbation to an integrable system. The vast majority of the irrational tori continue to exist in some distorted fashion consistent with

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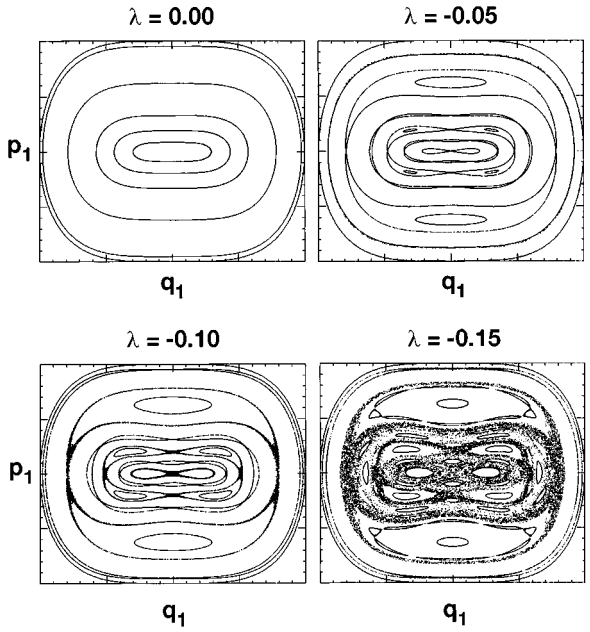

FIG. 1. $q_2 = 0$ Poincaré sections for a system of coupled quartic oscillators governed by the Hamiltonian Eq. (4.1). As the perturbation is turned on, the resonant tori of the integrable ($\lambda = 0.00$) case are replaced by island chains. For stronger coupling, chaotic regions begin to develop.

the theorem of Kol'mogorov, Arnol'd, and Moser [9]. They constitute a relative measure of the available phase space near unity. Yet the rational tori have all disappeared being replaced by chains of resonances on all scales; see Fig. 1. Considering that the periodic orbits were originally on the rational tori, a number of problems arise in attempting to apply the trace formula blindly. Though the stable and perturbatively introduced unstable periodic orbits may now be isolated in a mathematical sense, one cannot expect the vast majority of periodic orbits to be locally linearizable over a volume related to Planck's constant $\hbar$. This is true independently of how deep the system is into the short-wavelength regime. The Gutzwiller expression for the prefactors will generally hold for at most a few orbits, diverge for certain multiple retracings, and not be applicable to others.

Ozorio de Almeida considered the question of isolated resonances [10], i.e., the most significant by-product of a generic perturbation, and provided a semiclassical expression for their creation. In the decade following his work, little concrete application or exploration of his ideas have taken place. One difficulty is that, although he gave a semiclassical theory, his main result is the derivation of an integral, which is generally not easily evaluated. He suggested an approximation scheme that is rather restrictive and does not give a full interpolation between the Berry-Tabor and Gutzwiller limits.

In this paper, we give a full description of our work briefly reported in a Letter [11]. Our main goals here are to derive (for systems with two degrees of freedom) a more general form fully interpolating the two limits following Ozorio de Almeida's approach, loosening the most restrictive assumption, to discuss how to relate the parameters of the theory to the properties of the periodic orbits, and to verify the applicability of the generalized approach with a paradigm for studies of the regular-to-chaotic-motion transition. Ozorio de Almeida and Hannay [12] also discuss satellite periodic orbits coalescing with central ones and give the appropriate normal forms. This generates standard diffraction catastrophe integrals. Recent work [13] has investigated the most important diffraction case for the paradigm presented here and we shall not discuss the coalescence problem further. Atkins and Ezra have also very recently discussed certain resonances [14], but not the generalization of Ozorio de Almeida's theory presented here.

Finally, mixed phase space systems are characterized by widespread chaotic motion with significant embedded Kol'mogorov-Arnol'd-Moser (KAM) regions, i.e., regions whose phase spaces are structured like near-integrable systems. Mixed systems are extremely interesting because they form the most generic class of systems and are quite prevalent. Examples abound in the dynamical models (anharmonic oscillators) of vibrational motion in simple molecules, atomic physics problems such as the diamagnetic Hydrogen atom, and others. These systems are the most complicated and very little has been written about the form that their trace formulas should possess. To begin with, all the dynamical complications of the near-integrable regime are associated with the KAM regions as well and the expressions given in this paper do apply to the KAM regions of mixed systems. Nevertheless, although our ultimate goal is to treat mixed systems, we just address the near-integrable regime in this paper. Some of the additional problems of such systems that remain to be understood are (i) the chaos-KAM borders that also have structure on all scales, (ii) trapping in the border regions introducing intermittency in the chaotic part of the dynamics, and (iii) that there often exist miniscule stable islands of motion deep within the chaotic region.

This paper is organized as follows. We begin in Sec. II with an overview of integrable and near-integrable systems, starting with the ideas of Berry-Tabor for nonisolated periodic orbits and introducing in a second stage the semiclassical theory of Ozorio de Almeida. In Sec. III we then derive an extended expression for interpolating the Berry-Tabor and Gutzwiller amplitudes. A method of implementing the resonance expressions is part of the development. At this point, a method of analysis is introduced, in Sec. III D, that can be thought of as ''inverse-$\hbar$ spectroscopy.'' Finally, in Sec. IV the two-degree-of-freedom coupled quartic oscillators are introduced as a simple paradigm that can be conveniently examined classically and quantum mechanically [15]. The periodic orbits, their actions, stabilities, etc., and long stretches of the quantum spectrum can be accurately computed. The coupling of the oscillators is tuned across the entire near-integrable regime to implement the interpolating expressions. Excellent agreement is found between the quantum mechanics and semiclassical theory. We also note some interesting features arising from the emergence of a resonance within a resonance as a system parameter is varied.

II. INTEGRABLE AND NEAR-INTEGRABLE SYSTEMS

We begin with some description of our intent in labeling a system as belonging to the near-integrable class and with the challenges posed by near-integrable dynamics. A purely classical definition of integrability is easily stated, it being

roughly the existence of N constants of the motion in the dynamics of an N-degree-of-freedom system; the trajectories wind around on N-tori in phase space. Starting with the image of a weak, generic perturbation to some integrable system, the KAM theorem states that many irrational tori survive the perturbation in some distorted fashion, whereas the rational tori are destroyed and replaced by resonances. We might therefore be tempted to define a purely classical criterion for determining near integrability as being those systems whose phase space measure of surviving tori compared to the measure of the full energy surface of interest remains close to one. However, our principal interest here is in semiclassical trace formulas wherein $\hbar$ plays a critical role. The classical dynamics most relevant to the quantum mechanics occurs within a Heisenberg time τ_H determined with the energy-time uncertainty relation; the energy scale is just given by the mean level spacing in the spectral region of interest. We therefore really have in mind more of an $\hbar$-dependent notion of what ''near-integrable'' means. Specifically, we will have to deal with the creation of resonances and some further complications (see the results), but understanding the dynamics up to τ_H does not include having to deal with chaos explicitly nor the interface between chaotic and regular phase space domains. These problems are inherent to the mixed phase space regime and are beyond the scope of this work. In other words, if $(\mathbf{I},\varphi)$ are action-angle variables for an unperturbed two degree-of-freedom integrable system, then up to τ_H, the full Hamiltonian

$$H(\mathbf{I},\varphi)=H_0(\mathbf{I})+\epsilon\mathcal{H}(\mathbf{I},\varphi) \tag{2.1}$$

is essentially identical to the integrable dynamics generated by averaging over the fast angle variable

$$H(\mathbf{I},\varphi_1)=H_0(\mathbf{I})+\frac{\epsilon}{2\pi}\int_0^{2\pi} d\varphi_2\mathcal{H}(\mathbf{I},\varphi), \tag{2.2}$$

which retains the resonances but eliminates any chaos.

The most obvious complications introduced by a perturbation are apparent in Fig. 1, where the surface of section of an integrable system is pictured next to the same surface for the system with an added perturbation. At the center, there is an isolated periodic orbit with other isolated periodic orbits around it too closely intertwined to be treated independently. Farther from the center lies our main concern, the multiple resonances that are too narrow to treat with a simple linearization as leads to the Gutzwiller amplitudes, but far enough from the central orbit to be dealt with independently. The problem of multiple, simultaneous resonances was also briefly discussed in [12].

A. Background

We give a brief background on the work of Gutzwiller [1], Berry and Tabor [3], and Ozorio de Almeida [10] to remind the reader of the current status of the subject and also to fix our notation for the rest of the paper. Consider a system governed by a Hamiltonian whose quantum form is denoted $\hat{\mathcal{H}}(\hat{\mathbf{p}},\hat{\mathbf{q}})$ and whose classical form is denoted $\mathrm{H}(\mathbf{p},\mathbf{q})$. The density of states $\rho(E)$ at energy E is expressible in terms of the energy-dependent Green's function $G(\mathbf{q}'',\mathbf{q}';E)=\langle\mathbf{q}''|(E-\hat{\mathcal{H}})^{-1}|\mathbf{q}'\rangle$:

$$\rho(E)=\mathrm{Tr}\{\delta(E-\hat{\mathcal{H}}(\hat{\mathbf{p}},\hat{\mathbf{q}}))\}=-\frac{1}{\pi}\mathrm{Im}\int d\mathbf{q}G(\mathbf{q},\mathbf{q};E). \tag{2.3}$$

The semiclassical approximation then can be used to relate the quantum $\rho(E)$ to properties of the underlying classical system. $\rho(E)$ decomposes into an average and a fluctuating component $\rho(E)=\overline{\rho(E)}+\rho_{\mathrm{fl}}(E)$, respectively, where

$$\overline{\rho(E)}=\frac{1}{(2\pi\hbar)^N}\int d\mathbf{p}\,d\mathbf{q}\delta(E-H(\mathbf{p},\mathbf{q})) \tag{2.4}$$

$$\rho_{\mathrm{fl}}(E)=-\frac{1}{\pi}\mathrm{Im}\left\{\frac{1}{i\hbar(2\pi i\hbar)^{(N-1)/2}}\int d\mathbf{q}\sum_t |D_t|^{1/2}\right.$$
$$\left.\times\exp\left(\frac{iS_t(\mathbf{q},\mathbf{q};E)}{\hbar}-i\eta_t\frac{\pi}{2}\right)\right\}, \tag{2.5}$$

$$D_t=\begin{vmatrix}\partial^2S/\partial\mathbf{q}''\partial\mathbf{q}' & \partial^2S/\partial\mathbf{q}''\partial E\\ \partial^2S/\partial\mathbf{q}'\partial E & \partial^2S/\partial E\partial E\end{vmatrix}=\frac{1}{\dot{q}_N\dot{q}_N'}\left|\frac{\partial^2S}{\partial\tilde{\mathbf{q}}\partial\tilde{\mathbf{q}}'}\right|$$
$$[\tilde{\mathbf{q}}=(q_1,q_2,\ldots,q_{N-1})]. \tag{2.6}$$

The equation for $\overline{\rho(E)}$ expresses the notion that a quantum state occupies a cell in ''phase space'' of volume $(2\pi\hbar)^N$. Other than $\overline{\rho(E)}\sim O(\hbar^{-N})$, it is of no further interest in this paper. The sum in $\rho_{\mathrm{fl}}(E)$ runs over all classical trajectories t starting at $\mathbf{q}$ and returning to $\mathbf{q}$ *at energy* E. S_t is the action $\int\mathbf{p}\,d\mathbf{q}$ along the trajectory and η_t is a topological phase index counting conjugate points. Finally, D_t is the determinant involving second derivatives of the action evaluated at $\mathbf{q}''=\mathbf{q}'=\mathbf{q}$ (see Sec. 2 of [1] and also the discussion in Sec. III of [16]).

Gutzwiller evaluated this integral with the method of stationary phase finding [1]

$$\rho_{\mathrm{fl}}(E)=\frac{1}{\pi\hbar}\sum_{\mathcal{P}}\frac{T}{r|\mathrm{Det}(M-\mathbf{1})|^{1/2}}\cos\left(\frac{S}{\hbar}-\sigma\frac{\pi}{2}\right). \tag{2.7}$$

The stationary phase condition restricts the trajectory sum to periodic orbits $\mathcal{P}$. S, T, M, and σ are the orbit's action, period, monodromy matrix, and Maslov index, respectively. r is the number of retracings for a given primitive orbit. The assumption that the orbits are isolated generates the forms for the amplitude.

B. Berry-Tabor amplitudes

For nonisolated stable periodic orbits (i.e., rational tori), we follow the second derivation of Berry and Tabor [3(b)] except that we start from the energy-dependent Green's function instead of the propagator and restrict ourselves to $N=2$ systems. Assuming now that the Hamiltonian is classically integrable, it can be expressed in action-angle variables $(\mathbf{I},\varphi)$ $(\varphi_1,\varphi_2\in[0,2\pi])$ as $H(\mathbf{I})$. For a given torus we note $\omega_i=\partial H/\partial I_i$ $(i=1,2)$, the corresponding angular frequencies, and $\alpha\equiv\omega_1/\omega_2$, the rotation number of the torus. The actions (I_1,I_2) are constants of motion since $\dot{I}_i=\partial H/\partial\varphi_i=0$. Periodic orbits are associated with tori such that the rotation number is rational, i.e., $\alpha=\mu_1/\mu_2$, where μ_1 and μ_2 are coprime integers. They can be labeled by the

two integers $\mathbf{M}=(M_1,M_2)=(r\mu_1,r\mu_2)$, where (μ_1,μ_2) specifies the primitive periodic orbit and r is the number of repetitions. M_i $(i=1,2)$ is thus the number of windings of φ_i in a complete round-trip on the orbit (r repetitions of the primitive).

Focusing now on the contribution to the fluctuating part of the density of states $\rho_{\mathbf{M}}$ of the orbit $\mathbf{M}$,

$$\rho_{\rm fl}=\sum_{\mathbf{M}}\rho_{\mathbf{M}}, \tag{2.8}$$

$$\rho_{\mathbf{M}}(E)=\frac{1}{\pi\hbar}\mathrm{Re}\left\{\int\frac{d\mathbf{q}}{\sqrt{2\pi i\hbar}}|D_{\mathbf{M}}|^{1/2}\times\exp\left(\frac{iS^0_{\mathbf{M}}(\mathbf{q},\mathbf{q})}{\hbar}-\frac{i\eta_{\mathbf{M}}\pi}{2}\right)\right\}. \tag{2.9}$$

Denoting $\mathbf{I_M}$ the actions of the corresponding torus, the action $S^0_{\mathbf{M}}$ along the orbit is given by (note the 2π factor between S and I)

$$S^0_{\mathbf{M}}=\oint_{\rm orbit}\mathbf{p}\cdot d\mathbf{q}=\oint_{\rm orbit}\mathbf{I}\cdot d\boldsymbol{\varphi}=2\pi I_{\mathbf{M}}\cdot\mathbf{M}. \tag{2.10}$$

As always, it is the prefactor that remains to be evaluated. This, however, can be derived in a straightforward manner if one uses a system of coordinates for which one direction is taken along the orbit [1,16]. These coordinates are given explicitly by the standard canonical transformation $(\mathbf{I},\varphi)\to(\mathbf{J},\theta)$ generated by $F_2(\mathbf{J},\varphi)=(\mu_2\varphi_1-\mu_1\varphi_2)J_1+\varphi_2J_2$:

$$\theta_1=\mu_2\varphi_1-\mu_1\varphi_2,\qquad J_1=I_1/\mu_2,$$
$$\theta_2=\varphi_2,\qquad J_2=I_2+(\mu_1/\mu_2)I_1, \tag{2.11}$$

for which, *on the torus* $\mathbf{I_M}$, θ_1 is constant along a trajectory. On $\mathbf{I_M}$, θ_1 thus specifies the particular trajectory and θ_2 the position on the trajectory. Recall that for the transformation Eq. (2.11) to be one to one, θ_2 should be taken in the range $[0,2\pi\mu_2]$ rather than $[0,2\pi]$. With r repetitions, the trajectory launched at $\theta=(\theta_1,\theta_2)$ is such that the final position θ' is $(\theta_1',\theta_2')=(\theta_1,\theta_2+2\pi r\mu_2)$.

In these coordinates the action $S^0_{\mathbf{M}}$ is unchanged, being canonically invariant. Moreover, when performing the change of variables $(q_1,q_2)\to(\theta_1,\theta_2)$ in the integral Eq. (2.9) (the action variables are fixed to $I_{\mathbf{M}}$), it can be seen that the determinant $D_{\mathbf{M}}$ transforms as a density, i.e.,

$$D_{\mathbf{M}}(\mathbf{q})dq_1dq_2=D_{\mathbf{M}}(\theta)d\theta_1d\theta_2, \tag{2.12}$$

where $D_{\mathbf{M}}(\theta)$ is defined by Eq. (2.6) but in the $(\mathbf{J},\theta)$ coordinates. This property basically justifies working from the beginning in action-angle coordinates (as done, for instance, in [3(b)] or in [10]), although the exact quantum Green's function is only defined in the original $\mathbf{q}$ variables. Because the justification of this point involves some subtleties, we shall discuss it in more details in Appendix I.

Using the right-hand side form of Eq. (2.6), the prefactor can be put in the form

$$|D_{\mathbf{M}}(\theta)|^{1/2}=\frac{1}{\omega_2}\left|\left(\frac{\partial\theta_1'}{\partial J_1}\right)_{\theta_1}\right|^{-1/2}. \tag{2.13}$$

The main point is that the evolution $(\theta_1,J_1)\to(\theta_1',J_1')$ (here with $J_1'=J_1$) is a Poincaré mapping between two $\theta_2=$const Poincaré sections. E, θ_2, and θ_2' are constant. Using relations implied by Eq. (2.11)

$$\theta_1'(J_1,\theta_1)=\theta_1+2\pi r\mu_2^2(\alpha-\mu_1/\mu_2) \tag{2.14}$$

and

$$\left(\frac{\partial\theta_1'}{\partial J_1}\right)_{\theta_1}=2\pi r\mu_2^2\left(\frac{\partial\alpha}{\partial J_1}\right)_E. \tag{2.15}$$

We introduce g_E (see Sec. IV of [15]), the function describing the energy surface E. It is such that for $I_2=g_E(I_1)$, the energy is fixed so that $H(I_1,I_2=g_E(I_1))=E$. Differentiating both sides of this last equality yields $dg_E/dI_1=-\alpha$, giving

$$\left(\frac{\partial\alpha}{\partial J_1}\right)_E=\mu_2\left(\frac{\partial\alpha}{\partial I_1}\right)_E=-\mu_2\frac{d^2g_E}{dI_1^2}. \tag{2.16}$$

$D_{\mathbf{M}}(\theta)$ is therefore inversely proportional to the curvature of the line $H(I_1,I_2)=E$ and is, as expected, independent of θ. The $\mathbf{M}$ torus contribution reduces to

$$\rho_{\mathbf{M}}(E)=\frac{1}{\pi\hbar}\mathrm{Re}\left\{\frac{1}{\sqrt{2i\pi\hbar}}\frac{1}{|2\pi r\mu_2^3g_E''|^{1/2}}\times\int_0^{2\pi}d\theta_1\exp\left[\frac{iS^0_{\mathbf{M}}}{\hbar}-\frac{i\eta_{\mathbf{M}}\pi}{2}\right]\int_0^{2\pi\mu_2}\frac{d\theta_2}{\omega_2}\right\}. \tag{2.17}$$

The integral over θ_2 is the single traversal period $T_{\mathbf{M}}/r$ of the periodic orbit, which on a torus is independent of θ_1. Later we shall need to be more careful evaluating the θ_2 integral. This is automatically taken care of by rewriting Eq. (2.17) as a partial derivative with respect to energy

$$\begin{aligned}\rho_{\mathbf{M}}(E)&=\frac{1}{\pi\hbar}\mathrm{Re}\left\{\frac{1}{\sqrt{2i\pi\hbar}}\frac{1}{|2\pi M_2^3g_E''|^{1/2}}\times\int_0^{2\pi}d\theta_1T_{\mathbf{M}}\exp\left[\frac{iS^0_{\mathbf{M}}}{\hbar}-\frac{i\eta_{\mathbf{M}}\pi}{2}\right]\right\}\\&=\frac{1}{\pi\hbar}\mathrm{Re}\left\{\frac{1}{\sqrt{2i\pi\hbar}}\frac{1}{|2\pi M_2^3g_E''|^{1/2}}\times\frac{\hbar}{i}\frac{\partial}{\partial E}\int_0^{2\pi}d\theta_1\exp\left[\frac{iS^0_{\mathbf{M}}}{\hbar}-\frac{i\eta_{\mathbf{M}}\pi}{2}\right]\right\},\end{aligned} \tag{2.18}$$

where the second form follows using the relation $T=\partial S/\partial E$. On a torus the integral over θ_1 gives a factor 2π. Thus the contribution of the orbits of topology $\mathbf{M}$ for an integrable system is

$$\rho^{\rm BT}_{\mathbf{M}}=\frac{T_{\mathbf{M}}}{\pi\hbar^{3/2}M_2^{3/2}|g_E''|^{1/2}}\cos\left(\frac{S^0_{\mathbf{M}}}{\hbar}-\frac{\eta_{\mathbf{M}}\pi}{2}-\frac{\pi}{4}\right). \tag{2.19}$$

The Maslov index $\eta_{\mathbf{M}}$ of the semiclassical Green's function is expressed in terms of the Maslov indices (ν_1,ν_2) of the paths on which the actions variables are defined as (see Appendix II)

$$\eta_{\mathbf{M}}=(M_1\nu_1+M_2\nu_2)-\Theta(g_E''), \tag{2.20}$$

where Θ is the Heaviside step function. For two-dimensional systems Eq. (2.19) is equivalent to the expression given by Berry and Tabor in [3].

C. The nearly integrable regime

Following Ozorio de Almeida, we begin with a Hamiltonian H close to integrability written in the form

$$H(\mathbf{I},\varphi)=H^0(\mathbf{I})+\epsilon\mathcal{H}(\mathbf{I},\varphi), \tag{2.21}$$

where the perturbation $\epsilon\mathcal{H}$ is ''small'' (in a sense to be specified later). We shall here investigate how the contribution $\rho_{\mathbf{M}}$ of the periodic orbits of ''topology'' $\mathbf{M}=(M_1,M_2)$ to the density of states is modified by the perturbing term.

For a sufficiently small perturbation, the change in $\rho_{\mathbf{M}}$ of Eq. (2.9) is essentially due to the modification of the phase, since the action is multiplied by the large factor $1/\hbar$ and the variation of the determinant $D_{\mathbf{M}}$ gives a higher-order correction. Therefore, in the evaluation of the integral, one should keep the (unperturbed) zeroth-order approximation for $D_{\mathbf{M}}$ and look for the first correction of the action. Indeed, since (I_1,I_2) are no longer constants of the motion, $S_{\mathbf{M}}$ is not given by Eq. (2.10), but a position-dependent term $\delta S(\mathbf{q})$ has to be added to $S^0_{\mathbf{M}}$.

Classical perturbation theory tells us that the first-order correction to the action is given by the integral [17]

$$\delta S(\mathbf{q})=-\epsilon\oint\mathcal{H}dt \tag{2.22}$$

taken on the *unperturbed trajectory* starting and ending at $\mathbf{q}$. Thus δS depends on the unperturbed trajectory on which $\mathbf{q}$ lies, but not on the position along the trajectory. (This property, though not surprising, is, nevertheless, not completely obvious since the perturbed trajectories starting and ending at a given point usually differ when one is moving along an unperturbed trajectory.) In terms of the coordinates $(\mathbf{J},\theta)$ defined by Eq. (2.11), this means that δS depends only on θ_1, but not on θ_2.

From Eq. (2.17), Ozorio de Almeida found that the effect of the perturbation is merely to replace the $\cos(S^0_{\mathbf{M}}/\hbar-\eta_{\mathbf{M}}\pi/2-\pi/4)$ by $\mathrm{Re}[R\exp i(S^0_{\mathbf{M}}/\hbar-\eta_{\mathbf{M}}\pi/2-\pi/4)]$ in the expression Eq. (2.19) of $\rho^{\mathrm{BT}}_{\mathbf{M}}$, where

$$R=\frac{1}{2\pi}\int d\theta_1\exp[i\,\delta S(\theta_1)/\hbar]. \tag{2.23}$$

The multiplicative factor R takes into account the small dephasing between different closed orbits in configuration space of topology M due to the fact that the resonant torus on which they exist is slightly broken by the perturbation. Thus an orbit of topology M closed in configuration space is generally no longer periodic.

Ozorio de Almeida suggested writing $\delta S(\theta_1)$ in term of its Fourier series

$$\delta S=\sum_{n=0}^{\infty}\Delta S_n\cos(n\theta_1-\chi_n). \tag{2.24}$$

The benefit is that the coefficients ΔS_n usually decay rapidly as a function of n. A natural simplifying ansatz would therefore be that only the first harmonic of the above expansion has to be taken into account. The constant $n=0$ term can be included in the unperturbed motion. Setting the origin of θ_1 at χ_1, δS reduces to

$$\delta S=\Delta S\cos(\theta_1). \tag{2.25}$$

In that case the integral Eq. (2.23) is the Bessel function $J_0(\Delta S/\hbar)$ and the contribution $\rho_{\mathbf{M}}$ to be used in Eq. (2.9) is [10]

$$\rho_{\mathbf{M}}=\rho^{\mathrm{BT}}_{\mathbf{M}}J_0(\Delta S/\hbar), \tag{2.26}$$

where the Berry-Tabor contribution $\rho^{\mathrm{BT}}_{\mathbf{M}}$ is given by Eq. (2.19).

III. RESONANCES: GENERALIZATION AND IMPLEMENTATION

It turns out that postulating the form Eq. (2.25) of the perturbative action generates rather strong restrictions on the applicability of the uniform approximation in Eq. (2.26). Generically, because of the Poincaré-Birkhoff theorem, only two orbits survive the destruction of the resonant torus: one stable s and one unstable u. We suppose that the actions S_s and S_u and the monodromy matrices M_s and M_u of these two orbits are known or can be computed. We shall see below that if Eq. (2.25) holds,

$$\mathrm{Det}(M_s-\mathbf{1})+\mathrm{Det}(M_u-\mathbf{1})\simeq 0. \tag{3.1}$$

Consider that $\mathrm{Det}(M_s-\mathbf{1})$ is confined to the interval $[0,4]$ and $\mathrm{Det}(M_u-\mathbf{1})$ to the interval $[-\infty,0]$. Almost all of the possible range of $\mathrm{Det}(M_u-\mathbf{1})$ is beyond the simplifying ansatz behind Eq. (2.25). Generically, under increasing perturbation Eq. (3.1), and thus Eq. (2.25) as well, quickly fails to hold. This is confirmed later in Sec. IV for coupled quartic oscillators.

A second concern is that in practice, especially if one is considering a resonance inside a KAM island of a mixed system, the unperturbed Hamiltonian H^0 expressed in action-angle variables and $\epsilon\mathcal{H}$ are unknown. A method is needed to evaluate the different parameters entering the formulas of Eqs. (2.19) and (2.26), including the generalization given ahead, without having to refer to action-angle coordinate systems. The most important parameters are the curvature g_E'' of the line $H(I_1,I_2)=E$ and the amplitude ΔS of the correction to the action. In addition, a criterion is needed to indicate under what circumstances the theory will apply. It happens that all this information is encoded in the characteristics of the perturbed, isolated periodic orbits.

A. Pendulum mapping

Instead of truncating the series as in Eq. (2.25), we map the problem onto the pendulum. Let

$$S_{\mathbf{M}}(\theta_1)=\overline{S_{\mathbf{M}}}(\epsilon)+\Delta S(\epsilon)\cos(\xi), \tag{3.2}$$

where $\theta_1=f(\xi)$ and

$$\overline{S_{\mathbf{M}}}(\epsilon)=\frac{1}{2\pi}\int_0^{2\pi} d\xi S(\theta_1). \tag{3.3}$$

This is possible since $S_{\mathbf{M}}(\theta_1)$ has but a single maximum and minimum occurring each interval on 2π. In principle, all the angular complexity of the function $S_{\mathbf{M}}(\theta_1)$ has been transferred to the parametric relationship $\theta_1=f(\xi)$. The advantage here is that $\Delta S(\epsilon)\cos(\xi)$ is the action variation of the standard pendulum from Eq. (2.22). The relationship between the variables θ_1 and ξ is smooth and nearly linear.

Because $dS_{\mathbf{M}}(\theta_1)/d\theta_1=J_1'-J_1$ (both initial θ_1 and final $\theta_1'=\theta_1$ angles are varied), the periodic orbits correspond to extremal actions. Thus $\xi=0$ or π for the stable and unstable periodic orbits. Choosing the unstable orbit as the origin of ξ, the amplitude $\Delta S(\epsilon)$ is related to the actions of the periodic orbits by

$$\Delta S(\epsilon)=\frac{S_u-S_s}{2} \tag{3.4}$$

and the average action $\overline{S_{\mathbf{M}}}$ by

$$\overline{S_{\mathbf{M}}}(\epsilon)=\frac{S_s+S_u}{2}. \tag{3.5}$$

To complete the derivation of a uniform approximation for $\rho_{\mathbf{M}}$, we need to specify the mapping of θ_1 onto ξ. As a function of either variable, the action is periodic on 2π intervals. The difference between the variables is therefore periodic as well. Keeping only the longest-wavelength oscillation in a Fourier decomposition of the difference, we approximate

$$\theta_1\approx\xi-a(\epsilon)\sin(\xi+\phi). \tag{3.6}$$

This approximation is quite different from truncating Eq. (2.24) after the $n=1$ term. In fact, it is possible to invert Eq. (3.6) as a Taylor series in the ''small'' parameter $a(\epsilon)$ as

$$\xi=\sum_{n=0}^{\infty} c_n(\theta)\frac{a(\epsilon)^n}{n!}, \tag{3.7}$$

where $c_n(\theta)$ can be found recursively. Inserting this expression into the cosine argument of Eq. (3.2) and expanding appropriately (and tediously) would generate an infinite series of the form of Eq. (2.24) with some decreasing set of ΔS_n as $n\to\infty$ depending on the value of $a(\epsilon)$.

In the same way the actions of the stable and unstable orbits determine the amplitude $\Delta S(\epsilon)$, their stability, i.e., their monodromy matrices M, is related to the second derivative of the action $d^2S_{\mathbf{M}}(\theta_1)/d\theta_1^2$. More precisely, one can apply a general identity used in the derivation of the Gutzwiller trace formula (see Sec. 4 of [1] or Sec. IV B of [16]; for $N=2$ systems, we give a short derivation in Appendix III). The result is

$$\frac{d^2S_{\mathbf{M}}(\theta_1)}{d\theta_1^2}=-\frac{\mathrm{Det}(M-\mathbf{1})}{(\partial\theta_1'/\partial J_1)_{\theta_1}}, \tag{3.8}$$

where $\theta_1'(\theta_1,J_1)$ is the Poincaré map whose zeroth-order (unperturbed) approximation is given by Eq. (2.14).

Using the chain rule,

$$\begin{aligned}\frac{d^2S_{\mathbf{M}}(\theta_1)}{d\theta_1^2}&=-\Delta S(\epsilon)\left[\cos(\xi)\left(\frac{d\xi}{d\theta_1}\right)^2+\sin(\xi)\frac{d^2\xi}{d\theta_1^2}\right]\\&=\mp\Delta S(\epsilon)\left(\frac{d\xi}{d\theta_1}\right)^2\end{aligned} \tag{3.9}$$

where $-$ is for the unstable orbit and $+$ is for the stable orbit. Two relations for the stability determinants of the periodic orbits follow now from Eqs. (3.8), (2.15), and (2.16);

$$\mathrm{Det}(M_u-\mathbf{1})=-\frac{2\pi r\mu_2^3 g_E''\Delta S(\epsilon)}{[1-a(\epsilon)\cos\phi]^2}, \tag{3.10a}$$

$$\mathrm{Det}(M_s-\mathbf{1})=+\frac{2\pi r\mu_2^3 g_E''\Delta S(\epsilon)}{[1+a(\epsilon)\cos\phi]^2}. \tag{3.10b}$$

There are two ways to view these equations. First, g_E'' can be independently evaluated; one method is described in [15]. There are then two equations, but only one unknown: $\tilde{a}(\epsilon)=a(\epsilon)\cos\phi$. The consistency of the two equations is a measure of the validity of the approximation in Eq. (3.6). The second viewpoint is just to assume that the system is in the near-integrable regime and the approximation is valid. Generally, the independent evaluation of g_E'' can be rather laborious and time consuming. Instead, one can use the equations to solve simply and quickly for both g_E'' and $\tilde{a}(\epsilon)$. In this way, every quantity necessary for our theory is given by properties of the periodic orbits alone. Then so long as g_E'' is approximately constant and equal to the value obtained as $\epsilon\to0$, the mapping is a valid approximation. We shall follow the second route, although for the calculations of Sec. IV we perform an additional analytical computation of g_E'' that verifies that, as $\epsilon\to0$, the two determinations are identical.

Taking the ratio of the two cases and doing some algebra fixes the value of $\tilde{a}(\epsilon)$ to be

$$\tilde{a}(\epsilon)\equiv a(\epsilon)\cos\phi=\frac{\kappa-1}{\kappa+1}, \tag{3.11}$$

where

$$\kappa=\left(-\frac{\mathrm{Det}(M_u-\mathbf{1})}{\mathrm{Det}(M_s-\mathbf{1})}\right)^{1/2}. \tag{3.12}$$

Ozorio de Almeida's results are recovered in cases where $\kappa\to1$, i.e., under the condition that Eq. (3.1) holds. g_E'' follows trivially from either of Eqs. (3.10).

The integral of Eq. (2.18) can now be evaluated straightforwardly using the integral

$$\int_0^{2\pi} d\theta_1 \exp\left[\frac{i\Delta S(\epsilon)}{\hbar}\cos(\xi)\right]$$
$$= \int_0^{2\pi} d\xi [1-a(\epsilon)\cos(\xi+\phi)]\exp\left[\frac{i\Delta S(\epsilon)}{\hbar}\cos(\xi)\right]$$
$$= 2\pi\left[J_0\left(\frac{\Delta S(\epsilon)}{\hbar}\right) - i\tilde{a}(\epsilon)J_1\left(\frac{\Delta S(\epsilon)}{\hbar}\right)\right]. \quad (3.13)$$

Note that the above expression depends only on $\tilde{a}(\epsilon)$ and not on $a(\epsilon)$ and $\cos\phi$ independently. It is thus entirely specified by S_u, S_s and κ. Denoting $s_\epsilon = \Delta S(\epsilon)/\hbar$, the final result for the contribution to the density of states is

$$\rho_{\mathbf{M}}(E) = \frac{1}{\pi|\hbar^3 M_2^3 g_E''|^{1/2}}\mathrm{Re}\left\{\frac{\hbar}{i}\frac{\partial}{\partial E}\exp\left(\frac{i\overline{S_{\mathbf{M}}}(\epsilon)}{\hbar} - \frac{i\eta_{\mathbf{M}}\pi}{2} - \frac{i\pi}{4}\right)[J_0(s_\epsilon) - i\tilde{a}(\epsilon)J_1(s_\epsilon)]\right\}$$
$$= \frac{1}{\pi|\hbar^3 M_2^3 g_E''|^{1/2}}\mathrm{Re}\left\{\exp\left(\frac{i\overline{S_{\mathbf{M}}}(\epsilon)}{\hbar} - \frac{i\eta_{\mathbf{M}}\pi}{2} - \frac{i\pi}{4}\right)\times\left[\overline{T}[J_0(s_\epsilon) - i\tilde{a}(\epsilon)J_1(s_\epsilon)] + i\Delta T\left[J_1(s_\epsilon) + \frac{i\tilde{a}(\epsilon)}{2}[J_0(s_\epsilon) - J_2(s_\epsilon)]\right]\right]\right\}, \quad (3.14)$$

where $J_0(z)$, $J_1(z)$, and $J_2(z)$ are the standard Bessel functions. The average period $T=(T_s+T_u)/2$ is half the sum of the two periodic orbit's periods and the difference is $\Delta T=(T_u-T_s)/2$, consistent with the corresponding notation for the actions.

B. Limiting cases

The limiting cases of the Berry-Tabor result and the Gutzwiller results are easily recovered. The former is obtained trivially as $\Delta S(\epsilon)\to 0$ (likewise $\Delta T\to 0$) since $\overline{S_{\mathbf{M}}}(\epsilon)\to S_{\mathbf{M}}^0$ and the Bessel function expression in parentheses reduces to unity. The other limit follows using the asymptotic expression for Bessel functions of large arguments:

$$J_n(z)\to\sqrt{\frac{2}{\pi z}}\cos\left(z - n\frac{\pi}{2} - \mathrm{sgn}[z]\frac{\pi}{4}\right), \quad z \text{ real}. \quad (3.15)$$

Then, after some algebra and the application of Eq. (3.10),

$$\rho_{\mathbf{M}}(E)\to\frac{1}{\pi\hbar}\frac{1}{|2\pi M_2^3 g_E''\Delta S(\epsilon)|^{1/2}}\left\{(\overline{T}-\Delta T)[1+\tilde{a}(\epsilon)]\times\cos\left(\frac{\overline{S}-\Delta S}{\hbar} - (\eta+\gamma_s)\frac{\pi}{2}\right) + (\overline{T}+\Delta T)[1-\tilde{a}(\epsilon)]\times\cos\left(\frac{\overline{S}+\Delta S}{\hbar} - (\eta+\gamma_u)\frac{\pi}{2}\right)\right\}$$
$$\to\frac{1}{\pi\hbar}\left\{\frac{T_s}{r|\mathrm{Det}(M_s-\mathbf{1})|^{1/2}}\cos\left(\frac{S_s}{\hbar} - \sigma_s\frac{\pi}{2}\right) + \frac{T_u}{r|\mathrm{Det}(M_u-\mathbf{1})|^{1/2}}\cos\left(\frac{S_u}{\hbar} - \sigma_u\frac{\pi}{2}\right)\right\}, \quad (3.16)$$

where S_s, T_s and S_u, T_u are the actions and periods of the full orbits (i.e., not the primitives). $\gamma_u=\Theta(\Delta S)=\Theta(g_E'')$ and $\gamma_s=\Theta(-\Delta S)=\Theta(-g_E'')$ (Θ is the Heaviside step function) arise because of the $\mathrm{sgn}[z]$ in Eq. (3.15) and we define

$$\sigma_u \equiv \eta_{\mathbf{M}} + \gamma_u = (M_1\nu_1 + M_2\nu_2), \quad (3.17a)$$

$$\sigma_s \equiv \eta_{\mathbf{M}} + \gamma_s = (M_1\nu_1 + M_2\nu_2) - \mathrm{sgn}[g_E'']. \quad (3.17b)$$

Noting that the Maslov index σ in Eq. (2.7) is, by definition [1], equal to $\eta_{\mathbf{M}}+\Theta[-d^2S/d\theta_1^2]$ and that $d^2S/d\theta_1^2$ is here given by Eq. (3.9), Eq. (3.16) is seen to be precisely the contribution of the stable and unstable orbit to the Gutzwiller trace formula.

Here a remark is in order. The term proportional to ΔT in Eq. (3.16) arises because in Eq. (3.14) the θ_1 dependence of not only δS, but also $T_{\mathbf{M}}$, has been taken into account. We began by saying that the perturbation of the determinant prefactor can be neglected, so it would seem reasonable to neglect the variation of T as well. In addition, Eq. (3.10) has essentially been derived for the unperturbed system. However, the combined result of accounting for the period variation and using Eq. (3.10) to determine $g''(E)$ is that the Gutzwiller amplitude is recovered *exactly* for large $\Delta S/\hbar$. Thus, our expressions being correct to the extent that the Gutzwiller trace formula is valid for large $\Delta S/\hbar$, it will be seen to hold even for very large classical perturbations in spite of a derivation whose starting point is first-order classical perturbation theory.

C. Discrete symmetries

The theory given so far for a generic perturbation must be slightly modified if the system possesses discrete symmetries including the perturbation terms. Instead of a single stable and a single unstable orbit created as the rational torus is destroyed and replaced by a resonance, it is possible that multiple orbits survive, which together build up the full resonance structure. Let l denote the number of surviving stable (or unstable, it is the same) orbits. The value of l depends on the discrete symmetry and the torus. Each of the l stable (unstable) orbits will map onto any of the other similarly created stable (unstable) periodic orbits through the applica-

tion of one of the operators of the discrete symmetry group. There are thus l multiple copies of identical pendulum structures in the resonance. Crudely speaking, each periodic orbit is l times too short to explore the full resonance. In other words, θ and ξ are not periodic on the same angular intervals. As ξ covers $[0,2\pi]$, θ only covers $[0,2\pi/l]$. Equation (3.6) must be replaced by

$$l\theta_1 \approx \xi - a(\epsilon)\sin(\xi+\phi). \tag{3.18}$$

With a little simple algebra, it can be seen that $\tilde{a}(\epsilon)$ retains its same definition as given in Eq. (3.11), but that the proportionality of the curvature g_E'' to the $\mathrm{Det}(M-1)$ is modified by a factor l^2 to become

$$\mathrm{Det}(M_u-\mathbf{1}) = -\frac{2\pi r l^2 \mu_2^3 g_E'' \Delta S(\epsilon)}{[1-\tilde{a}(\epsilon)]^2}, \tag{3.19a}$$

$$\mathrm{Det}(M_s-\mathbf{1}) = +\frac{2\pi r l^2 \mu_2^3 g_E'' \Delta S(\epsilon)}{[1+\tilde{a}(\epsilon)]^2}. \tag{3.19b}$$

All the rest of the semiclassical treatment follows without further modification.

D. Inverse-$\hbar$ spectroscopy

Because many oscillating terms contribute to the total density of states, it is difficult to verify the role of specific orbits directly in the spectrum. As has been previously considered [18], the spectrum can be transformed in order to separate orbit contributions by their classical actions. A convenient scheme begins with the simple observation that in Eq. (3.14) and in the diffraction integrals that arise, classical actions appear divided by $\hbar$. With t denoting $\hbar^{-1}$, the variables of action S and the inverse Planck constant t can be taken as a Fourier transform pair with the transform kernel $k(t)=e^{-iSt}$. Instead, it is useful to introduce some minor modifications. First, we add an exponential damping to the kernel because later we will not have access to an infinite range of t (i.e., we will have only a finite stretch of the spectrum). Second, adding a factor $t^{-1/2}$ turns out to generate compact analytic forms as a function of S for the complete periodic orbit expressions. The form we use is equivalent to Gaussian damping, but in the variable $t^{1/2}$. Other choices are possible, but this version is quite convenient.

The density of states must now be considered both as a function of t and E. In other words, as $\hbar$ changes the energy levels move, forming continuous curves when drawn in the (t,E) plane. The energy curves will intersect a fixed energy value only at special or ''quantized'' values of t. It is the transformation of this ''t spectrum'' that allows a precise view of the effects of the individual orbits. We therefore consider the action function

$$R(S,E) = \int_0^\infty dt k(t)\rho(t,E) = \int_0^\infty dt\ t^{-1/2} e^{-(\alpha-iS)t}\rho(t,E). \tag{3.20}$$

Expressing the density of states as a sum over periodic orbit contributions, each labeled by j, gives

$$R(S,E) = \sum_j R_j(S,E),$$

$$R_j(S,E) = \int_0^\infty dt t^{-1/2} e^{-(\alpha-iS)t}\rho_j(t,E). \tag{3.21}$$

The actual expression for $R_j(S,E)$ now depends on the orbit and whether it belongs to a resonance as covered by Eq. (3.14) or one of the diffraction integrals discussed elsewhere [13]. For resonances one obtains [introducing $\mathsf{p}_j(E)=\alpha-i(S-\overline{S_j})$]

$$\begin{aligned} R_j(S,E) &= \int_0^\infty dt t e^{-(\alpha-iS)t} \frac{1}{\pi|M_2^3 g_E''|^{1/2}} \\ &\quad \times \mathrm{Re}\left\{ \frac{1}{ti}\frac{\partial}{\partial E}\exp\left(i\overline{S_j}t - \frac{i\eta_{\mathbf{M}}\pi}{2} - \frac{i\pi}{4}\right)\right. \\ &\quad \left. \times [J_0(\Delta S_j t) - i\tilde{a}(\epsilon)J_1(\Delta S_j t)]\right\} \\ &= \frac{i\exp(i\eta_{\mathbf{M}}\pi/2 + i\pi/4)}{2\pi|M_2^3 g_E''|^{1/2}} \frac{\partial}{\partial E} \\ &\quad \times \frac{1+[i\tilde{a}(\epsilon)/\Delta S_j](\sqrt{\mathsf{p}_j^2+\Delta S_j^2}-\mathsf{p}_j)}{\sqrt{\mathsf{p}_j^2+\Delta S_j^2}}. \end{aligned} \tag{3.22}$$

In evaluating the integral, the Re{ } restriction may be replaced by 1/2 of the complex conjugate expression since for S and $\overline{S_j}$ of opposite sign the integral is essentially zero. Equation (3.22) is the functional dependence that we expect resonances to show in the similarly transformed exact quantum spectrum. The final expression after carrying out the derivative (note $\partial\mathsf{p}_j/\partial E = iT_j$) is

$$\begin{aligned} R_j(S,E) &= \frac{\exp(i\eta_{\mathbf{M}}\pi/2 + i\pi/4)}{2\pi|M_2^3 g_E''|^{1/2}} \\ &\quad \times \left[\frac{\overline{T_j}[\mathsf{p}_j + i\tilde{a}(\epsilon)\Delta S_j] - \Delta T_j[\tilde{a}(\epsilon)\mathsf{p}_j + i\Delta S_j]}{(\mathsf{p}_j^2+\Delta S_j^2)^{3/2}} \right. \\ &\quad \left. + \frac{\tilde{a}(\epsilon)\Delta T_j}{\Delta S_j^2}\left(1 - \frac{\mathsf{p}_j}{(\mathsf{p}_j^2+\Delta S_j^2)^{1/2}}\right)\right]. \end{aligned} \tag{3.23}$$

For completeness, we also give the expression deriving from the Gutzwiller trace formula

$$\begin{aligned} R_j(S,E) &= \frac{T_u \exp(i\sigma_u\pi/2)}{4r|\pi\mathrm{Det}(M_u-\mathbf{1})|^{1/2}[\alpha - i(S-S_u)]^{3/2}} \\ &\quad + \frac{T_s \exp(i\sigma_s\pi/2)}{4r|\pi\mathrm{Det}(M_s-\mathbf{1})|^{1/2}[\alpha - i(S-S_s)]^{3/2}} \end{aligned} \tag{3.24}$$

and the Berry-Tabor result

$$R_{\mathbf{M}}(S,E) = \frac{\overline{T_{\mathbf{M}}^0}\exp(i\eta_{\mathbf{M}}\pi/2 + i\pi/4)}{2\pi|M_2^3 g_E''|^{1/2}[\alpha - i(S-\overline{S_{\mathbf{M}}^0})]^2}. \tag{3.25}$$

IV. COUPLED QUARTIC OSCILLATORS

Any of a number of systems, such as the diamagnetic hydrogen atom in certain field regimes, are suitable for verifying the theory of the preceding section. We have studied two coupled quartic oscillators in depth previously because of its transition from integrable to chaotic motion as the coupling increases. The most detailed information can be found in Ref. [15], where numerical techniques enabling us to calculate tens of thousands of quantum levels to high precision are described. This will make it possible to resolve various orbit contributions with a very sharp precision. Previous work by several groups has been published on the quartic oscillator's periodic orbit theory [19–21]. However, these works focus on the strongly chaotic coupling regime, whereas our interest here lies in the near-integrable and ultimately mixed phase space regimes.

A. Classical oscillators

Let us first recall the salient features of the dynamics. The quartic oscillator's Hamiltonian can be written as

$$H(\lambda)=\frac{p_1^2+p_2^2}{2}+V(q_1,q_2),$$

$$V(q_1,q_2)=a(\lambda)\left(\frac{q_1^4}{b}+bq_2^4+2\lambda q_1^2q_2^2\right), \tag{4.1}$$

where $a(\lambda)$ is a largely irrelevant constant chosen for technical convenience in making the quantum calculations and λ is the parameter governing the coupling between the oscillators and is responsible for the variation of the system from integrable ($\lambda=0$) to chaotic dynamics ($-0.6>\lambda>-1.0$). [The value of the constant is given by $a(\lambda)=(4m^2/9\pi^2\hbar^4)K^2(1-\lambda/2)$, where $K(z)$ is a complete elliptic integral of the first kind and effectively $m=\hbar=1$, $K(1/2)=1.854\,074\,677\,301\,372.$] The range ($0.0>\lambda>-0.15$) approximately corresponds to the near-integrable regime where the chaos is narrowly contained and far from having a global covering of phase space. Nevertheless, we show in Fig. 1 a sequence of surfaces of section with λ decreasing towards -0.15 to illustrate the significant changes in the dynamics in the interval $\lambda\in[-0.15,0.0]$. One sees that $\lambda=-0.15$ is by no means a ''weak'' perturbation to the integrable system. But for the reasons described at the beginning of Sec. II and the results found later, it shall still be considered as belonging to the near-integrable regime. The parameter $b=\pi/4$ is set differently from one in such a way that, in addition to time reversal invariance, the system has the symmetry C_{2v} of the rectangle generated by the reflection P_1 and P_2 across to the lines $q_1=0$ and $q_2=0$; $l=2$ in Eq. (3.19) for the resonances pictured in Sec. V. The potential $V(\mathbf{q})$ is homogeneous in (q_1,q_2) which leads to scaling relations in the dynamics. Any trajectory $[\mathbf{q}^E(t),\mathbf{p}^E(t)]$ on the energy surfaces E can be mapped onto a trajectory $[\mathbf{q}^0(t),\mathbf{p}^0(t)]$ on the energy surface $E^0=1$. With $\gamma=(E/E^0)^{1/4}$,

$$\mathbf{p}^E(t)=\gamma^2\mathbf{p}^0(\gamma t),\quad \mathbf{q}^E(t)=\gamma\mathbf{q}^0(\gamma t). \tag{4.2}$$

For the period T and action S of some period orbit, Eq. (4.2) leads to

$$T^E=\gamma^{-1}T^0,\quad S^E=\gamma^3S^0. \tag{4.3}$$

Using the relation $\partial S/\partial E=T$ and Eq. (4.3), $S^0=4E^0T^0/3$.

In Sec. III, our goal had been to express quantal properties of a system in terms of classical quantities such as the action and monodromy matrix of periodic orbits. This is of practical interest because, especially in the nearly integrable regime, there exist efficient methods to compute numerically these quantities even when it is not possible to obtain them analytically. The approach used here is the one suggested by Baranger *et al.* [22], which consists in starting from known orbits and following them by continuity as a parameter is varied. We have in fact essentially implemented their algorithm to which we refer the reader for a detailed description. We stress though that this algorithm allows for a simultaneous computation of both the periodic orbits and their associated monodromy matrix. The main difference here is that, instead of varying the energy as was done by Baranger *et al.*, it is kept fixed (and equal to $E_0=1$) and the parameter varied is the coupling λ between the two oscillators.

As a starting point, we use the periodic orbits of the integrable system $\lambda=0$ for which the motion of the two oscillators is decoupled and governed, respectively, by the one-dimensional Hamiltonians

$$H_1=p_1^2/2+(a_0/b)q_1^4,$$

$$H_2=p_2^2/2+(a_0b)q_2^4 \tag{4.4}$$

[$a_0=a(\lambda=0)=0.154\,800\,436\,631\,7$].

Determining the changing periodic orbits of interest as λ moves away from zero involves two steps. The first one consists of determining the resonant tori (i.e., the families of periodic orbits) of the $\lambda=0$ Hamiltonian. This part is rather straightforward since to any rational rotation number $\alpha=\mu_1/\mu_2$, where μ_1 and μ_2 are coprime integers, the resonant torus of topology (μ_1,μ_2) is determined by the conditions

$$\alpha=\frac{\mu_1}{\mu_2}=\frac{T_2}{T_1}, \tag{4.5}$$

$$E_1+E_2=E^0=1. \tag{4.6}$$

The periods T_1 and T_2 of the two one-dimensional quartic oscillators can then be expressed in term of the energies E_1 and E_2 in the corresponding modes as

$$T_1=\xi\left(\frac{b}{a_0E_1}\right)^{1/4},\quad T_2=\xi\left(\frac{1}{a_0bE_2}\right)^{1/4} \tag{4.7}$$

[with $\xi=\Gamma(\frac{1}{4})^2/(2\sqrt{\pi})$]. This readily yields

$$E_1=\frac{\mu_1^4}{\mu_1^4+b^{-2}\mu_2^4},\quad E_2=\frac{\mu_2^4}{\mu_2^4+b^2\mu_1^4}, \tag{4.8}$$

which uniquely specify the resonant torus.

A given resonant torus corresponds to a one-parameter family of periodic orbits. As soon as the perturbing coupling

is turned on, however, the usual scenario, as described by the Poincaré-Birkhoff theorem, is that all of them are instantaneously destroyed, except for two trajectories (in the absence of symmetries), one stable and one unstable. We shall in the following denote by $S\mu_1\mu_2(\lambda)$ and $U\mu_1\mu_2(\lambda)$ these surviving orbits. Of course, we need to locate from where on the torus the surviving orbits originate. In general, this requires some further computation. However, for the Hamiltonian in Eq. (4.1) the symmetries of the system simplify the problem. Considering a given resonant torus (μ_1,μ_2) and working, for instance, in a $q_2=0$ Poincaré section, the surviving periodic orbits for infinitesimal, but nonzero, coupling are the extrema of the action $\delta S(q_1,p_1)=-\oint \delta V dt$, where $\delta V(\mathbf{q})$ is the perturbing potential, and the integral is taken along the unperturbed orbit starting and ending at (q_1,p_1). In spite of the notation used, q_1 and p_1 are not independent variables since (q_1,p_1) is constrained to be on the intersection of the resonant torus with the Poincaré section. It can be seen that, because of the symmetries, δS is necessarily an even function of both q_1 and p_1. Therefore δS has to be extremal whenever either q_1 or p_1 is equal to zero. It then suffices to check that the extrema on the q_1 axis do not correspond to the same periodic orbit as the one on the p_1 axis to ensure that both $U\mu_1\mu_2$ and $S\mu_1\mu_2$ have been found. The rare orbits for which this is not true have to be treated separately. This consideration, together with Eq. (4.8), entirely specifies the original orbits, which we are going to follow from $\lambda=0.0$ to $\lambda=-0.15$ covering the full near-integrable regime of coupling.

B. Quantum oscillators

The Schrödinger equation and scaling relations are summarized as

$$E\Psi(\mathbf{q})=-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial q_1^2}+\frac{\partial^2}{\partial q_2^2}\right)\Psi(\mathbf{q})+a\hat{V}(\mathbf{q})\Psi(\mathbf{q}),$$

$$E_i^a=a^{1/3}E_i^0,\Psi_i^a(\mathbf{q})\Rightarrow\Psi_i^0(a^{-1/6}\mathbf{q}). \tag{4.9}$$

A nice simplification of using this homogeneous potential is the relation between the energy eigenvalues $\{E_n\}$ found at fixed $\hbar$ and the $\hbar$ eigenvalues $\{\hbar_n\}$ found at fixed energy E. For our choice of constant $a(\lambda)$, the following exact relation holds for all λ and $n=1,2,3,\ldots\infty$:

$$\left(\frac{E_n}{E}\right)^{3/4}=\frac{\hbar}{\hbar_n}=\frac{t_n}{t}. \tag{4.10}$$

The Hamiltonian (4.1) is invariant under reflections about the q_1 and q_2 axes and under time reversal with the symmetries of the eigenstates classified as

$$P_i\Psi(\mathbf{q})=\pi_i\Psi(\mathbf{q}), \tag{4.11}$$

where $\pi_i=\pm 1$.

For the entire near-integrable regime $\lambda\in\{-0.15,0.0\}$, we calculate the level curves for the first 12 000 levels. This is sufficient for the purpose of isolating a resonance and showing its contribution to the density of states making a full transition from the Berry-Tabor amplitude to the Gutzwiller amplitude; much longer level sequences are easily generated, but are unnecessary here. To compare with the theoretical expectations, the quantum spectrum must be transformed according to Eq. (3.20). Using

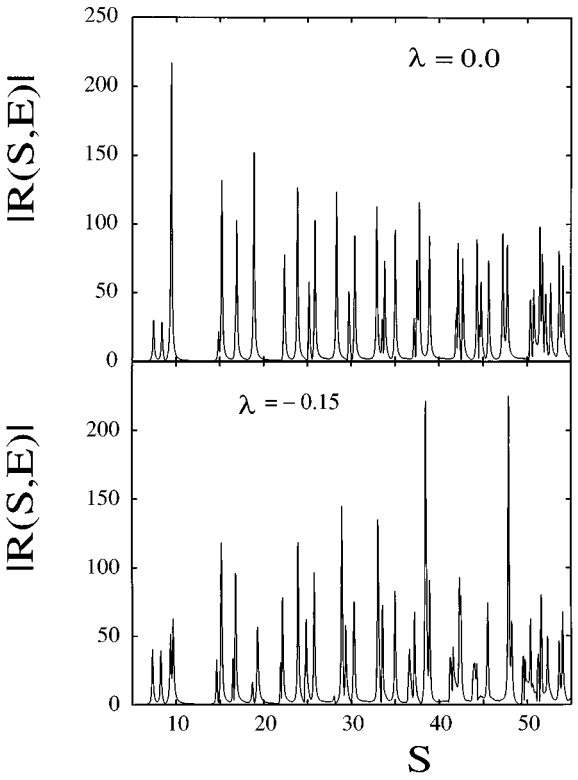

FIG. 2. Quantum action function $|R(S,E=1)|$ for two different couplings: the integrable case $\lambda=0.00$ and the large perturbation limit of the near-integrable regime to nearly the mixed phase space regime $\lambda=-0.15$.

$$\rho(t,E)=\sum_{n=0}^{\infty}\delta(E-E_n(t)) \tag{4.12}$$

and noting that Eq. (4.10) is equivalent to $E_n(t)=E_n(\hbar=1)t^{-4/3}$, it is straightforward to show that

$$R(S,E=1)=\frac{3}{4}\sum_{n=1}^{\infty}[E_n(\hbar=1)]^{3/8}e^{-(\alpha+iS)[E_n(\hbar=1)]^{3/4}}, \tag{4.13}$$

which is to be compared with Eqs. (3.21) and (3.22), evaluated with the classical actions and stabilities.

V. RESULTS

Before verifying the theory, we first illustrate in Fig. 2 the spectrum of peaks produced by the inverse-$\hbar$ transformation of the quantum spectrum. The two spectra shown cover opposite limiting frontiers of the near-integrable regime, namely, $\lambda=0.0$ and $\lambda=-0.15$. Note the general features one can expect. First, some of the peaks have begun or appear to have split. Next, the positions of the peaks shift very little. Finally, there is a significant rearrangement of some of the magnitudes of the peaks even though both curves belong to the same near-integrable regime. Furthermore, even

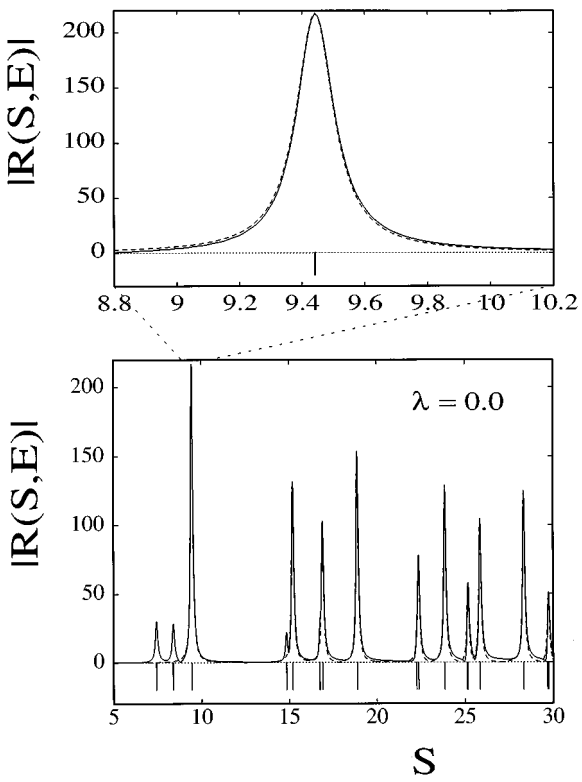

FIG. 3. Comparison of the quantum action function and the semiclassical theory for integrable systems ($\lambda=0$). The solid curve is the quantum results and the dashed curve the Berry-Tabor formula. The short vertical lines below mark the actions of the classical tori. The $\mathbf{M}=(1,1)$ peak is shown expanded as an inset to show the quality of agreement better. Note that $E=1$.

though the Berry-Tabor amplitudes are larger than the Gutzwiller amplitudes by $\hbar^{-1/2}$ and one might have expected the amplitudes to decrease, the perturbation of the system forms several new peaks as large as or larger than the Berry-Tabor magnitudes. The new large peaks exist for λ values quite far from integrability.

A. Integrable systems

We begin with the Berry-Tabor formula, which has existed for about 20 years. Its precision in predicting magnitudes has sometimes been found to be a little disappointing [3,14]. This motivated, for instance, the authors of [3] to include complex trajectories to obtain better accuracy. Here we have long spectral sequences that can be used to shed some light on this difficulty. Because there is no harmonic component in the quartic oscillator's potential, neither Berry-Tabor nor Gutzwiller amplitudes are applicable to tori having one of their coprime integers equal to zero as in $\mathbf{M}=(\mu_1,0)$ or $\mathbf{M}=(0,\mu_2)$. It is not of sufficient interest here to derive formulas specific to these special tori and no attempt is made to include their effects in the comparison to the semiclassical theory. With that exception, in Fig. 3 we find excellent agreement, to within a couple of percent or better, between the Berry-Tabor theory compared to the quantum results. We conclude that Berry-Tabor theory works extremely well, except perhaps too close to the ground-state region of the spectrum. The best accuracy is found for tori with smaller actions. In particular, the $\mathbf{M}=(1,1)$ torus contribution shown expanded in Fig. 3 is good to about 1% of the magnitude in the peak region with the phase error not worse than about 2°. This sets the general scale for the quality of results we would like to see across the near-integrable regime for the comparison of the theory for resonances presented here.

On closer inspection, it can be seen that some degradation shows up in the tails and some peaks for tori with larger actions. As a general rule, semiclassical approximations have a tendency to break down at longer propagation times. Moreover, it can be seen from the definition Eq. (3.20) that contributions of a resonance to $R(S,E)$ is dominated by different part of the spectrum depending on whether the central peak or the tail is considered. Indeed, for $S\simeq\bar{S}$ the integral Eq. (3.20) is dominated by t (i.e., $\hbar^{-1}$) of the order α^{-1}. Therefore if α can be chosen small enough, this corresponds to quantum levels well within the semiclassical regime. On the contrary, the tails are dominated by contributions from t of the order $(S-S_j)^{-1}$ independently of how small α becomes. Thus the tails are dominated more by the lower levels in the spectrum and it is natural for errors in the semiclassical approximation to appear there first. An additional effect for larger values of the action is the increased density of periodic trajectories. Several poorly reproduced tails may overlap and lead to cumulative errors. Nevertheless, the Berry-Tabor theory works beautifully for the quartic oscillators in our energy regime.

B. Near-integrable regime

In surveying the quantum results, we found the following properties. There were no peaks appearing unrelated to some classical orbit, i.e., no ghost orbits [23] in this regime. Several of the peaks that appeared to be splitting under perturbation were just the consequence of two quite distinct tori beginning nearly degenerate in action and moving apart. Many magnitudes were left almost unchanged, yet others were greatly affected. One can also find examples of constructive interference where amplitudes increased as orbits crossed paths. It happened that very few resonances in our present calculation (just 12 000 levels per value of λ) could be followed from the Berry-Tabor well into the Gutzwiller regime (two separated contributions to the density of states). They are all for tori with $\mathbf{M}=(k,k)$ $k=1,2,3,\ldots$. For the other resonances $\Delta S/\hbar$ is not sufficiently large to observe peak splitting. In addition, although the number of destroyed tori increases with the perturbation, the behavior of g_E in the neighborhood of the surviving ones is only slightly affected even for significant couplings. This is seen in Fig. 4 where the curve $g_E(I_1)$ at $\lambda=-0.10$ appears almost on top of its unperturbed analog wherever both are defined. Derivatives of g_E magnify the differences between the perturbed and unperturbed results; nevertheless, g_E'' shows only small variation throughout the nearly integrable regime. Note that in the gaps of g_E corresponding to resonances, derivatives can only be taken through an extrapolation. A purely *classical* value of g_E'' cannot be defined without ambiguity, but far from bifurcations (see below) the results are always consistent with Eqs. (3.10) and (3.11).

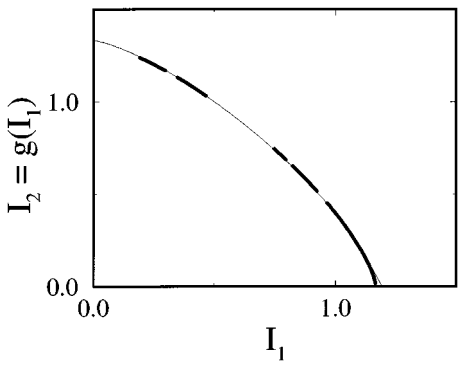

FIG. 4. Comparison of the classically computed function $I_2 = g_E(I_1)$ at $\lambda = 0.00$ (thin) and $\lambda = -0.10$ (thick). In the coupled case, the curve is only defined for the tori that have not been destroyed by the perturbation. Despite the strong perturbation, the curve appears almost unchanged.

The best resonance to begin testing the theory is for $\mathbf{M}=(1,1)$ for several reasons. To begin with, it is isolated well enough from other orbits to follow unambiguously. Its stable and unstable orbits are well separated by $\lambda = -0.15$; i.e. its entire transition from the Berry-Tabor to Gutzwiller limits emerges. Also for this case, the independently calculated value of g_E'' for the integrable case ($\lambda = 0$) leads to consistency with Eqs. (3.10) to better than 5% across the entire near-integrable regime. This is illustrated in Fig. 5. The value of g_E'' for $\lambda = 0$ was calculated by explicit construction of the energy surface in the neighborhood of $\mathbf{M}=(1,1)$ and evaluating its curvature analytically. The other

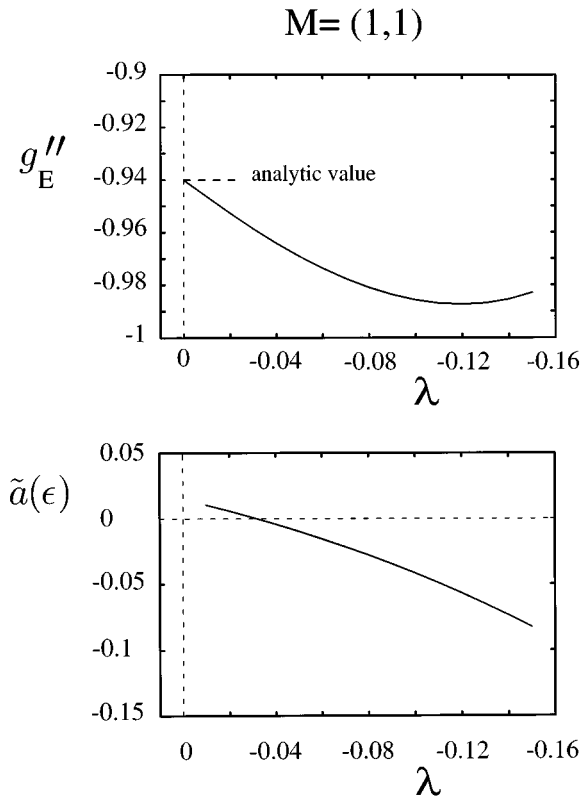

FIG. 5. Drawn are $g''(\mathbf{I_M})$ and $\tilde{a}(\epsilon)$ as functions of the coupling strength calculated from Eqs. (3.10) and (3.11) for $\mathbf{M}=(1,1)$.

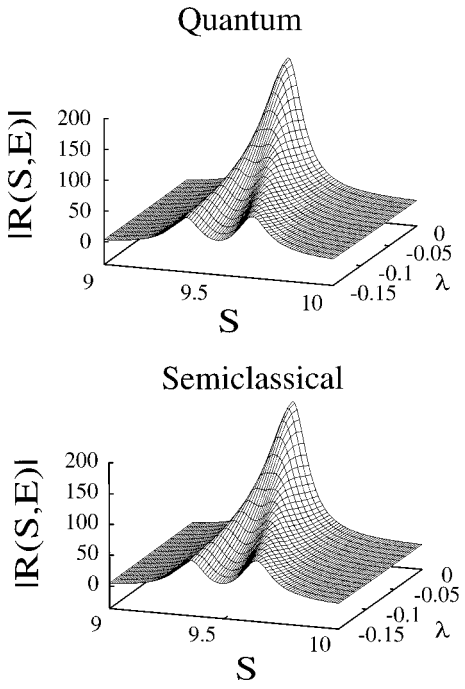

FIG. 6. Comparison of the quantum and semiclassical theory of the $\mathbf{M}=(1,1)$ resonance as a function of action S and perturbation strength λ. Note that $E=1$.

g_E'' values near $\mathbf{M}=(1,1)$ for different perturbations were derived via the relations given in Eq. (3.10). There is excellent agreement between the $\lambda \to 0$ limit from the derived values of g_E'' and the analytic result, which validates the use of Eq. (3.10). Finally, the asymmetry of the stable and unstable orbits as measured by $\tilde{a}(\epsilon)$ varies smoothly with λ and does not exceed 10%. It is interesting to note that $\tilde{a}(\epsilon)$ does not appear to approach zero as $\lambda \to 0$. So the ratio $-\mathrm{Det}(M_u - 1)/\mathrm{Det}(M_s - 1)$ does not approach 1 even for infinitesimal classical perturbations to the integrable system; recall Eq. (2.25) deriving from Ozorio de Almeida's ansatz. Of course, the asymmetric term in Eq. (3.14) must vanish as $\lambda \to 0$, but this is attained because $\Delta S, \Delta T \to 0$ and the Bessel function $J_1(0) = 0$ and not because $\tilde{a}(\epsilon) \to 0$. In Fig. 6 we show a comparison of the semiclassical theory with the quantum results using the g_E'' and $\tilde{a}(\epsilon)$ values given in Fig. 5 The agreement is excellent, being better than 3% in error in the domain of the peak for all the values of λ; see, for example, Fig. 7.

If we use $\tilde{a}(\epsilon) = 0$ and g_E'' of the integrable system (Ozorio de Almeida's ansatz), the errors in the semiclassical theory may be significantly larger, depending on the resonance. The benefit of accounting for ΔT, $\tilde{a}(\epsilon)$, and a varying g_E'' become more pronounced for the $\mathbf{M}=(2,2)$ orbits whose amplitudes would be poorly reproduced otherwise. The asymmetry between the stable and unstable orbits is amplified by the second tracing of the $\mathbf{M}=(1,1)$ orbits. This is illustrated in Fig. 8. We plot $|R(S,E)|$, but only along the emerging ridges associated with the stable and unstable orbits as a function of λ, i.e., $|R(S_s(\lambda),E)|$ and $|R(S_u(\lambda),E)|$. The curves generated by the Ozorio de Almeida ansatz, the Gutzwiller trace formula, and the theory presented in this paper are plotted along with the curve gen-

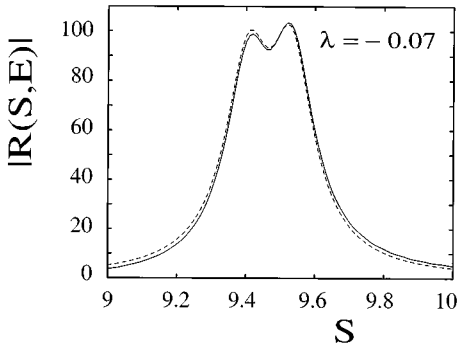

FIG. 7. Cross section through Fig. 6 for the perturbation coupling parameter $\lambda = -0.07$.

erated by the quantum spectrum for comparison. As expected, our theory goes asymptotically to the Gutzwiller expression for large perturbation. Whereas Gutzwiller's result begins at infinity for the integrable system, our result and the ansatz begin at the Berry-Tabor value. The last two curves follow each other closely up to $\lambda = -0.04$ and diverge for stronger perturbations. Our theory in this case continues to follow the quantum spectral results closely.

In general, it is expected that the amplitudes should decrease with increasing perturbation since the Gutzwiller amplitudes are lower order in $\hbar$ than the Berry-Tabor amplitudes. In fact, this happens up to a point at which the stable orbit branch passes through a minimum (its stability determinant passes through a maximum, here 4). Its amplitude then increases rapidly and, in all the quartic oscillator results we checked, it always, at some perturbation strength, exceeds the initial Berry-Tabor amplitudes. Consider the $\mathbf{M}=(3,3)$ case. Although these orbits are just the third traversal of the $\mathbf{M}=(1,1)$ orbits, the theory presented here can no longer follow the quantum results. A first signal that something is going wrong is that the behavior of g''_E and $\tilde{a}(\epsilon)$ derived from Eqs. (3.10) and (3.11) is much more dramatic; see Fig. 9. In principle, although we allow some variation of g''_E with the perturbation, its value remains associated (at a given λ) to a torus and should not depend on repetition numbers. Therefore g''_E should be the same for all the $\mathbf{M}=(k,k)$, $k=1,2,3$. This is actually the case for $\mathbf{M}=(1,1)$ and (2,2). However, as observed in Fig. 9, for $\mathbf{M}=(3,3)$ this is true only for small couplings, and as λ approaches -0.15, g''_E evolves towards zero, indicating an infinity in the prefactor of the semiclassical theory and $\tilde{a}(\epsilon)$ towards -1 [i.e., $-\mathrm{Det}(M_u-1)/\mathrm{Det}(M_s-1)\to\infty$].

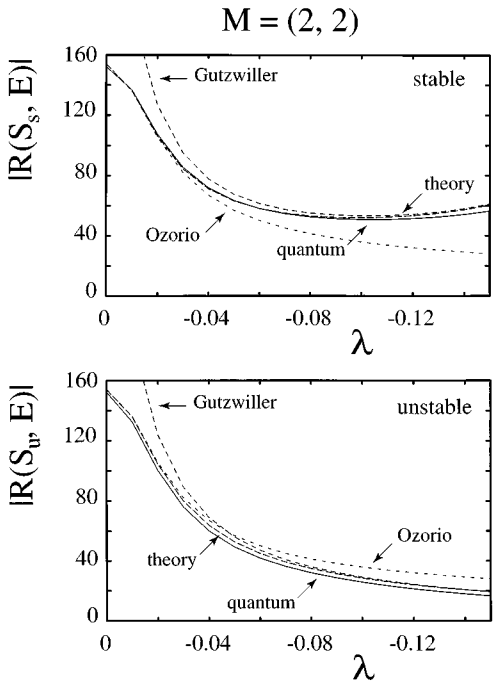

FIG. 8. Comparison of the quantum (solid) and semiclassical (dashed) action functions $|R(S_u(\lambda))|$ and $|R(S_s(\lambda))|$ for the $\mathbf{M}=(2,2)$ resonance. The semiclassical predictions from the Gutzwiller amplitude, Ozorio de Almeida ansatz, and our work are plotted for comparison.

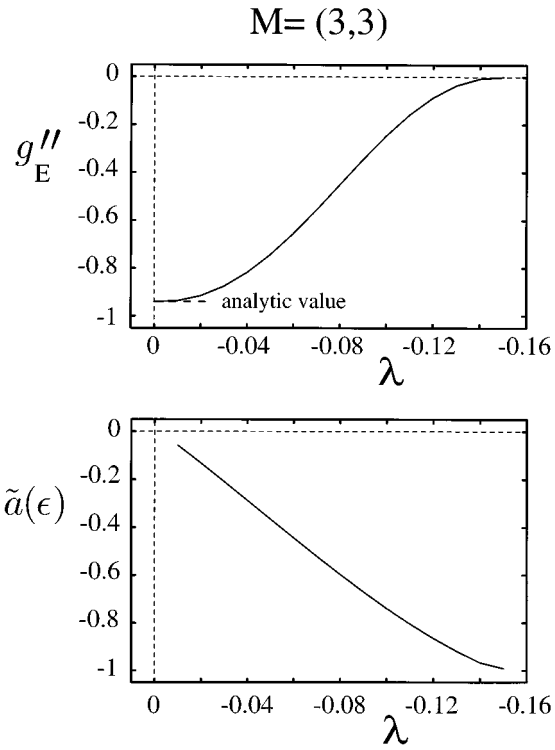

FIG. 9. Drawn are $g''(\mathbf{I_M})$ and $\tilde{a}(\epsilon)$ as functions of the coupling strength calculated from Eqs. (3.10) and (3.11) for $\mathbf{M}=(3,3)$.

The difficulty encountered here is actually the same as that originally pointed out by Gutzwiller in his derivation of the trace formula, namely, that for elliptic orbit a divergence appears as $\mathrm{Det}(M_s-\mathbf{1})\to 0$. This situation corresponds generically to a bifurcation of the elliptic orbit and for the $\mathbf{M}=(1,1)$ resonance to the creation of a 2/3 resonance in the neighborhood of the stable orbit—a resonance within a resonance; see Fig. 10. For large $\Delta S/\hbar$ [as is the case here for the $\mathbf{M}(3,3)$ resonance near the bifurcation] our result is strictly equivalent to the one obtained using the Gutzwiller trace formula, yielding the usual description: the stable orbit contribution is infinitely stronger than the unstable one (i.e., only the stable branch is diverging). The essence of this behavior is reflected in the quantum results; see Fig. 11. The initial quantum peak splits asymmetrically and the stable branch rises above its integrable system value after initially decreas-

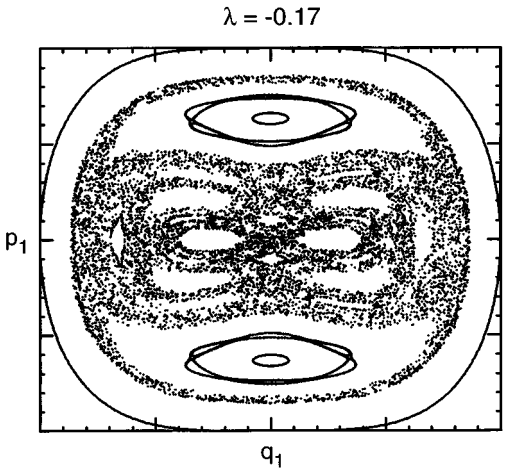

FIG. 10. Blowup of the stable island surrounding the stable orbit of the primary resonance $\mathbf{M}=(1,1)$ for a coupling strength $\lambda=-0.17$, which is slightly stronger than the bifurcation value $\lambda_{\mathrm{bif}}\simeq-0.15$. Note that for symmetry reasons, six islands are visible instead of three.

ing. Of course, there is no singularity in the quantum magnitude as in the semiclassical theory, which is breaking down. Actually all the tall action peaks emerging at large perturbation can be associated with this kind of structure. Interestingly in our results, the coalescences more than compensate the reduction in order of $\hbar$ in going from the Berry-Tabor to the Gutzwiller limit. One method to properly account (in the large $\Delta S/\hbar$ regime) for the magnitude of these peaks near the classical bifurcation points would be to follow Ozorio de Almeida and Hannay's work [12] where normal forms are given along with some theory.

It should be kept in mind that resonances with small $\Delta S/\hbar$ cannot be described properly near a bifurcation by our method even though the theory is not equivalent there to the Gutzwiller theory. It happens that Eq. (3.10b) applied at a bifurcation [i.e., $\mathrm{Det}(M_s-\mathbf{1})=0$ but $\Delta S\neq 0$] constrains g_E'' to be null, which has no particular reason to be the case. This simply reflects that the mapping Eq. (3.6) cannot describe a bifurcation. In fact (we do not give the figure here), the

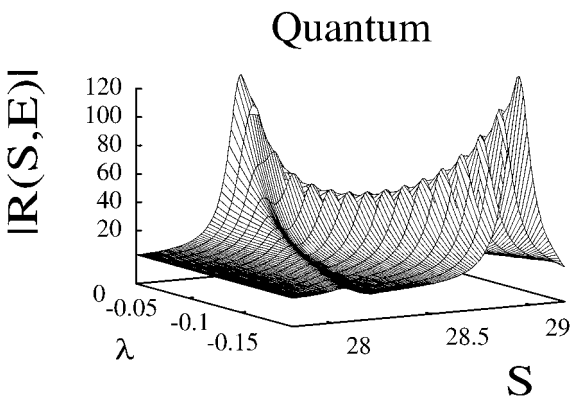

FIG. 11. Quantum action function of the $\mathbf{M}=(3,3)$ resonance as a function of action S and perturbation strength λ, showing the consequences of the bifurcation of the stable orbit. In a sense it is simpler to locate the classical bifurcation with the quantum spectrum than by calculating classical trajectories. Note that $E=1$.

$\mathbf{M}=(6,9)$ resonance falls into this class and one sees absolutely no increase in the amplitude near the bifurcation. It remains extremely close to the Berry-Tabor amplitude throughout. The alternative mapping $\xi=\theta_1+a\sin(\theta_1)$ (which, however, does not yield a closed form expression for $\rho_{\mathbf{M}}$) may be used to treat the bifurcation for $\Delta S/\hbar\simeq 1$ or less. It, however, does not provide a sufficiently good description of the actual bifurcation process to be used at larger values of $\Delta S/\hbar$.

We make a final related comment on the observation that several amplitudes appeared to change very little. As pointed out by Ozorio de Almeida [10], for primitive orbits, as either μ_1 or μ_2 increases, the action differences ΔS decrease rapidly. Except for the shortest orbits, ΔS is so small that the amplitude remains almost constant and the peak shifts just a little even for significant perturbation strengths. The theory presented here is still applicable to these orbits, but just remains essentially equal to the Berry-Tabor formula and this is borne out with the quantum spectrum. However, even though ΔS remains close to zero, the stability determinants do not. Indeed, writing $\mathrm{Det}(M_u-\mathbf{1})=-2\sinh(\zeta/2)$ and $\mathrm{Det}(M_s-\mathbf{1})=2\sin(\beta/2)$, a very rough order of magnitude of ζ and β can be obtained, assuming they are approximately proportional to the period of the corresponding orbit. The coefficient of proportionality can then be understood as a kind of mean Lyapunov exponent, which increases with the perturbation. Therefore the determinants of long orbits tend to move away from zero even faster than for the shortest periodic orbits. In particular, with increasing perturbation, the determinant of the stable orbit will leave and return to near zero, as $\beta\rightarrow 2\pi$, where the semiclassical theory given here fails, before the resonance contribution to the density of states moves away from the Berry-Tabor regime. For the majority of the longer periodic orbits, as one increases the perturbation strength beyond the near-integrable regime a new treatment will need to be found.

VI. CONCLUSION

The theory presented in this paper extends the semiclassical theory of Ozorio de Almeida for near-integrable systems. We present uniform expressions, fully interpolating the Berry-Tabor and Gutzwiller amplitudes across the whole nearly integrable regime. The functional forms obtained are expressed explicitly in terms of the canonical invariant properties of the periodic orbits, i.e., action, stability matrix determinant, phase index, and period. This has made it possible to perform a complete implementation of the theory for a model system and to give a fairly complete discussion of the semiclassical theory. The study directs our attention toward some rather interesting classical dynamical effects visible in the quantum system.

From a qualitative point of view, the phase space structure of an integrable system is unstable with respect to generic perturbations. It is foliated by tori that serve as geometrical structures for Einstein-Brillouin-Keller (EBK) quantization in the more familiar semiclassical theory. In a trace formula approach, i.e., Berry-Tabor theory, it is the resonant tori ($N-1$ parameter family of periodic orbits) that play the dominant role in the theory. As an infinitesimal perturbation is introduced, these rational tori are replaced by resonances

organized around two ''surviving'' periodic orbits, one stable and the other unstable. Discrete symmetries may increase this number and can be incorporated in the theory as well.

First, consider just the shortest periodic orbits; they are associated with the largest resonances. With increasing perturbation, their resonance structures grow quickly. At some perturbation strength, the two surviving short orbits become effectively isolated from one another in their contributions to the density of states. Excluding further orbit bifurcations for the moment, the stable and unstable orbit contributions should approach the sum of the individual Gutzwiller expressions for the amplitudes of isolated orbits. This was borne out with the quantum spectrum of the quartic oscillators in Sec. V where the entire transitional behavior from Berry-Tabor to Gutzwiller behavior was observed. The extended semiclassical theory followed the quantum results very accurately. The small residual errors were of the same relative size as occurring in the Berry-Tabor or Gutzwiller limits.

An interesting consequence of the fact that the theory presented fully interpolates the Berry-Tabor and Gutzwiller expressions is that it works well beyond where the first-order classical perturbation theory used in its derivation might be anticipated to be valid. Instead, it fails where the Gutzwiller theory does for nonzero perturbations, i.e., in circumstances where the stable orbit's $\mathrm{Det}(M_s-\mathbf{1})\to 0$. Still considering only the shortest periodic orbits, this occurs for perturbations strong enough to produce globalized chaos well into the mixed phase space regime (which we found very encouraging with respect to beginning to understand those systems). To be a little more explicit, the short orbit class is marked by having $\Delta S/\hbar$ exceed 1 without the perturbation sending $\mathrm{Det}(M_s-\mathbf{1})$ through 0 and for this class our treatment works extremely well.

Turning now to the longer orbits, we need to distinguish two classes, those that are repetitions of some short orbit and those that are not. The distinction is important due to the behavior of ΔS and the eigenvalues of M_s. For the rth repetition of some orbit, ΔS is r times the action difference of the primitive periodic orbit $(r=1)$. Likewise, the rth repetition of M_s has eigenvalues that are the rth power of the primitives, $\exp(\pm ir\lambda)$. In essence a much smaller perturbation will lead to $\mathrm{Det}(M_s-\mathbf{1})\to 0$ for a repetition, but since ΔS is also increasing proportionally to r, these orbits also generally attain $\Delta S/\hbar>1$ without their determinants passing through zero. They therefore also belong to the short orbit class. However, for them, the theory breaks down under smaller perturbations. All the newly created high peaks showing up in the perturbed $\hbar^{-1}$-transformed spectra were due to this effect. The stable orbits for $\mathbf{M}=(3,3)$, $(4,4)$, and $(5,5)$ emerge from their respective origins at zero perturbation by separating from the unstable orbit and decreasing in magnitude. Still within the near-integrable regime, they regrow into peaks taller than those that existed even for the integrable system. Since $\mathrm{Det}(M_s-\mathbf{1})\to 0$ indicates an orbit bifurcation from the stable orbit, a new resonance is being created within the original resonance. For these cases, there were thus very sizable effects in the quantum spectrum. Ozorio de Almeida and Hannay have discussed how to uniform the semiclassical theory for such cases [12], but we did not enter the subject here.

As pointed out by Ozorio de Almeida [10], for the remaining infinity of orbits the situation is different. For them, $\Delta S/\hbar$ does not exceed 1 for perturbations strong enough to make $\mathrm{Det}(M_s-\mathbf{1})=0$. ΔS for a given perturbation shrinks rapidly with increase in μ_1 or μ_2. In our spectra, even for $\mathbf{M}=(2,3)$, for example, we found that $\Delta S/\hbar$ was much less than one across the entire near-integrable regime. Not surprisingly then, its contribution remained, to a high degree of accuracy, equal to the Berry-Tabor amplitude throughout. The extended theory remains valid for these orbits up to a perturbation sufficiently strong to make $\mathrm{Det}(M_s-\mathbf{1})=0$ just as with the short orbit class. However, here the theory is not that interesting since it predicts correctly an approximate equivalence to the Berry-Tabor amplitude up to the point where it fails (although it does suggest using S_j and T_j substituted for the action and period of the motion on the original torus). In addition, even the repetition $\mathbf{M}=(6,9)$ behaved in the same way with no change from the Berry-Tabor amplitude. This is in spite of the fact that its $\mathrm{Det}(M_s-\mathbf{1})=0$ near the large perturbation end of the near-integrable regime. That it showed no evidence of the bifurcation is natural in the sense that the resonance is so narrow as to be indistinguishable from a torus, so the resonance within the resonance structure appears to play no role. At some point for a strong enough perturbation though, one would expect this equivalence to Berry-Tabor to fail for long orbits, but apparently not by following the same Bessel function interpolation as found for the shorter orbits.

This points to one of the key problems remaining to be solved in order to understand mixed phase space dynamics and the associated trace formulas. It is necessary to extend our approach to the case of a larger number of periodic orbits within the resonance. From a technical point of view, we recall the assumption made in our derivation that δS has only two extrema. Because these extrema correspond to the orbits surviving the perturbation, this assumption is precisely equivalent to restricting ourselves to the range of perturbation weak enough that there is no bifurcation. Extending the range of applicability of the semiclassical theory further toward the mixed regime will therefore require relaxing this constraint, though still keeping the desire to express all the parameters of the theory in terms of the periodic orbits' canonically invariant quantities. Although certainly not a simple task, this might provide one approach to tackling the study of semiclassical trace formulas for the mixed phase space regime.

ACKNOWLEDGMENTS

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APPENDIX A: TRANSFORMATION OF $D_{\mathbf{M}}$

In this appendix we show that in the change of variable Eq. (2.11), the determinant Eq. (2.6) of the Green's function actually transforms as a density, i.e., that

$$D_{\mathbf{M}}(\mathbf{q})dq_1dq_2 = D_{\mathbf{M}}(\boldsymbol{\theta})d\theta_1 d\theta_2 .$$

A general result [24] is that for point transformations, that is, for canonical transformation $(\mathbf{p},\mathbf{q})\rightarrow(\mathbf{P},\mathbf{Q})$ such that the new position $\mathbf{Q}$ does not depend on the old momentum $\mathbf{p}$, $D_{\mathbf{M}}$ transforms as a density. The difficulty here is that the canonical transformation Eq. (2.11) *is not* a point transformation.

Let us thus introduce a new set of canonical variables $(\mathbf{P},\mathbf{Q})$ defined by

$$\mathbf{Q}(\mathbf{q}) = \theta(\mathbf{q},\mathbf{J}_{\mathbf{M}}). \tag{A1}$$

On the torus $\mathbf{J}_{\mathbf{M}}$, $\mathbf{Q}$, and θ are equivalent, but this is no longer the case as one considers a point outside of this torus. Because Eq. (A1) is a point transformation, one has indeed for any phase space point $\mathbf{r}$ on the torus $\mathbf{J}_{\mathbf{M}}$

$$D_{\mathbf{M}}(\mathbf{q})dq_1dq_2 = D_{\mathbf{M}}(\mathbf{Q})dQ_1dQ_2 ,$$

and since one remains on the torus the measure $d\theta_1 d\theta_2$ is equal to dQ_1dQ_2. Thus, applying the right-hand side of Eq. (2.6), what remains to be shown is that $\partial^2 S/\partial Q_1\partial Q_1' = \partial^2 S/\partial\theta_1\partial\theta_1'$, i.e., $\partial Q_1'/\partial P_1 = \partial\theta_1'/\partial J_1$.

For this purpose, consider two Poincaré sections, $\mathcal{P}_\theta$ at $\theta_2 = \text{const}$ and $\mathcal{P}_{\mathbf{Q}}$ at $Q_2 = \text{const}$, containing the point $\mathbf{r}$. Let T be the mapping such that a trajectory started at (θ_1, J_1) in $\mathcal{P}_\theta$ crosses $\mathcal{P}_{\mathbf{Q}}$ at $(Q_1,P_1) = T(\theta_1,J_1)$ and dT is its linearization at $\mathbf{r}$. Finally, we note M^Q and M^θ the monodromy matrices in $\mathcal{P}_{\boldsymbol{\theta}}$ and $\mathcal{P}_{\mathbf{Q}}$. Because $\theta_1 \equiv Q_1$ on the torus $\mathbf{I}_{\mathbf{M}}$, $dT = \begin{pmatrix} 1 & t_{12} \\ t_{21} & t_{22} \end{pmatrix}$. Moreover, $M_{\boldsymbol{\theta}}$ is a sheer, i.e., $M^\theta = \begin{pmatrix} 1 & m_{12}^\theta \\ 0 & 1 \end{pmatrix}$ $(m_{12}^\theta = \partial\theta_1'/\partial J_1)$. Therefore

$$\begin{aligned} M^Q &= (dT)M^\theta(dT)^{-1} \\ &= \begin{pmatrix} t_{22} - t_{21}(m_{12}^\theta + t_{12}) & m_{12}^\theta \\ t_{21}^2 m_{12}^\theta & t_{22} + t_{21}(m_{12}^\theta - t_{12}) \end{pmatrix} \end{aligned}$$

and $m_{12}^Q = m_{12}^\theta$, which is the desired property.

APPENDIX B: COMPUTATION OF THE MASLOV INDICES

In Sec. II, we have introduced three kinds of Maslov indices: η, σ, and the pair (ν_1,ν_2), associated, respectively, with the semiclassical Green's function, the Gutzwiller trace formula, and the two independent closed paths $\mathcal{C}_1$ and $\mathcal{C}_2$ of a torus on which the actions (I_1,I_2) are computed. All three of them are ''true'' Maslov indices, in the sense that they represent the number of times a curve defined on a specified Lagrangian manifold crosses a line where the projection of the manifold on the configuration space is singular (the index depends therefore both on the curve and on the manifold). This is the case in particular for the index σ [16], although here we have only used it in the way it was original defined by Gutzwiller [1] [see the text just after Eq. (3.17)], which allows a direct and simple expression in term of η.

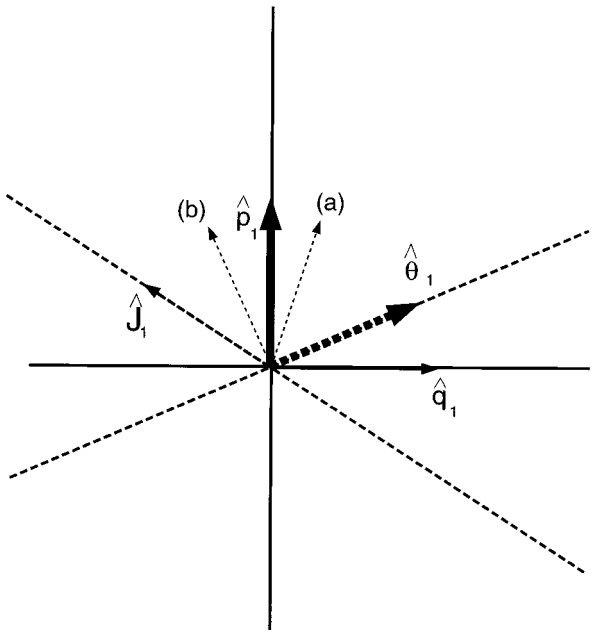

FIG. 12. Schematic representation of the motion of the tangent to the invariant torus (thick dashed arrow) and to the Lagrangian manifold on which the semiclassical Green's function is constructed (thick solid arrow) in a $\theta_2 = \text{const}$ Poincaré section. Because the torus is an invariant manifold, the former $(\hat{\theta}_1)$ is mapped onto itself after winding $(M_1\nu_1 + M_2\nu_2)/2$ times around the periodic orbit. By continuity $\hat{p}_1$ therefore crosses $M_1\nu_1 + M_2\nu_2$ or $M_1\nu_1 + M_2\nu_2 - 1$ depending on whether $\partial p_1'/\partial q_1$ is positive [final position (a)] or negative [final position (b)].

The aim of this appendix is to prove Eq. (2.20), i.e., that for a given torus $\mathbf{I}_{\mathbf{M}}$,

$$\eta_{\mathbf{M}} = (M_1\nu_1 + M_2\nu_2) - \Theta[g_E'']$$

(Θ is the Heaviside step function). To see this, let us first consider $\tilde{\eta}_{\mathbf{M}}$, the Maslov index of the periodic orbit $\mathbf{M}$ on the torus $\mathbf{I}_{\mathbf{M}}$. By definition of the topology (M_1,M_2) of the periodic orbit, the trajectory winds M_1 times around $\mathcal{C}_1$ and M_2 times around $\mathcal{C}_2$ and therefore $\tilde{\eta}_{\mathbf{M}} = (M_1\nu_1 + M_2\nu_2)$. Now $\tilde{\eta}_{\mathbf{M}}$ and $\eta_{\mathbf{M}}$ correspond to the same curve (a periodic orbit of topology $\mathbf{M}$), but not to the same manifold: the former is associated with the invariant torus, whereas the latter is the manifold on which the semiclassical Green's function $G(\mathbf{r},\mathbf{r}')$ is constructed, namely, the set of trajectories started at $\mathbf{r}$ with arbitrary momentum (on the energy surface E). Figure 12 then contains all the information required to relate $\tilde{\eta}_{\mathbf{M}}$ and $\eta_{\mathbf{M}}$. Crossings of the singularities of the manifold correspond to places where the tangent of the manifold becomes vertical. Considering the linearized motion around the orbit in a Poincaré section attached to the orbit, this means that the Maslov index is actually the number of traversals of the vertical, counted positively for clockward traversal and negatively for an anticlockward traversal, of the image of the vector tangent to the manifold at the starting point $\mathbf{r}$. This is, respectively, $\hat{\theta}_1$ for $\tilde{\eta}_{\mathbf{M}}$ and $\hat{p}_1$ for $\eta_{\mathbf{M}}$. There is, however, a slight complication for $\hat{p}_1$ since its original position is precisely on the vertical. The prescription

for the Green's function is then to consider that $\hat{p}_1$ is actually on the right upper quadrant (i.e., has an infinitesimal positive component on the q_1 axis). Now, since on the torus $\mathbf{I_M}$ the Poincaré map is the identity, $\hat{\theta}_1$ makes exactly $\tilde{\eta}_{\mathbf{M}}/2$ turns in one iteration of the periodic orbit. By continuity, $\hat{p}_1$ makes the same number of traversal of the vertical as $\hat{\theta}_1$ if $\partial q_1'/\partial p_1$ is positive and one less if $\partial q_1'/\partial p_1$ is negative. Since, moreover, the Poincaré map is a sheer in the (θ_1, J_1) coordinates, $\mathrm{sgn}[\partial q_1'/\partial p_1] = \mathrm{sgn}[\partial \theta_1'/\partial J_1] = \mathrm{sgn}[-g_E''']$ [where the last equality is deduced from Eqs. (2.15) and (2.16)] and therefore $\eta_{\mathbf{M}} = \tilde{\eta}_{\mathbf{M}} - \Theta[g_E''']$.

APPENDIX C: DERIVATION OF EQ. (3.8) FOR $N=2$

Consider in a Poincaré section $q_2 = \mathrm{const}$ a fixed point (periodic orbit) (q_1^0, p_1^0) of the Poincaré map. Introducing $\delta q_1 = q_1 - q_1^0$ and $\delta p_1 = p_1 - p_1^0$, the linearized motion around the orbit can be characterized either by the monodromy matrix $M = (m_{ij})$ $(i,j = 1,2)$

$$\delta q_1' = m_{11}\delta q_1 + m_{12}\delta p_1,$$

$$\delta p_1' = m_{21}\delta q_1 + m_{22}\delta p_1$$

(with $\mathrm{Det}M = 1$) or by the quadratic approximation to the action

$$S(q_1, q_1') = S^0 + p_1^0(\delta q_1' - \delta q_1) + \left[\frac{A}{2}(\delta q_1)^2 + \frac{B}{2}(\delta q_1')^2 + C\,\delta q_1 \delta q_1'\right].$$

Using the relations $\partial S/\partial q_1 = -p_1$ and $\partial S/\partial q_1' = p_1'$ gives

$$\delta p_1 = -A\,\delta q_1 - C\,\delta q_1',$$

$$\delta p_1' = +C\,\delta q_1 + B\,\delta q_1'$$

and thus $A = m_{11}/m_{12}$, $B = m_{22}/m_{12}$, and $C = -1/m_{12}$. With $S(q_1) = S(q_1, q_1)$, one has therefore $d^2S/dq_1^2 = A + B + 2C = (\mathrm{Tr}M - 2)/(2m_{12})$, which, noting that $\mathrm{Det}M = 1$ implies $\mathrm{Det}(M-1) = 2 - \mathrm{Tr}M$, gives the desired results

$$\frac{d^2S}{dq_1^2} = -\frac{\mathrm{Det}(M - \mathbf{1})}{\partial q_1'/\partial p_1}.$$

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