Semiclassical Trace Formulas of Near-Integrable Systems: Resonances

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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 expressions depend critically on the nature of the classical dynamics. The near-integrable regime is most importantly characterized by the destruction of rational invariant tori being replaced by chains of resonances, yet without globalized chaos being introduced. We give new, generalized expressions appropriate for resonances and apply them to a system that has served as a paradigm for the transition from regular to chaotic dynamics.

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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 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 dynamical 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.

When discussing the various possible system dynamics, it is advantageous to take a more global viewpoint than just classifying every periodic orbit with regards 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. In the latter case, periodic orbits are usually well isolated, and the form of the amplitude derived by Gutzwiller can be used. For integrable systems where there exist as many constants of the motion as degrees of freedom (N), the trajectories lie on N-dimensional tori in the $2N$-dimensional phase space. 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. To fill out a rational torus typically requires an $(N-1)$-parameter continuous family of neighboring periodic orbits. Therefore the form of the amplitude given by Gutzwiller cannot be used in this case, and has to be replaced by expressions such as the ones given by Balian and Bloch [2], and later by Berry and Tabor [3] in a general action-angle formalism.

Systems belonging to the extreme cases of integrable or fully chaotic dynamics are quite rare. The most generic situation for a low-dimensional Hamiltonian is to have a mixed phase space (i.e., significant regions of both near-integrable and chaotic motions). However, a good understanding of the nearly integrable regime would already be extremely useful. First of all, integrable systems are structurally unstable, and many experimental systems considered *a priori* integrable are better described as nearly integrable. In addition, near-integrable theory will be one of the necessary ingredients for mixed phase space systems, since their regular phase space regions may locally be treated as if they were nearly integrable. Finally, the most visible features, and sometimes the only ones which can be observed [4], of these mixed systems come from these regular regions.

The near-integrable regime is characterized by imagining a generic perturbation to a integrable system. The vast majority of the irrational tori continue to exist in some distorted fashion consistent with the KAM theorem of Kolmogorov, Arnol'd, and Moser [5]. Yet the rational tori have all disappeared being replaced by chains of resonances on all scales. Considering that the periodic orbits originally composed 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 $\hbar$, no matter how near the short wavelength limit a system finds itself. 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.

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Ozorio de Almeida was the first to consider the question of resonances [6] and to provide a semiclassical expression for the transition toward the limit where the Gutzwiller expressions hold. Remarkably, however, nearly a decade after publication, little concrete application or exploration of his ideas has taken place. The main difficulty is that although he gave a semiclassical theory, he derived an integral which is generally not easily evaluated. He suggested an approximation scheme for weak perturbations that is rather restrictive and does not give a full interpolation between the Berry-Tabor and Gutzwiller limits. We find generalized, effective expressions that resolve this dilemma in which all the necessary information is encoded in the periodic orbits. Application to the coupled quartic oscillators [7] demonstrates the excellent accuracy of the new expressions.

Consider a Hamiltonian system. The density of states $\rho(E)$ at energy E is expressible in terms of the energy dependent Green function: $\rho(E) = -(1/\pi) \times \mathrm{Im} \int d\mathbf{q}\, G^+(\mathbf{q},\mathbf{q};E)$. It decomposes into an average and a fluctuating component, $\rho(E) = \overline{\rho}(E) + \rho_{\mathrm{fl}}(E)$, respectively, where in the semiclassical approximation

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

The relation for $\overline{\rho}(E)$ is of no interest here and not given. 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 $\int \mathbf{p}\cdot d\mathbf{q}$ along the trajectory, η_t is a topological phase index counting conjugate points, and D_t is the determinant involving second derivatives of the action evaluated at $\mathbf{q}'' = \mathbf{q}' = \mathbf{q}$. Gutzwiller approximated this integral, finding

$$\rho_{\mathrm{fl}}(E) = \frac{1}{\pi\hbar}\sum_j \frac{T_j\cos(S_j/\hbar - \eta_j\pi/2)}{r_j|\mathrm{Det}(M_j - \mathbf{1})|^{1/2}}. \tag{2}$$

The stationary phase condition restricts the trajectory sum to periodic orbits labeled by the index j. S_j, T_j, M_j, η_j, and r_j are, respectively, the orbit's action, period, monodromy matrix, topological phase, and the number of traversals of the primitive orbit.

Turning now to a classically integrable system whose periodic orbits are not isolated, its Hamiltonian can be expressed in action-angle variables $(\mathbf{I},\boldsymbol{\varphi})$ $(\varphi_1,\varphi_2 \in [0,2\pi])$ as $H(\mathbf{I})$; we restrict the discussion to systems with 2 degrees of freedom. Periodic orbits are associated with tori such that the rotation number α is rational. These orbits can be labeled by integers $\mathbf{M} = (M_1, M_2) = (r\mu_1, r\mu_2)$, where (μ_1,μ_2) are coprime integers specifying the primitive periodic orbit ($\alpha = \mu_1/\mu_2$) and r is the number of repetitions. Considering the contribution $\rho_{\mathbf{M}}$ to ρ_{fl} of the orbit of topology $\mathbf{M}$, and denoting by $\mathbf{I}_{\mathbf{M}}$ the action variables of the corresponding torus, the action integral along the orbit is the same for all members of the family, and given by $S^0_{\mathbf{M}} = 2\pi\mathbf{I}_{\mathbf{M}}\cdot\mathbf{M}$. The determinant $D_{\mathbf{M}}$ is best evaluated in a system of coordinates $(\theta_1 = \mu_2\varphi_1 - \mu_1\varphi_2, \theta_2 = \varphi_2)$ such that, *on the torus* $\mathbf{M}$, the variable θ_1 is constant along the trajectory. Making the change of variable from the coordinates (q_1,q_2) to (θ_1,θ_2) in the configuration space integral of Eq. (1), the prefactor can be seen to be a constant and the integral over the variables θ_1 and θ_2 reduces to a multiplication by the size of the domain of integration. Evaluation of these factors yields the Berry-Tabor expression for the contribution of the orbit of topology $\mathbf{M}$: $\rho^{\mathrm{BT}}_{\mathbf{M}} = \mathrm{Re}[T_{\mathbf{M}}\mathcal{G}^{\mathrm{BT}}_{\mathbf{M}}]$,

$$\mathcal{G}^{\mathrm{BT}}_{\mathbf{M}} = \frac{\exp(iS^0_{\mathbf{M}}/\hbar - i\eta_{\mathbf{M}}\pi/2)}{\pi(i\hbar^3M_2^3|g''_E|)^{1/2}}, \tag{3}$$

where g_E (see Sec. IV of [7]) is the function describing the energy surface E in action space, i.e., $H(I_1, I_2 = g_E(I_1)) = E$.

The treatment of nearly integrable systems begins with the Hamiltonian H written in the form $H(\mathbf{I},\boldsymbol{\varphi}) = H^0(\mathbf{I}) + \epsilon\mathcal{H}(\mathbf{I},\boldsymbol{\varphi})$, where the perturbation $\epsilon\mathcal{H}$ is "small." Still labeling the closed orbits by the topology $\mathbf{M}$ of the unperturbed family, the action $S_{\mathbf{M}}(\mathbf{q})$ is no longer constant, expressing the breaking of the resonant torus by the perturbation. Using classical perturbation theory, however, the first order correction to the action is $\delta S_{\mathbf{M}}(\mathbf{q}) = \oint \epsilon\mathcal{H}\,dt$ 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. In the (θ_1,θ_2) coordinates the integral along θ_2 is again trivial, but the θ_1 dependence of δS has to be taken into account. In Ref. [6], Ozorio de Almeida showed that for nearly integrable systems $\rho^{\mathrm{BT}}_{\mathbf{M}}$ has to be replaced by $\rho^{\mathrm{res}}_{\mathbf{M}} = \mathrm{Re}[C_{\mathbf{M}}\mathcal{G}^{\mathrm{BT}}_{\mathbf{M}}]$, where $\mathcal{G}^{\mathrm{BT}}_{\mathbf{M}}$ is given by Eq. (3) and $C_{\mathbf{M}}$ is a damping factor originating from the dephasing of the orbit contribution in the family $\mathbf{M}$:

$$C_{\mathbf{M}}(E) = \frac{1}{2\pi}\int_0^{2\pi} d\theta_1\, T_{\mathbf{M}}\exp\frac{i\delta S_{\mathbf{M}}(\theta_1)}{\hbar}. \tag{4}$$

Typically, Eq. (4) is difficult to evaluate exactly, particularly for regular regions of mixed phase space systems for which the integrable system of reference is generally not known. As an approximation, Ozorio de Almeida suggested keeping just the first term $\Delta S\sin(\theta_1)$ of the Fourier expansion of $\delta S(\theta_1)$ yielding a Bessel function correction to the Berry-Tabor amplitude $\rho^{\mathrm{res}}_{\mathbf{M}} = \rho^{\mathrm{BT}}_{\mathbf{M}}J_0(\Delta S/\hbar)$ [6]. Following the Poincaré-Birkoff theorem, two periodic orbits survive the destruction of the rational torus $\mathbf{M}$: one stable, s, and one unstable, u. Their actions are the extrema of $\delta S(\theta_1)$, thus the difference $\Delta S = (S_u - S_s)/2$ determines the Bessel function argument. Keeping only the first harmonic of $\delta S(\theta_1)$ implies the monodromy matrices of the surviving periodic orbits satisfy $\mathrm{Det}(M_s - \mathbf{1}) \simeq -\mathrm{Det}(M_u - \mathbf{1})$. Under increasing perturbation, this constraint quickly fails to hold depending on the system and particular resonance. Our task is to approximate Eq. (4) in a controllable way (i.e., a criterion is given for the validity of the approximation) so that the periodic orbits determine all the parameters.

Instead of truncating the Fourier series of $\delta S_{\mathbf{M}}$, we map the problem onto the pendulum [absorbing $\overline{\delta S_{\mathbf{M}}} = (1/2\pi)\int_0^{2\pi} d\xi\, \delta S_{\mathbf{M}}(\theta_1)$ into $S^0_{\mathbf{M}}$]

$$\delta S_{\mathbf{M}}(\theta_1) = \Delta S(\epsilon)\cos(\xi), \tag{5}$$

where $\theta_1 = f(\xi)$. This is possible since $S_{\mathbf{M}}(\theta_1) = S^0_{\mathbf{M}} + \delta S_{\mathbf{M}}(\theta_1)$ has but a single maximum and minimum occurring each interval on 2π. In principle, all the angular complexity of the function $\delta S_{\mathbf{M}}(\theta_1)$ has been transferred to the functional relationship $\theta_1 = f(\xi)$. However, because $\Delta S(\epsilon)\cos(\xi)$ is the action variation of the standard pendulum, the relationship between θ_1 and ξ is smooth and nearly linear, and can be approximated in the form (equivalent to a resummed version of an infinite series of terms in the Fourier expansion of $\delta S_{\mathbf{M}}$)

$$\theta_1 \approx \xi - a(\epsilon)\sin(\xi) \tag{6}$$

in all the nearly integrable regimes.

In the same way as above, the two surviving periodic orbits have an action which is extremal, that is, $\xi = 0$ or π. Choosing the unstable orbit as the origin of ξ, one has therefore $\Delta S(\epsilon) = (S_u - S_s)/2$, and $S^0_{\mathbf{M}} = (S_s + S_u)/2$. Similarly, the stabilities of the orbits allow an unambiguous determination of the parameter $a(\epsilon)$. We start from a general relation used in the derivation of the Gutzwiller trace formula [1] and valid for both periodic orbits

$$\frac{d^2 S_{\mathbf{M}}(\theta_1)}{d\theta_1^2} = \mathrm{Det}(M - \mathbf{1})\, \frac{\partial^2 S(\theta_1, \theta_1')}{\partial\theta_1 \partial\theta_1'}\bigg|_{\theta_1'=\theta_1}. \tag{7}$$

The partial derivative on the RHS of Eq. (7) can then be evaluated on the unperturbed system, yielding $\partial^2 S/\partial\theta_1\partial\theta_1' = (2\pi r \mu_2^3 g_E'')^{-1}$. Using the chain rule

$$\frac{d^2 S_{\mathbf{M}}(\theta_1)}{d\theta_1^2} = \zeta \Delta S(\epsilon)\left(\frac{d\xi}{d\theta_1}\right)^2 \tag{8}$$

(where $\zeta = +1$ or -1 for, respectively, the stable and unstable orbits). This gives two relations for the stability determinants of the periodic orbits:

$$\mathrm{Det}(M - \mathbf{1}) = \zeta\, \frac{2\pi r \mu_2^3 g_E'' \Delta S(\epsilon)}{[1 + \zeta a(\epsilon)]^2}. \tag{9}$$

There are two ways to view these equations. First, g_E'' can, with some work, be independently evaluated (see Sec. 4.1 of [7]) giving two equations but only one unknown. The self-consistency is then a measure of the validity of Eq. (6). The second viewpoint just assumes the approximation is valid. Instead of a laborious calculation, the equations are easily solved for both g_E'' and $a(\epsilon)$. All quantities necessary for our theory are then given by properties of the periodic orbits alone.

Taking the ratio of the two cases and doing some algebra fixes the value of $a(\epsilon)$ to be $a(\epsilon) = (\kappa - 1)/(\kappa + 1)$, where

$$\kappa = \left(-\frac{\mathrm{Det}(M_u - \mathbf{1})}{\mathrm{Det}(M_s - \mathbf{1})}\right)^{1/2}. \tag{10}$$

Ozorio de Almeida's suggestion is essentially recovered in cases where $\kappa \to 1$.

The integral of Eq. (4) gives our main result [denoting $s_\epsilon = \Delta S(\epsilon)/\hbar$]

$$C_{\mathbf{M}} = T^0_{\mathbf{M}}[J_0(s_\epsilon) - i a(\epsilon) J_1(s_\epsilon)] + i\Delta T\left[J_1(s_\epsilon) + \frac{i a(\epsilon)}{2}[J_0(s_\epsilon) - J_2(s_\epsilon)]\right], \tag{11}$$

where $J_n(z)$ are the standard Bessel functions. The term proportional to ΔT arises from the θ_1 dependence of the period $T_{\mathbf{M}}(\theta_1) = \partial S_{\mathbf{M}}(\theta_1)/\partial E$. The average period $T^0_{\mathbf{M}} = (T_s + T_u)/2$ 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. Using $\rho^{\mathrm{res}}_{\mathbf{M}} = \mathrm{Re}[C_{\mathbf{M}} \mathcal{G}^{\mathrm{BT}}_{\mathbf{M}}]$ [see Eq. (3)], and, except for the discussion of the Maslov indices not given here, the Berry-Tabor expression is obtained trivially as $\Delta S \to 0$ and the Gutzwiller limit follows using the asymptotic expression for Bessel functions of large arguments.

As has been previously considered [8], the spectrum can be essentially Fourier transformed in $\hbar^{-1}$ in order to separate orbit contributions by their classical actions; the transform variables are $(t = \hbar^{-1}, S)$. In addition, we multiply by an exponential damping because we only have a finite stretch of the spectrum and by a factor $t^{-1/2}$, which generates compact analytic forms as a function of S. We therefore work with the action function

$$R(S,E) = \int_0^\infty dt\, t^{-1/2} e^{-(\alpha - iS)t} \rho(t,E) \tag{12}$$

in the discussion ahead.

To test our approach, let us consider a model system of a two-dimensional quartic oscillator of mass $m = 1$ driven by the potential

$$V(q_1, q_2) = a(\lambda)\left(\frac{q_1^4}{b} + b q_2^4 + 2\lambda q_1^2 q_2^2\right). \tag{13}$$

The parameter b is taken equal to $\pi/4$, and $a(\lambda)$ is a largely irrelevant constant chosen for technical convenience. λ is the parameter responsible for the variation of the system from integrable ($\lambda = 0$) to chaotic dynamics ($-0.6 > \lambda > -1.0$). The range ($0.00 > \lambda > -0.15$) approximately corresponds to the near-integrable regime where the chaos is narrowly contained [7]. The potential $V(\mathbf{q})$ is homogeneous in (q_1, q_2), which leads to scaling relations in the dynamics.

For the entire near-integrable regime $\lambda \in \{-0.15, 0.0\}$, we calculate the level curves for the first 12 000 levels and

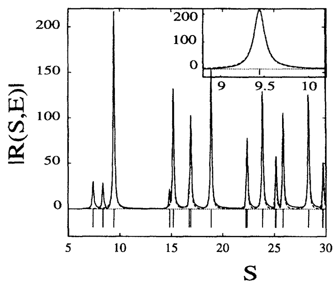

FIG. 1. Comparison of the quantum action function and the semiclassical theory for integrable systems ($\lambda = 0$). The solid curve is the quantum results and the dashed curve the Berry-Tabor formula. The short vertical lines mark the actions of the classical tori. The $\mathbf{M} = (1, 1)$ peak is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

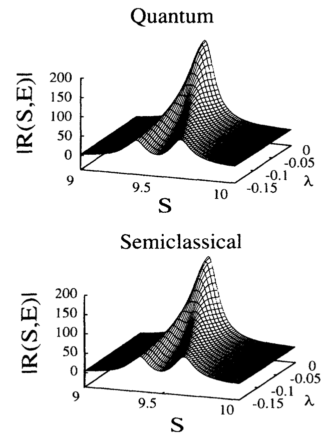

FIG. 2. Comparison of the quantum and the semiclassical theory of the $\mathbf{M} = (1, 1)$ resonance as a function of action, S, and perturbation strength, λ. Note $E = 1$.

the necessary information about the periodic orbits. We first show results for the integrable case. The Berry-Tabor formula has sometimes been found to be a little imprecise. With the exception of the "tori" $\mathbf{M} = (m_1, 0)$ or $\mathbf{M} = (0, m_2)$, which are isolated orbits of no interest here, in Fig. 1 we find excellent agreement to within a couple of percent or better between the Berry-Tabor theory compared to the quantum results. The best accuracy is found for smaller action tori with some degradation showing up in the tails and peaks for larger action tori. In particular, the $\mathbf{M} = (1, 1)$ torus contribution shown expanded is good to 1% of the magnitude in the peak region with the phase error not worse than about 2°. This sets the scale for the quality of results we demand across the near-integrable regime for the comparison of the theory for resonances presented here.

This same resonance is isolated from other orbits, and its stable and unstable orbits are well separated by $\lambda = -0.15$. Its independently calculated value of g_E'' leads to consistency with Eqs. (9) to better than 5% across the entire near-integrable regime. In Fig. 2, we show the comparison of the semiclassical theory with the quantum results. The agreement is excellent being better than 3% error near the peak for all values of λ. The agreement found using the aforementioned $J_0(\Delta S/\hbar)$ expression leads to 10% errors for this resonance. For other resonances such as $\mathbf{M} = (3, 3)$, the improvement using Eq. (11) is far more significant. This point and the behaviors of other resonances will be discussed in a full exposition of this work [9].

In conclusion, we have extended periodic orbit theory for near-integrable systems for which Ozorio de Almeida derived a semiclassical formalism a decade ago, but without giving the connection to periodic orbits. We have obtained new expressions, valid in the whole nearly integrable regime and fully interpolating the Berry-Tabor and Gutzwiller expressions, whose parameters have been identified with properties of the periodic orbits. This has made it possible to perform the first complete implementation of the theory for a model system, and the results are found to be excellent.

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