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\hbar expansion for the periodic-orbit quantization of hyperbolic systems

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Using Feynman path integrals and the stationary-phase method, we develop a semiclassical theory for quantum trace formulas in classically hyperbolic systems. In this way, we obtain corrections to the Gutzwiller-Selberg trace formula as an asymptotic series in powers of the Planck constant. The first coefficient of this series is given explicitly. We illustrate the theory with the calculation of complexwave-number resonances for the two-disk scatterer and show that effects beyond the Gutzwiller leading approximation are at the origin of a lengthening of the resonance lifetimes at low energy. PACS number(s): 03.65.Sq, 03.40.Kf, 05.45.+^b

In recent years, there has been an increased interest in semiclassical methods for quantizing the classically chaotic systems found in highly excited atoms and molecules. Several important results have been obtained thanks to the Gutzwiller-Selberg trace formula [1], which has been applied to calculate the energy eigenvalues or the scattering resonances of systems such as the anisotropic Kepler problem [1], the disk scatterers [2,3], the helium atom [4], the hydrogen negative ion [5], and others [6—8], in terms of their classical periodic-orbits.

In semiclassical methods, the action W of a path $q(t)$ is expanded around the classical trajectories with respect to the differences $q(t) - q_{cl}(t)$. The first variation in the action vanishes according to classical mechanics, $\delta W = 0$. As a consequence,

$$
W[\mathbf{q}(t)] = \int_0^T L(\mathbf{q}, \dot{\mathbf{q}}) dt = W_{\rm cl} + \frac{1}{2} \delta^2 W + \frac{1}{3!} \delta^3 W + \frac{1}{4!} \delta^4 W + \cdots, \qquad (1)
$$

where *L* is the Lagrangian, W_{cl} is the action of the classical trajectory, and $\delta^n W$ is the *n*th-order variation. The Gutzwiller-Selberg trace formula only uses the quadratic variation in (1). For special geodesic ffows on surfaces of constant negative curvature, it is known that the Gutzwiller-Selberg trace formula establishes an exact relationship between the quantum energy levels and the periodic orbits [1].

However, evidence has accumulated that this trace formula is not exact for more general systems. In the threedisk scatterer, the complex energies calculated from the ζ function and the curvature expansion appear to differ systematically from the exact quantum-mechanical values [3]. Similar discrepancies have been observed more recently for the energy eigenvalues obtained with the Riemann-Siegel look-alike formula for several bounded systems, which raised some criticism about the method [7]. Moreover, for the two- and three-disk scatterers, the Selberg trace formula is unable to reproduce a lengthening of the resonance lifetimes at low energy [9,10]. In view of these problems, the higher-order terms of the action (1) can no longer be ignored in the periodic-orbit quantization method.

In the present Rapid Communication, our purpose is to show that these higher-order variations in the action are at the origin of contributions to the semiclassical

trace formula that are in powers of the Planck constant \hbar . In this way, we develop an alternative theory for obtaining the periodic-orbit quantization condition to all orders in the semiclassical approximation. Our theory is based on the evaluation of the Feynman path integrals by the stationary-phase method, keeping all the terms of the expansion in powers of \hbar . For a one-variable integral with an arbitrary function $\phi(x)$ having one stationary point where $\partial_x \phi(x_0) = 0$, we have ϵ + ∞

$$
\int_{-\infty}^{\infty} e^{(i/\hbar)\phi(x)} dx
$$
\n
$$
= e^{(i/\hbar)\phi_0} \left[\frac{2\pi i \hbar}{\phi_0^{(2)}} \right]^{1/2} \left[1 - \frac{i \hbar \phi_0^{(4)}}{8(\phi_0^{(2)})^2} + \frac{5i \hbar (\phi_0^{(3)})^2}{24(\phi_0^{(2)})^3} + O(\hbar^2) \right], (2)
$$

with the notation $\phi_0^{(n)} = \partial_x^n \phi(x_0)$. Thanks to the stationary-phase method, the oscillatory integral is reduced to a series of moments of an imaginary Gaussian integral. Our aim is to apply the expansion (2) to the Feynman path integral defining the trace formula.

Let us consider a system with f degrees of freedom described by the Hamiltonian $\hat{H} = -(\hbar^2/2)\nabla^2 + V(q)$, possibly with boundary conditions on hard walls or symmetry surfaces. The classical dynamics is assumed to be hyperbolic, i.e., that all the periodic orbits are unstable and of the saddle type. The energy eigenvalues or the scattering resonances are known to be poles of the trace of the resolvent of the Hamiltonian at real or complex energies 1]. Since the resolvent is related to the propagator $\hat{U}(T) = \exp(-i\hat{H}T/\hat{n})$ by $\hat{U}(T)$ =exp($-i\hat{H}T/\hbar$) by

$$
\frac{1}{E - \hat{H}} = \frac{1}{i\hbar} \int_0^\infty dT e^{(i/\hbar)ET} \hat{U}(T) , \qquad (3)
$$

 $E-H$ in θ o
with ImE > 0, we first consider the trace of the propagator that can be directly evaluated as the Feynman path integral

$$
\operatorname{tr} \hat{U}(T) = \left[\frac{N}{2\pi i \hbar T} \right]^{Nf/2} \int d\mathbf{q}_0 \cdots d\mathbf{q}_{N-1}
$$

$$
\times \exp \left[\frac{i}{\hbar} W(\mathbf{q}_0, \dots, \mathbf{q}_{N-1}) \right], \qquad (4)
$$

where the propagation has been subdivided into N small time intervals $\Delta t = T/N$ and where W denotes the discretized path action (1). The trace of the resolvent will be calculated afterwards.

The trace has the effect of closing the paths in (4) :

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 $\mathbf{q}_0 = \mathbf{q}_N$. Hence the stationary phase condition $\partial W / \partial q_n = 0$ selects the following solutions of Newton's equations $\ddot{\mathbf{q}} = -\partial_{\mathbf{q}} V$. (i) There are the fixed points where $\partial_{q}V(q_s) = 0$ for the critical energies $E_s = V(q_s)$. We shall describe the fixed points elsewhere because they are absent in several known examples of hyperbolic systems [3—8]. (ii) There are the periodic orbits, which are unstable and isolated due to the assumption of hyperbolicity. Because the time T may be some multiple $r \ge 1$ of the fundamental periods $T_p(E)$, which vary with the energy in anharmonic potentials, the periodic orbits are found at the different energies satisfying $T = rT_p(E_{pr})$.

Since the periodic orbits are one-dimensional solutions, one among the positions $\{q_n\}$ remains arbitrary while the

others are determined by Newton's equations and the fixed value of T. We take q_{01} as the arbitrary position that parametrizes the periodic orbit. Thereafter, the action in (4) is expanded in Taylor series around the classical solution according to (1). The $(Nf-1)$ -component vector $\{\xi^a\} = \{q_n - q_c(n \Delta t)\}_{n=0}^{N-1}$ denotes the separation of the path with respect to the classical solution. In the double index $a = (i, n)$, the first index *i* refers to the *i*th space component of q ($i = 1,...,f$) and the second index n to the time $t = n\Delta t$ $(n = 0, \ldots, N-1)$. $W_{,a} \ldots$ denotes the partial derivative $\partial \cdots \partial W / \partial \xi^a \cdots \partial \xi^z$ evaluated at the classical solution $\xi^a=0$. We adopt the convention of summation over repeated indices. We get

$$
\text{tr}\,\hat{U}(T)\Big|_{\text{PO}} = \sum_{p,r} \left[\frac{N}{2\pi i\hbar T}\right]^{Nf/2} \exp\left[\frac{i}{\hbar}W_{\text{cl}}\right] \int dq_{01}d^{Nf-1}\xi \exp\left[\frac{i}{2\hbar}W_{,ab}\xi^a\xi^b\right] \times \left[1 + \frac{i}{6\hbar}W_{,abc}\xi^a\xi^b\xi^c + \frac{i}{24\hbar}W_{,abcd}\xi^a\xi^b\xi^c\xi^d + O(\xi^5/\hbar) - \frac{1}{72\hbar^2}W_{,abc}W_{,def}\xi^a\xi^b\xi^c\xi^d\xi^e\xi^f + O(\xi^7/\hbar^2) + O(\xi^9/\hbar^3)\right].
$$
 (5)

The second derivative matrix $D_{ab} = W_{,ab}$ carries information on the linear stability of the periodic orbits. Its elements are

$$
\frac{\partial^2 W}{\partial q_i(t)\partial q_j(t)} = \frac{2N}{T} \delta_{ij} - \frac{T}{N} \frac{\partial^2 V}{\partial q_i \partial q_j}(t) + O(N^{-2}),
$$

$$
\frac{\partial^2 W}{\partial q_i(t)\partial q_j(t \pm \Delta t)} = -\frac{N}{T} \delta_{ij} + O(N^{-2}),
$$
 (6)

and zero otherwise. The higher derivatives are

$$
\frac{\partial^m W}{\partial q_{i_1}(t)\cdots\partial q_{i_m}(t)} = -\frac{T}{N} \frac{\partial^m V}{\partial q_{i_1}\cdots\partial q_{i_m}}(t) + O(N^{-2}), \qquad (7)
$$

and zero otherwise. As announced with (2), the Feynman path integral (4) has now been reduced to the series (5) of moments of imaginary Gaussian integrals. Because the periodic orbits are unstable and isolated, odd moments are vanishing while even moments are given by

$$
\int d^{Nf-1}\xi \exp\left[\frac{i}{2\hbar}D_{ab}\xi^a\xi^b\right]\xi^{c_1}\xi^{c_2}\cdots\xi^{c_{2L-1}}\xi^{c_{2L}}
$$

$$
=\left[\frac{(2\pi i\hbar)^{Nf-1}}{\det\mathbf{D}}\right]^{1/2}(i\hbar)^L
$$

$$
\times\left[(\mathbf{D}^{-1})^{c_1c_2}\cdots(\mathbf{D}^{-1})^{c_{2L-1}c_{2L}}+\cdots\right],
$$
(8)

where the sum contains all the terms obtained by grouping the indices two by two. At the Gutzwiller approximation given by the first term of (5), we only need the functional determinant detD, which has been derived in Ref. [11] for the trace of the propagator. The higher approximations require the knowledge of the inverse matrix D^{-1} . Remembering the convention on the indices $a = (i,m)$ and $b = (j,n)$ and recovering the continuous time limit, the inverse matrix can be expressed like $(D^{-1})^{ab} = G_{ij}(m \Delta t, n \Delta t)$ in terms of the classical Green function, which is the solution of

$$
\frac{d^2}{dt^2}G_{ij}(t,t')+\frac{\partial^2 V}{\partial q_i\partial q_k}[\mathbf{q}_{cl}(t)]G_{kj}(t,t')=-\delta_{ij}\delta(t-t') ,\quad (9)
$$

for the periodic orbit $q_{cl}(t)$. The associated boundary conditions are

$$
G_{1j}(t_0, t') = G_{1j}(t_0 + T, t') = 0, \quad G_{ij}(t_0, t') = G_{ij}(t_0 + T, t'),
$$
\n(10)

with $i = 2, \ldots, f$ and $j = 1, \ldots, f$. The initial time t_0 corresponds to the position on the periodic orbit that is fixed by the value of q_{01} .

Gathering the results, the terms in ξ^4 and ξ^6 of Eq. (5) divided by the leading term take the form $i\hbar C_1$ with

$$
C_{1} = \frac{1}{8T} \int_{0}^{T} dt_{0} \int_{t_{0}}^{t_{0}+T} dt \frac{\partial^{4} V(t)}{\partial q_{i} \partial q_{j} \partial q_{k} \partial q_{l}} G_{ij}(t, t) G_{kl}(t, t)
$$

+
$$
\frac{1}{24T} \int_{0}^{T} dt_{0} \int_{t_{0}}^{t_{0}+T} dt dt' \frac{\partial^{3} V(t)}{\partial q_{i} \partial q_{j} \partial q_{k}} \frac{\partial^{3} V(t')}{\partial q_{i} \partial q_{j} \partial q_{m}} [3 G_{ij}(t, t) G_{kl}(t, t') G_{mn}(t', t') + 2 G_{il}(t, t') G_{jm}(t, t') G_{kn}(t, t')] . \qquad (11)
$$

The next terms are given by similar integrals. All these integrals can be written in terms of diagrams of a kind considered in quantum field theories $[12-16]$ according to the following rules. A vertex with m legs is associated with each $\frac{\partial^m V(t)}{\partial q_{i_1} \cdots \partial q_{i_m}}$. A line is associated with each classical Green function $G_{ij}(t,t')$ that joins two free legs either of the same vertex or between two different vertices. Integrals are then performed over the times of the different vertices. Finally, a time average $T^{-1} \int_0^t dt_0$ is carried out over the initial time t_0 . In the series, we find connected and disconnected diagrams. A very important property is that the series of all the diagrams can be transformed into the exponential of a

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series involving only the connected diagrams. Finally, we get that the periodic orbits contribute to the trace by the terms

$$
\operatorname{tr}\hat{U}(T)\Big|_{\text{PO}} = \sum_{\substack{p,r \\ (T=r_p)}} \frac{T_p \exp\left[\frac{i}{\hbar}rW_p - i\frac{\pi}{2}r\mu_p + i\frac{\pi}{4}\text{sgn}\partial_E T_p + \sum_{n=1}^{\infty} (i\hbar)^n C_n (rT_p)\right]}{|2\pi\hbar r(\partial_E T_p) \det(\mathbf{M}_p^r - \mathbf{I})|^{1/2}}\,. \tag{12}
$$

 W_p is the action of the prime periodic orbit p over the fundamental period T_p ; μ_p is its Morse index; M_p is the linearized symplectic first return map in the neighborhood of p . In the exponential, we find a a new asymptotic series with all the corrections in \hbar^n . For geodesic flows on surfaces of constant negative curvature, these corrections are vanishing $C_n = 0$, so that a Selberg trace formula is then recovered [1].

We now turn to the trace of the resolvent (3). According to the stationary-phase method, the integral (3) over the time T has several types of critical points. (i) There is $T=0$, which leads to the average level density of Fermi, Thomas, Weyl, and Wigner [17]. (ii) There are the periods $T = rT_p$ determined by the condition $\partial T_W + E = 0$. (iii) There are the fixed points. As explained before, we focus on the unstable periodic orbits. Introducing the reduced action $S(E) = ET + W(T)$ and using $T_p = \partial_E S_p$, we finally obtain our main formula for the contribution of the periodic orbits to the trace of the resolvent,

$$
\operatorname{tr}\frac{1}{E-\hat{H}}\Bigg|_{\text{PO}} = \sum_{\substack{p,r}} \frac{T_p \exp\left(\frac{i}{\hbar}rS_p - i\frac{\pi}{2}r\mu_p\right)}{i\hbar|\det(\mathbf{M}_p^r - 1)|^{1/2}} \exp\left\{i\hbar\left(C_1(rT_p) - \frac{\partial_E^2 B_{pr}}{2r(\partial_E^2 S_p)B_{pr}} + \frac{(\partial_E^3 S_p)^2}{6r(\partial_E^2 S_p)^3} - \frac{\partial_E^4 S_p}{8r(\partial_E^2 S_p)^2}\right)\right\},\tag{13}
$$

where $S_p = S(E)/r$, C_1 is the first correction given by Eq. (11), and

$$
B_{pr}(E) = \frac{T_p}{|\partial_E T_p \det(\mathbf{M}'_p - \mathbf{I})|^{1/2}} \tag{14}
$$

Equations (13) and (14) give the correction in \hbar to the Gutzwiller trace formula. The next corrections can be obtained systematically.

To illustrate the theory, we apply the preceding method to the scattering of a point particle on two disks fixed in the plane, which is one of the simplest classically hyperbolic systems. Its classical repeller consists of the single unstable periodic orbit for which the particle

remains trapped between the two disks. This scatterer can be viewed as a model of unimolecular dissociation [2]. To obtain the energies and the lifetimes of the quantum resonant states, we have to solve the Schrödinger equation $(\Delta + k^2)\psi = 0$ with the Dirichlet boundary condition $\psi=0$ on the border of the disks. Because the wave number k is related to the energy by $E = \hbar^2 k^2 / (2m)$, the small parameter is k^{-1} instead of \hbar . Using the free quantum Green function $\mathcal{G}_0 = (-i/4)H_0^{(1)}(k|\mathbf{q}-\mathbf{q}'|)$, the full quantum Green function is obtained by a multiplescattering expansion: $g = \sum_{m=0}^{\infty} \hat{Q}^m g_0$ [18–20]. The scattering resonances are obtained as the zeros of the characteristic equation

$$
0 = \det(I - \hat{Q}) = \exp\left[-\sum_{m=1}^{\infty} \frac{1}{m} \text{tr} \hat{Q}^m\right] = \exp\left[-\sum_{m=1}^{\infty} \frac{2^m}{m} \oint ds_1 \cdots ds_m \frac{\partial S_0}{\partial n_1}(m, 1) \cdots \frac{\partial S_0}{\partial n_m}(m - 1, m)\right],
$$
\n(15)

for complex wave numbers k . $\partial/\partial n$ denotes the normal derivative exterior to the disks. The integer m is the number of collisions of the path on the disks. The arguments $(j, j+1)$ of the quantum Green functions refer to the free flights between the *j*th and $(j+1)$ th collisions. The integrals are performed over the infinitesimal arc of perimeter ds_i , running along the border of the disks.

We have carried out a systematic k^{-1} -expansion of (15) beyond the leading approximation, which is known to give the Gutzwiller-Selberg ζ function [20]. Our calculation required the extension of the method described in the preceding paragraphs from smooth potentials to billiards. Instead of Feynman path integrals, we are dealing here with ordinary multiple integrals where the role of the classical Green functions (9) is played by finite matrices controlling the quadratic stability of the periodic orbits under the defocusing collisions on the disks. We have obtained the following periodic-orbit quantization condition:

$$
0=1-\frac{1}{\Lambda^{1/2}}\exp[ikL+ik^{-1}c_1-k^{-2}c_2+O(k^{-3})] \ . \qquad (16)
$$

If the two disks of unit radius have their centers separated by a distance $R = 6$, the length of the periodic orbit is $L = 8$; its stability eigenvalue is $\Lambda = 97.989795$; and we finally get the first two coefficients $c_1 = 0.625000$ and $c_2 = -0.750$ 12 from our semiclassical theory, the details of which will be given elsewhere. We remark that the real parts of the resonance wave numbers are modified by the k^{-1} term because it gives a real correction to the term kL . On the other hand, because the k^{-2} term is imaginary with respect to kL it brings a correction to the imaginary parts of the zeros, i.e., to the lifetimes of the resonances. This behavior is indeed confirmed by the comparison with the exact quantum-mechanical values of the resonances provided for us by Wirzba [9,10]. Except for the first resonance where the series in (16) cannot converge since $|k_1|$ < 1, Table I shows that our semiclassical expan-

sion considerably improves the leading Gutzwiller approximation; in particular, by two digits at large wave numbers. Moreover, we see in Table I that our theory carried out till the k^{-2} approximation, explains the lengthening of the resonance lifetimes at low energy, which remained unraveled at the Gutzwiller k^0 approximation. The lengthening has its origin in the quantum fluctuations due to the high-order variations in the action (1) around the classical periodic orbit. Besides, we recover the inverse of the Ruelle ζ function of the two-disk repeller if we neglect the k^{-n} corrections in (16). In this regard, our result shows how the ζ functions must be modified to incorporate the quantum corrections in the periodic-orbit quantization condition. We can show that similar results hold for quantum maps [21,22].

In conclusion, we think that the h expansion described in this Rapid Communication provides a foundation for the periodic-orbit quantization method, which is no longer restricted to the leading approximation. In this respect, the \hslash expansion can be fruitfully applied to classically chaotic systems, not only to improve the accuracy of the semiclassical evaluation of the energy levels of highly excited atoms or molecules, but also to obtain the lifetimes of autoionizing states of He or H^- , which are not attainable [4,5] at the leading approximation.

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