Semiclassical Path-Integral Quantization of Nonintegrable Hamiltonian Systems

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The periodic-orbit quantization approach of Gutzwiller, which is a semiclassical approximation of Feynman's path-integral formalism, is used to calculate finite-resolution densities of states for a Hamiltonian system whose classical motion is dominated by chaos, viz., the hydrogen atom in a uniform magnetic field. In spectral regions where the resolution obtained is larger than the mean level spacing, it is possible to extract approximate eigenvalues of the quantized system. The particular role of stable periodic orbits and their direct quantization are elaborated. Remarkable agreement with exact quantum calculations results.

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For integrable Hamiltonian systems, direct semiclassical quantization schemes such as the WKB or Einstein-Brillouin-Keller method are well established and widely applied.[1] However, it is still unknown how to extend these methods to nonintegrable systems, although this represents one of the oldest outstanding problems of elementary quantum mechanics. An alternative to the direct semiclassical quantization is the "global" periodic-orbit quantization approach of Gutzwiller, which is a semiclassical approximation of Feynman's path-integral formalism.[2] In contrast to the direct methods, where a classical orbit with quantized actions defines a semiclassical eigenstate, the spectrum of the global approach emerges from the *superposition* of contributions arising from periodic orbits only. Generally the global approach is much more complicated, which accounts for its lack of popularity. Yet, it is the only known semiclassical quantization procedure which applies to both integrable and nonintegrable (including classically chaotic) systems. For integrable systems the theory yields the same results as the direct methods,[3] whereas for some classically chaotic systems the method is equivalent to solving the Schrödinger equation.[4] That periodic orbits influence quantum spectra strongly was shown very recently, both experimentally[5,6] and theoretically.[7,8] However, little is known about the quantitative applicability of the method. Gutzwiller applied the theory to the anisotropic Kepler problem, which turns out to be classically chaotic.[9] Using a coding scheme, he was able to include all the periodic orbits of the system. The calculated eigenvalues agreed well with quantum results.[10] However, it is difficult to assess how the method works when coding schemes are not available and only the simplest periodic orbits are known.

In this Letter we apply the theory to calculate, for the first time, a smoothed density of states for a Hamiltonian system whose classical motion is dominated by global chaos. The action of the longest periodic orbit included limits in the density resolution. In spectral regions, where this resolution is larger than the mean level spacing, it is possible to approximate the quantized energy levels. In addition, the particular role of stable orbits for direct quantization will be explicated.

The essential formulas are reviewed in Berry and Mount[1] and Berry.[11] We only sketch the way in which periodic orbits enter the central formulas of the theory.[12] The quantum Green's function G is the Fourier transform of the time-evolution propagator written as a Feynman path integral

$$G(\mathbf{q}',\mathbf{q}'',E) = -\frac{i}{\hbar}\int_0^\infty dt \left\{ e^{iEt/\hbar} \int_{\mathbf{q}'}^{\mathbf{q}''} D[\mathbf{q}] e^{(i/\hbar)\int_0^T L(\mathbf{q},\dot{\mathbf{q}},t)dt} \right\}, \tag{1}$$

where L is the Lagrangian. The semiclassical approximation now consists in evaluating the integrals by the method of stationary phase. Then only classical paths γ form $\mathbf{q}'$ to $\mathbf{q}''$ with energy E contribute to the integrals:

$$G_{sc}(\mathbf{q}',\mathbf{q}'',E) \simeq \sum_\gamma A_\gamma e^{(i/\hbar)S_\gamma - \text{phases}}, \tag{2}$$

where $S_\gamma(\mathbf{q}',\mathbf{q}'',E)$ is the classical action along the path γ, and $A_\gamma(E)$ is an amplitude to be discussed later. The semiclassical density of states d is now

$$d(E) = -\frac{\Im m}{\pi} \int d\mathbf{q}' G_{sc}(\mathbf{q}',\mathbf{q}'')\,|_{\mathbf{q}'=\mathbf{q}''}. \tag{3}$$

It depends only on the classical paths which start and end at the same point. Again the stationary phase approximation is used to integrate Eq. (3) and only orbits with stationary actions S contribute. These orbits are of two types: paths of zero length (this is the limit of the direct paths as $\mathbf{q}' \to \mathbf{q}''$), and periodic orbits, which have the same momentum $\mathbf{p}' = \mathbf{p}''$, when they return in coordinate space. The paths of zero length give rise to a (smoothly) energy dependent mean level density $\bar{d}(E)$, known as the Thomas-Fermi term. A single periodic orbit gives an oscillatory contribution to the density of

states[2]:

$$d(E)=\bar{d}(E)+\Im m\sum_r \frac{T_r}{\pi\hbar}\sum_{j\neq 0}\frac{\exp\{ij[S_r/\hbar-\alpha_r\pi/2]\}}{[\det(M_r^j-1)]^{1/2}}. \quad (4)$$

The sum in the trace formula (4) runs over all primitive periodic orbits r and all repetitions j of a primitive orbit with period T_r, action S_r, and Maslov index α_r. M_r is the 2×2 stability matrix, whose eigenvalues define the type of fixed point of the periodic orbit in the Poincaré surface of section. The determinant in (4) is given, dependent on the type of fixed point, by[2,13]

$$\tfrac{1}{2}[\det(M^j-1)]^{1/2}=\begin{cases}-i\sinh(j\lambda/2), & \text{hyperbolic}, \quad (5a)\\ \cosh(j\lambda/2), & \text{inverse hyperbolic}, \quad (5b)\\ \sin(j\pi\nu), & \text{elliptic}, \quad (5c)\end{cases}$$

where λ is the Liapunov exponent for an unstable periodic orbit and ν is the stability angle divided by 2π.

It is instructive to study the contribution to the level density of a single periodic orbit with all its repetitions j. For unstable periodic orbits, the sum over j in (4) yields nearly Lorentzian contributions[2] centered on the energies E_n given by $S(E_n)=2\pi\hbar(n+\alpha/4)$. Thus, a single unstable periodic orbit manifests itself as a modulation of the level density rather than a sequence of quantum states. It is the interference of the modulations coming from different orbits, which leads to singularities (quantum states) in the density of states. For stable periodic orbits, Eq. (4) can be summed analytically and gives δ functions in the density of states at energies E_{nk} satisfying[14]

$$S(E_{nk})=2\pi\hbar[n+(k+\tfrac{1}{2})\nu+\alpha/4]. \quad (6)$$

The quantum number n counts the number of nodes along the periodic orbit while k gives the excitation of the normal-mode frequency of harmonic perturbations about the periodic orbit. For nonvanishing de Broglie wavelengths the harmonic approximation for transversal excitation generally breaks down at some finite value of k, but the essential point is that the theory predicts sequences of regularly spaced quantum states associated with each stable periodic orbit.

We now use the above theory to calculate the density of states for a hydrogen atom in a uniform magnetic field $\mathbf{B}=(0,0,\gamma B_0)$, $B_0=2.35\times 10^5$ T. The Hamiltonian (in a.u.)

$$H=\tfrac{1}{2}p^2-r^{-1}+\tfrac{1}{8}\gamma^2(x^2+y^2) \quad (7)$$

fails to separate in any coordinate system of R^3; only the azimuthal quantum number m and parity π are good quantum numbers and can be separated off. The Hamiltonian (7) scales as

$$H(\mathbf{p},\mathbf{r};\gamma)=\gamma^{2/3}H(\gamma^{-1/3}\mathbf{p},\gamma^{2/3}\mathbf{r};\gamma=1),$$

which simplifies the application of Eq. (4) considerably, since all classical quantities on the right-hand side are energy and field strength independent (apart from scaling). The classical system displays a smooth transition from regularity to chaos as the parameter $\epsilon=E\gamma^{-2/3}$ is varied.[15] In the following we will study the density of states as a function of $\gamma^{-1/3}$ for fixed scaled energy ϵ and $m^\pi=0^+$. An algorithm to solve the Schrödinger equation for fixed scaled energy is described in Ref. 16. Quantum spectra studied here consist typically of 350–1600 levels.

To enumerate all the periodic orbits of the classical system is a difficult task. No general scheme to find them is available. By solving the equations of motion numerically, we calculated all periodic orbits up to a given scaled action $\tilde{S}_{\max}$, which obey two of the following properties: (i) orbits which pass through the origin, (ii) orbits which pass perpendicularly through a symmetry axis, and (iii) orbits which run on the boundary of the classically allowed region. There is some evidence that these orbits cover all the periodic orbits up to $\tilde{S}_{\max}=3$. Details of these calculations will be published elsewhere.

We first turn to the problem of direct quantization of stable periodic orbits. The most simple periodic orbit (shortest period and shortest action) is the motion perpendicular to the field. This orbit remains stable up to $\epsilon_0=-0.1273$ and becomes unstable for $\epsilon>\epsilon_0$.[17] Equation (6) now predicts series of quantum states of equidistant spacing $\Delta\gamma^{-1/3}\sim 1/\tilde{S}$ given by the scaled action $\tilde{S}$ of the primitive periodic orbit. We searched for such states in quantum spectra for various values of the scaled energy ϵ and found them with excellent agreement. Since for this orbit the "local parity" $(-1)^k$ of the transversal excitation coincides with the exact z parity, only even k have to be considered in the $m^\pi=0^+$ spectra. Resummation over k then leads to an additional factor of 2 in the argument of the amplitude function (5c). Table I summarizes the results: Spacings and phases for $k=0$ and the amplitudes A_j for j traversals of the orbit are given both classically and quantum mechanically. The quantum amplitude of each cosine modulation in Eq. (4) is extracted from a Fourier transform of the quantum spectra.[7] The results for $\epsilon=-0.1$ given in Table I correspond to the case in which the orbit has become unstable and we have used Eq. (5a) in calculating the classical amplitudes. Then, it was not possible to identify a regularly spaced sequence of states in the corresponding quantum spectrum, in agreement with the theory which only predicts regular *modulations* in the density of states when the orbit is unstable. Again, the corresponding quantum value of the spacing of these modulations is extracted from a Fourier transform.

We now turn to the calculation of a smoothed density of states by application of Eq. (4). The mean level density is simply proportional to $\gamma^{-1/3}$ and we concentrate on the fluctuating part, that is the double sum in Eq. (4)

TABLE I. Spacings, phases, and modulation amplitudes A_j for the jth traversal associated with the periodic orbit perpendicular to the field for various values of the scaled energy ϵ. Values marked with an asterisk have some uncertainty or could not be determined because the corresponding peak in the Fourier transform was not fully resolved.

Scaled energy ϵ		−0.4	−0.35	−0.3	−0.25	−0.2	−0.15	−0.1
Spacing	Classical	0.921 70	0.948 01	0.975 35	1.003 71	1.033 05	1.063 35	1.094 57
	Quantum	0.921 71	0.948 01	0.975 35	1.003 71	1.033 03	1.063 23	1.094
Phase	Classical	0.898	0.885	0.870	0.852	0.829	0.794	3/4
	Quantum	0.899	0.886	0.870	0.852	0.827	0.793	3/4
A_1	Classical	0.54	0.54	0.56	0.60	0.71	1.17	1.0
	Quantum	0.48	0.47	0.48	0.54	0.65	1.23	1.1
A_2	Classical	0.93	2.14	4.25	1.04	0.65	0.69	0.5
	Quantum	0.83	2.12	4.8*	1.03	0.58	0.81	... *
A_3	Classical	0.81	0.58	0.57	0.91	3.33	0.62	0.3
	Quantum	1.02	0.48	0.49	0.94	2.9*	0.69	... *

only. We choose $\epsilon = -0.2$. For this value of the scaled energy, only a small part of the classical phase space is regular while the dominant part is occupied by chaotic trajectories. It has been shown that short-range fluctuation measures of the associated quantum spectrum are close to those of a random matrices, which prohibits an assignment of quantum numbers.[18]

Before carrying out the calculations, Eqs. (2) and (3) must be modified. The m^{π} subspaces possess discrete symmetries such as parity. The Green's function in Eq. (2) has to be adapted to this symmetry before taking the trace in Eq. (3).[9] As a consequence, periodic orbits contribute also with half their periods to the level density, if they are periodic under these symmetry transformations.

Figure 1(a) shows the "minimal version" of the theory. Only the contributions of the two simplest periodic orbits with up to one traversal are considered and plotted as a thin line. The smoothed fluctuating part of the exact quantum mechanically level density is shown as a thick line. This smoothed density has been obtained by replacing the δ function singularity of each quantum eigenstate by

$$\delta(x-x_i) \rightarrow \int_0^{S_{\max}} \left\{ \int_{-\infty}^{\infty} e^{-2\pi i S x} \delta(x-x_i)\, dx \right\} e^{2\pi i S x}\, dS ,$$

$x = \gamma^{-1/3}$, which corresponds to the same smoothing scheme in Fourier space as for the semiclassical calculation, where only orbits with actions $S < S_{\max}$ are included in the sum (4). Figure 1(a) shows that already this minimal version is able to reproduce the gross structure of the exact quantum spectrum with remarkable accuracy.

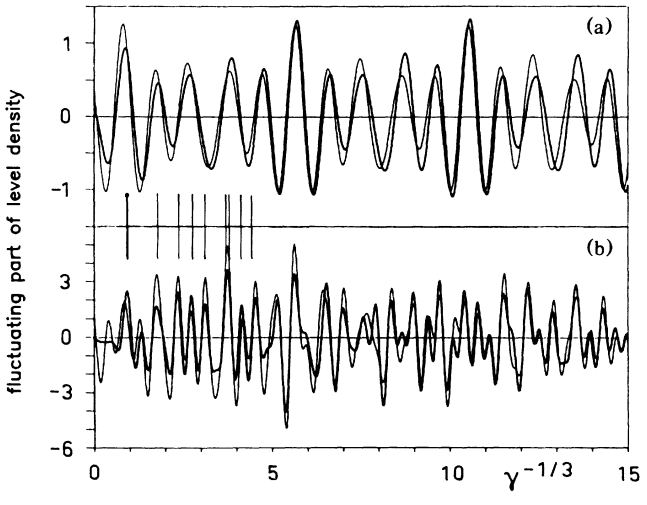

FIG. 1. Smoothed fluctuating part of the density of states. The quantum results (thick lines) are smoothed over the first 100 eigenstates. Semiclassical results (thin lines) are obtained by including two orbits with scaled actions $\tilde{S} < 1.33$ [(a), three contributions], and thirteen orbits with $\tilde{S} < 3$ [(b), nineteen contributions]. The lowest quantum eigenvalues are marked as vertical bars.

Figure 1(b) shows the results of the calculations when all orbits with actions up to $S_{\max} = 3$ are included. Nineteen contributions from thirteen different orbits are summed and plotted as a thin line. From these thirteen orbits, twelve have positive Liapunov exponents and are embedded in the chaotic part of the phase space. The thick line shows the smoothed fluctuating part of the exact quantum density of states. Again, close coincidence is observed not only for the gross structure, but even for the finer details.

As is shown in Fig. 1, the theory is able to describe a finite-resolution density of states. In spectral regions where this resolution is large compared to the mean separation of states, the peaks appearing in the level density are caused by individual resolved quantum states. This can be seen on the left of the figure where the positions of the first eigenstates are marked by vertical bars. Both the quantum eigenvalues and the positions of the first few semiclassical peaks appearing on the left of Fig. 1(b) are tabulated in Table II. Agreement within a few percent of the mean level spacing is obtained, even down to the ground state. This is surprising, because the present

TABLE II. Eigenvalues $\gamma_i^{-1/3}$ of the first nine states.

State i	$\gamma_i^{-1/3}$ Quantum	$\gamma_i^{-1/3}$ Semiclassical
1	0.91	0.85
2	1.79	1.75
3	2.36	2.36
4	2.75	2.73
5	3.12	3.13
6	3.70	2×3.75
7	3.80	
8	4.14	4.19
9	4.47	4.54

theory assumes $\hbar$ to be small and this is hardly fulfilled near the ground-state region. Furthermore, the results are even good up to the ninth eigenvalue, although only thirteen orbits have been included. Similar calculations for integrable systems needed the inclusion of many more periodic orbits to get reliable eigenvalues.[19]

In summary, we have calculated semiclassically a smoothed density of states for a nearly completely chaotic Hamiltonian system by the knowledge of the most simple periodic orbits of the system. The fluctuating part of this density agrees well with full quantum calculations. The analysis shows that the fluctuations are far from random, although they exhibit properties which can be simulated by random matrices. In spectral regions where the resolution obtained is larger than the mean level spacing, it is possible to extract approximate eigenvalues for the quantized energy levels. A stable periodic orbit gives rise to regular sequences of quantum states.

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