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Trace formula for level density of a spherical billiard

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Abstract. A trace formula for the oscillating part of the level density for a spherical billiard has been obtained in spherical polar coordinates. The Jacobian of stability and the length of the orbits are obtained from the classical mechanics of the problem. The same formula is applicable to both the planar and the diametric orbits. Numerical results have been obtained with this formula and compared with the results from exact quantum theory, EBK quantization, and Balian and Bloch.

Keywords. Semiclassical methods; periodic orbit theory; trace formula; spherical billiard.

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1. Introduction

The twentieth century began with radical departures from the classical Newtonian ideas and the ensuing exasperation was difficult to overcome. It now appears that physics is coming to a full circle with the new developments in semiclassical physics near the end of the century, which make it possible to use the classical ideas in quantum domain. The most important characteristic of quantum systems is the existence of discrete eigenvalues of quantities like energy. The quantum level density near the Fermi energy $g(E_{\rm F})$ becomes a quantity of fundamental importance which controls the properties of the system including its stability. It is possible to express this quantity as a sum of a smooth part $\tilde{g}(E)$ and a fluctuating part $\delta g(E)$ [1,2]. The semiclassical periodic orbit theory (POT) has successfully provided a relationship between the fluctuating part in level density $\delta g(E)$ to the classical periodic orbits in the corresponding classical system. This relationship, a trace formula due to Gutzwiller [3], may be written as

$$\delta g(E) = \frac{1}{\pi\hbar} \sum_{\rm PO} \frac{T_{\rm PPO}}{\sqrt{\det|\tilde{M}_{\rm PO} - I|}} \cos\left(\frac{S_{\rm PO}}{\hbar} - \sigma_{\rm PO}\frac{\pi}{2}\right). \tag{1}$$

The left hand side of (1) is a quantity quantum in nature whereas the right hand side contains only classical quantities. Here, $T_{\rm PPO}$ represents the time period of the primitive periodic orbit or, the fundamental orbit and $\tilde{M}_{\rm PO}$ is the Monodromy stability matrix. The oscillations are controlled by action $S_{\rm PO}$ of each periodic orbit and $\sigma_{\rm PO}$ is an integer

known as the Maslov index. It may be pointed out that expression (1) is applicable to only classically chaotic systems which display isolated periodic orbits. This formula fails for systems having continuous symmetries which have degenerate families of non-isolated periodic orbits.

In a related development, Balian and Bloch [4] also obtained a formula for the level density of 3-dimensional cavities with ideally reflecting wall of arbitrary shape; their expression remains valid for systems with continuous symmetries. Later Berry and Tabor [5] also obtained a periodic orbit sum to level density for integrable systems.

Strutinsky and coworkers [6,7] extended the Gutzwiller's trace formula to systems with continuous symmetries. Later on they applied this theory to particles bound in a spheroidal cavity [8]. They investigated the leading contributions to δg and to the energy shell corrections from the shortest periodic orbits for deformed harmonic oscillator and spheroidal cavities. In particular, they obtained the locations of minima of these quantities, corresponding to the ground state deformations, as a function of the Fermi energy or the particle number. A generalization of the Gutzwiller theory to systems with continuous symmetries has also been presented by Creagh and Littlejohn [9].

A spherical billiard is a system with continuous symmetries and therefore contains families of degenerate periodic orbits. Balian and Bloch [4] gave explicit results for a spherical hard wall cavity which were recently used to explain the supershell structure observed in sodium atom cluster [11]. Its two-dimensional counterpart, a circular billiard has found many applications in recent times to such diverse systems as mesoscopic atomic clusters [12,13], quantum dots [14] and nuclei [10] (see the review by Brack [15]). Frisk [10] used the trace formula of Berry and Tabor [5] to obtain the level density fluctuations in a circular billiard. More recently, Reimann *et al* [16] used the Gutzwiller's trace formula to obtain similar results for a circular billiard.

The aim of the present paper is to present a simple approach to the trace formula for a spherical billiard. The whole derivation has been carried out in spherical polar coordinates, a natural coordinate system for a sphere. While our derivation is based on classical equations of motion that of Balian and Bloch uses a geometrical approach. Our approach is simpler to follow, avoids many approximations and gives an expression which is complete in itself. Numerical results based on this trace formula are presented and compared with the exact quantal results and also those of Balian and Bloch, and EBK quantization.

2. Theory

The starting point of our formulation is the general expression for $\delta g(E)$ presented by Strutinsky *et al* [8], which is valid for systems with continuous symmetries. According to this, the oscillating component of single particle level density in cylindrical coordinate (ρ, ϕ, z) is given by

$$\delta g(E) = \frac{1}{\pi\hbar^2} \sum_{\beta,m} f_{\beta,m} \sin\left(\frac{S_{\beta,m}}{\hbar} + \sigma_{\beta,m}\right) \times \int\int \mathrm{d}\rho \mathrm{d}z \sqrt{|p_\rho \rho J(p_\rho p_z t_{\beta,m}; \rho' z' E)|}_{\rho' z' \to \rho z} \tag{2}$$

The factor $f_{\beta,m}$ equals to 1 for the diametric orbits and 2 for other orbits like triangles, squares etc. The time period for the path from the initial point $\vec{r}$ to final point $\vec{r'}$ at energy E is defined as

$$t_\beta = \frac{\partial S_\beta(\vec{r},\vec{r'},E)}{\partial E}. \tag{3}$$

The quantity J in eq. (2) is the Jacobian of transformation between two sets of classical quantities $(p_\rho, p_z, t_{\beta,m})$ and (ρ', z', E), which are related by the classical equations of motion. Here β denotes a family of orbit and m is the number of repeated cycles.

The maximum contribution to the gross-shell structure comes from the shortest periodic orbits. It has now become customary to carry out a smooth truncation of the contributions of longer periodic orbits by folding the level density with a Gaussian function of width γ/R [16],

$$\delta g_{\rm av}(E) = \sum_{\beta,m} \delta g(E) \mathrm{e}^{-(\gamma L_{\beta,m}/2R)^2}. \tag{4}$$

Here, $L_{\beta,m}$ is the length of a periodic orbit. The averaging width γ is larger than the mean spacing between the energy levels within a shell, but much smaller than the distance between the gross shells. This averaging ensures that all longer paths are strongly damped and only the shortest periodic orbits contribute to the oscillating part of the level density. This overcomes the convergence problem that arises in the summation over all the periodic orbits.

The Hamiltonian H is expressed in terms of the spherical polar coordinates (r, θ, ϕ) and the canonically conjugate momenta (p_r, p_θ, p_ϕ) as

$$H = \frac{1}{2M}\left(p_r^2 + \frac{1}{r^2}p_\theta^2 + \frac{1}{r^2\sin^2\theta}p_\phi^2\right) + V(r), \tag{5}$$

where M is the mass of the particle and

$$\begin{aligned} V(r) &= 0 : r < R_0 \\ &= \infty : r \geq R_0, \end{aligned} \tag{6}$$

R_0 being the radius of the spherical cavity.

The time dependent Hamilton–Jacobi equation leads to the time independent equation given by

$$\frac{1}{2M}\left[\left(\frac{\partial S_\beta}{\partial r}\right)^2 + \frac{1}{r^2}\left(\frac{\partial S_\beta}{\partial \theta}\right)^2 + \frac{1}{r^2\sin^2\theta}\left(\frac{\partial S_\beta}{\partial \phi}\right)^2\right] = E. \tag{7}$$

The three partial actions (s_r, s_θ, s_ϕ) are given by

$$s_\phi = \oint p_\phi \mathrm{d}\phi = 2\pi\ell_z, \tag{8}$$

$$s_\theta = \oint p_\theta \mathrm{d}\theta = \oint \sqrt{\epsilon^2 - \frac{\ell_z^2}{\sin^2\theta}}\mathrm{d}\theta = 2\pi(\epsilon - \ell_z), \tag{9}$$

$$s_r = \oint p_r \mathrm{d}r = \oint \sqrt{2ME - \frac{\epsilon^2}{r^2}}\mathrm{d}r, \tag{10}$$

where ℓ_z and ϵ are the separation constants. The limits of integration in eq. (10) are determined by noting that the particle motion is bounded between an upper limit provided by the radius of the sphere $r = R_0$ and a lower limit obtained from $p_r^2 = 0$,

$$r_{\min} = \frac{\epsilon}{\sqrt{2ME}}, \tag{11}$$

where

$$\epsilon = \sqrt{(2ME)}R_0 \cos\chi. \tag{12}$$

Solving eq. (10), we get

$$s_r = 2\sqrt{(2ME)}R_0(\sin\chi - \chi\cos\chi). \tag{13}$$

The constant ϵ is fixed by using the periodicity condition,

$$\frac{\omega_r}{\omega_\theta} = -\frac{\partial S_\theta/\partial\epsilon}{\partial S_r/\partial\epsilon} = \frac{n_r}{n_\theta}, \tag{14}$$

where n_r and n_θ are relatively prime integers. This implies that $\chi = \pi(n_\theta/n_r)$. The frequency of rotation for a three dimensional orbit is

$$\Omega_\beta = \frac{2\pi}{T_\beta} = \frac{\omega_r}{n_r} = \frac{\sqrt{2ME}}{MR_0}\,\frac{\pi}{n_r\sin\chi} \tag{15}$$

and,

$$T_\beta = \frac{M}{\sqrt{2ME}}L_\beta, \tag{16}$$

where $L_\beta = 2R_0 n_r \sin\chi$. It may be noted that (15) for the rotational frequency is exactly the same as obtained in the quantum treatment [19].

The action $S_\beta = \sqrt{2ME}L_\beta$ in (2) is determined by the length $L_\beta(n_r, n_\theta)$, which can easily be found from the time period in eq. (16). This length comes out to be exactly the same as obtained from the geometrical considerations viz. $L_\beta = 2n_r R_0 \sin(n_\theta\pi/n_r)$. A good description of the periodic orbits in a circle may be found in [16].

The Jacobian is obtained by using the Hamilton–Jacobi equation and is given by

$$J = -\frac{2M^2}{\sqrt{2ME}}\,\frac{1}{\sqrt{r^2 - a^2}}\left(\frac{1}{m}\right) \tag{17}$$

with $a = R_0\cos\chi$. The quantity ρp_ρ appearing in eq. (2) is given by

$$\rho p_\rho = \sqrt{2ME}\left[\sqrt{r^2 - a^2}\sin\theta + a\cos\theta\right]\sin\theta. \tag{18}$$

Using (17) and (18) in (2), the oscillating component of the level density is given by

$$\delta g(E) = \frac{1}{\pi\epsilon_0}\sqrt{kR_0}\sum_{\tau_{n_\theta}}\sum_{\tau_{n_r}>2\tau_{n_\theta}} \sin[kL(\tau_{n_r},\tau_{n_\theta})+\sigma(\tau_{n_r},\tau_{n_\theta})]$$
$$\times\int_{r=\cos\chi}^{1}\int_{\theta=0}^{\pi} -r\mathrm{d}r\mathrm{d}\theta\left(\left|\frac{2}{m}\left[\sin^2\theta+\frac{\cos\chi}{\sqrt{r^2-\cos^2\chi}}\sin\theta\cos\theta\right]\right|^{1/2}\right), \quad (19)$$

where $\tau_{n_r} = mn_r, \tau_{n_\theta} = mn_\theta$ and $\epsilon_0 = \hbar^2/2MR_0^2$. We have also multiplied eq. (19) by a factor $\sqrt{kR_0}$ to compensate for the degeneracy of the spherical cavity. It may be pointed out that whereas the action S_β is identical for repeated cycles of a periodic orbit and therefore can be multiplied by the number of repetitions to obtain the total action, the same is not true, in general, for the Maslov index. It was recently demonstrated explicitly by Brack and Jain [17,18] that for stable isolated orbits in a harmonic oscillator potential, the Maslov index does not repeat itself in successive cycles. In the present work, the Maslov index $\sigma(\tau_{n_r},\tau_{n_\theta})$ has been taken by us from Balian and Bloch [4]. Accordingly, the Maslov index is

$$\sigma(\tau_{n_r},\tau_{n_\theta}) = -\frac{3\pi}{2}\tau_{n_r} - (\tau_{n_\theta}-1)\pi + \frac{3\pi}{4}. \quad (20)$$

For diametric orbits, eq. (19) simplifies to

$$\delta g_{\mathrm{dia}}(E) = -\frac{1}{\pi\epsilon_0}\sum_{\tau_{n_\theta}}\frac{1}{\sqrt{2m}}\sin(kL(\tau_{n_r},\tau_{n_\theta})+\sigma(\tau_{n_r},\tau_{n_\theta})), \quad (21)$$

where $\tau_{n_r} = 2\tau_{n_\theta}$. The Maslov index $\sigma(\tau_{n_r},\tau_{n_\theta})$ in this case is taken as

$$\sigma(\tau_{n_r},\tau_{n_\theta}) = -\frac{3\pi}{2}\tau_{n_r} + \frac{3\pi}{4}. \quad (22)$$

It may be noted that Balian and Bloch [4] give separate expressions for the contribution to level density arising from planar orbits and diametric orbits. Our formula (19), however, is valid for both; it reduces to the diametric result on putting the required condition.

Using Weyl's formula for smooth part of the level density [18], we obtain

$$\tilde{g}(E) = \frac{1}{3\pi\epsilon_0 kR_0}\left[(kR_0)^2 - \frac{3\pi}{4}kR_0 + 1\right] \quad (23)$$

for a spherical cavity. The total level density $g(E)$, therefore becomes

$$g(E) = \tilde{g}(E) + \delta g(E) + \delta g_{\mathrm{dia}}(E). \quad (24)$$

3. Results

We have used the formula (19) to calculate the oscillating part of the level density and the results are shown in figures 1a and b. In figure 1a, we show the variation of δg as a function of kR_0 where the 3:1, 4:1, 5:1 and 6:1 orbits have been taken into account;

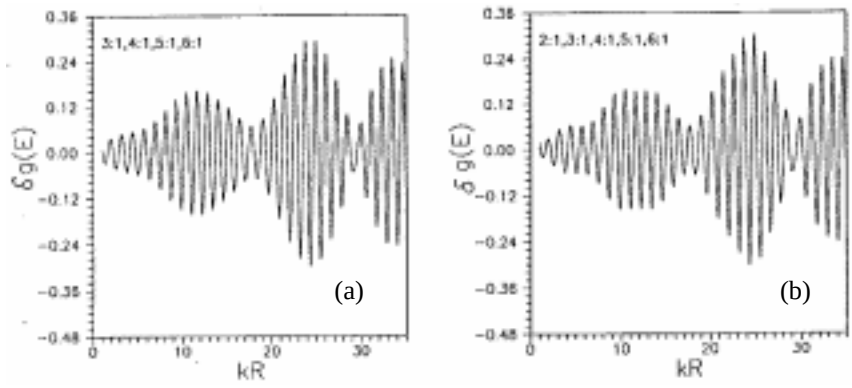

Figure 1. Plots of $\delta g(E)$ vs. kR for spherical cavity using our formula based on POT; $\delta g(E)$ is calculated in dimensionless unit. (**a**) Only four shortest periodic orbits except diameter orbit are included in the sum. (**b**) Diameter orbit is also included in the sum. The smoothing term with $\gamma = 0.6$ is included in both the cases.

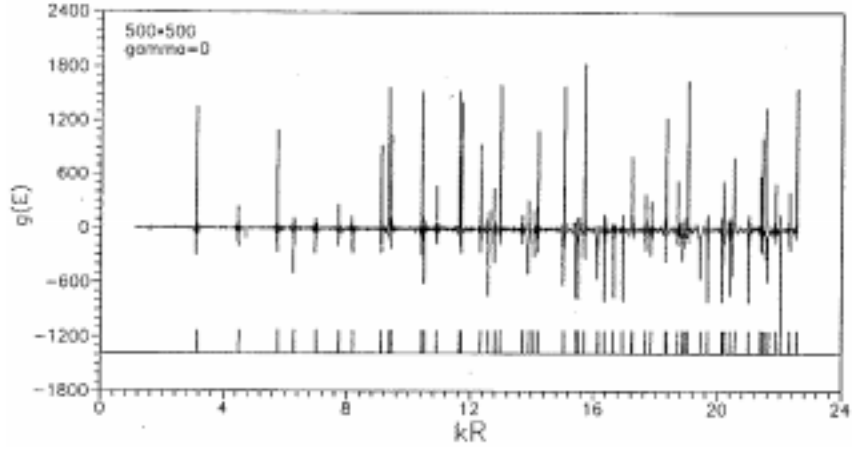

Figure 2. Plot of total level density $g(E)$ vs. kR when 500×500 shortest periodic orbits are included in the sum. Here $\gamma = 0$. Also shown in the strip at the bottom are the exact quantum eigenvalues.

the diametric orbits were not included and no sum was carried out over repeated cycles. The plot reveals the well known beating pattern or the supershell structure that arises out of the interference of mainly the triangular (3:1) and the rhomboidal (4:1) orbits. It may be noticed that δg oscillates at a higher frequency with $\Delta kR_0 \approx 1.1$ units and a supershell structure appears which oscillates with a slow frequency with $\Delta kR_0 \approx 12$ units. When the diametric orbits are included in the sum, the picture modifies to the one shown in figure 1b. Although the diametric orbits have a significantly smaller length than the 3:1 and other higher orbits included in the sum, they have a degeneracy factor lower by one unit than other orbits; hence, they do not lead to any significant modification in the supershell

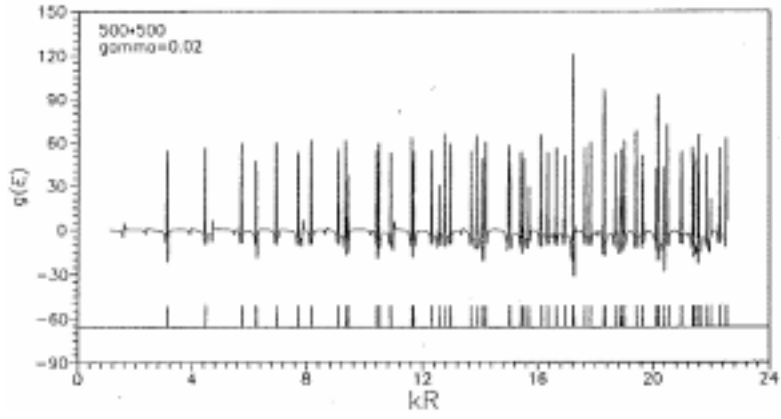

Figure 3. Same as figure 2 but with $\gamma = 0.02$. Again, the quantum results are shown at the bottom. A one-to-one correspondence between the POT and the exact results is seen.

Table 1. Comparison of numerical results for a spherical billiard using exact quantum theory, EBK quantization, Balian and Bloch (BB) formula and our trace formula.

Quantum	EBK	BB	Our trace formula
3.142	3.101	3.101	3.101
4.493	4.458	4.457	4.458
5.763	5.729	5.728	5.728
6.283	6.263	6.263	6.262
6.988	6.953	6.953	6.953
7.725	7.708	7.708	7.708
8.183	8.147	8.147	8.147
9.095	9.078	9.078	9.078
9.356	9.320	9.320	9.320
9.425	9.412	9.411	9.410
10.417	10.401	10.401	10.401
10.513	10.476	10.476	10.476
10.904	10.892	10.892	10.892
11.657	11.620	11.620	11.619
11.705	11.689	11.689	11.689
12.323	12.312	12.312	12.312
12.566	12.556	12.556	12.554
12.791	12.753	12.753	12.753
12.967	12.951	12.951	12.951
13.698	13.687	13.687	13.687
13.916	13.877	13.877	13.877
14.066	14.057	14.057	14.057

structure. In both the calculations, we have used $\gamma = 0.6$. The ultimate test of the trace formula is its ability to reproduce the exact quantum mechanical eigenvalues if sufficient number of orbits are included in the periodic orbit sum. In figures 2 and 3, we show the

results of total level density, when periodic orbits upto $n_r = 500$ and $n_\theta = 500$ are included in the sum. Figure 2 exhibits the results without smoothing while a smoothing width $\gamma = 0.02$ is considered in figure 3. The effect of smoothing is visible in terms of a cleaning up of many spurious peaks and also the negative amplitude decreases appreciably. A beautiful eigenvalue spectrum is obtained both with and without smoothing. The exact quantum eigenvalues are also shown in the graphs in the strip at the bottom for a direct comparison. It is satisfying to note that the observed peaks have a one-to-one correspondence with the quantum results.

A detailed comparison of our numerical results upto $kR_0 = 14$ with those of the exact quantum treatment, Balian and Bloch and the EBK quantization, is presented in table 1. In our calculations as well as those of Balian and Bloch, periodic orbits upto $n_r = 300$ and $n_\theta = 150$ were included in the sum. We find that our values are identical to those of Balian and Bloch. Also, both of them give results which are nearly same as the results of EBK quantization. The accuracy of all the three approaches thus appears to be same.

The formula for the level density of a spherical billiard presented here is a compact result free from approximations and the numerical results testify to its success. The spherical billiard is a system with a large number of possible applications in nuclei, atoms and mesoscopic systems. It is hoped that the formula presented here will facilitate new applications.

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