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The accuracy of semiclassical quantization for an integrable system—the hyperspherical billiard

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Abstract. The eigenvalues of the hyperspherical billiard are calculated in the semiclassical approximation. The eigenvalues where this approximation fails are identified and found to be related to caustics that approach the wall of the billiard. The fraction of energy levels for which the semiclassical error is larger than some given value is calculated analytically (and tested numerically) and found to be independent of energy. The implications for other systems, in particular integrable ones, are discussed.

1. Introduction

Exact solutions to physical problems are rare. In most cases one has to resort to approximate solutions. In quantum mechanics the Wentzel–Kramers–Brillouin (WKB) method, along with perturbation theory, is probably the most common method used to obtain approximate solutions (for reviews, see [1–3]). The WKB method is a formal $\hbar$ expansion for the wavefunction, that expresses its rapid oscillations in the semiclassical limit. Using this expansion combined with an appropriate boundary condition results in an approximate quantization condition. Therefore, high-order approximations for the wavefunction can be used to improve the accuracy of the eigenvalues. A systematic way to obtain approximate quantum eigenvalues using the WKB method was first developed by Dunham [4], improved by Bender and co-workers [5] and is summarized in [6]. In some cases the resulting series for the eigenvalues converge to the exact ones, but generally the resulting expansion will be an asymptotic series.

A surprisingly small number of papers were devoted to the accuracy of semiclassical methods, and even less for high orders or high-dimensional systems. A naive estimate for the accuracy of semiclassical methods is that the leading semiclassical approximation is accurate to order $\hbar$ and therefore the resulting error is of order $\hbar^2$. For example, substitution of the Van Vleck propagator into Schrödinger's equation will not solve the equation exactly, and a remainder of order $\hbar^2$ will result [7]. The mean level spacing scales as $\hbar^D$, where D is the dimension of the system, thus the relative error scales as $\hbar^{D-2}$ and the semiclassical method fails for high-dimensional systems. The prefactor of the semiclassical error is important (in particular for $D = 2$), since individual energies can be found semiclassically only if the error is less than the mean level spacing. For integrable systems the WKB expansion enables one to find analytic estimates for the error in the energies as is demonstrated for a class of such systems in this paper. In addition, it may also shed light on the accuracy of the semiclassical approximation for other dynamical systems. The common argument for the failure of the semiclassical approximation for chaotic systems in $D > 2$ and possibly for $D = 2$ was recently challenged by Primack and Smilansky [8]. For chaotic systems energy is the only quantum number and this is the only identity of a level. The mean level spacing is determined by the smooth Weyl term. This term can be determined for billiards to a high order in Planck's constant $\hbar$. Primack and Smilansky introduced a method to evaluate the error in the energy levels resulting from the fact that oscillatory terms are known only to the leading order in $\hbar$. They concluded that the error in the evaluation of single levels compared with the mean level spacing diverges, at most, as $|\ln \hbar|$ in the limit $\hbar \to 0$. Dahlqvist [9] estimated effects of diffraction for the $D = 2$ Sinai billiard and concluded that ignoring diffraction, as is done in the standard semiclassical approximation, may result in errors at least of the order of the mean level spacing.

Here we study the much simpler case of integrable systems when an expression for the energy levels can be obtained to arbitrary order in $\hbar$ and the levels that are poorly approximated in the leading order of the semiclassical approximation can be characterized. An estimate for the error of the semiclassical quantization for the hyperspherical billiard, that is a generalization of the circle billiard to arbitrary dimension D, is obtained. It was proposed as a model for the nucleus, where the $\mathcal{A}$ nucleons are described by a single point in the $3\mathcal{A}$-dimensional space [10]. The circular billiard was the subject of several works regarding the semiclassical accuracy. Prosen and Robnik explored the error for the energies of the circle billiard numerically [11]. They found that the mean error increases with the energy, and concluded that the semiclassical approximation fails in this simple system. Boasman used the boundary integral method to find the quantization error for several billiards, including the circle billiard [12]. The error was found to be a small fraction of the mean level spacing for general two-dimensional billiards. For the circle billiard he found that for most of the energies the semiclassical error is a constant, which is a small fraction of the mean level spacing. There were large errors for some eigenenergies, the corresponding eigenfunctions were found to be affected by caustics, and it was stated that the fraction of these poorly approximated states decreases with energy.

Following earlier work of Agam [13] we use a certain WKB expansion, keeping the classical quantities fixed, that gives identical quantization condition to the one obtained from the Debye expansion of the Bessel function. This expansion enables us to estimate the fraction of states where the error in the leading semiclassical approximation exceeds some value. The relation to caustics turns out to be transparent. For integrable systems this is a better measure than the mean error since some eigenenergies, that can be clearly characterized, may have extremely large errors. The reason is that for integrable systems, in contrast to chaotic ones, there are other quantum numbers in addition to the energy. These help to characterize the groups of quantum eigenstates that are badly approximated in the leading order of the semiclassical approximation.

The semiclassical expansion for the eigenvalues of the hyperspherical billiard to second order in $\hbar$ is derived in section 2, with the help of the standard semiclassical expansion, as well as the Debye expansion of the Bessel functions. In section 3 the density of eigenvalues where the semiclassical approximation is poor (a term that is defined in that section) is derived analytically and tested numerically. The results are summarized in section 4 and the implications for other systems are discussed.

2. The WKB expansion for the hyperspherical billiard

In this section the semiclassical quantization for the hyperspherical billiard is developed up to second order in $\hbar$. First, a short introduction to a systematic WKB expansion for one-dimensional problems is given. Then the Debye expansion for the Bessel function is used to derive the second-order quantization condition. This derivation is much simpler than the derivation that uses a systematic WKB expansion. In order to verify that the quantization condition derived from the Debye expansion of the Bessel function is indeed a result of a semiclassical expansion, a WKB series is developed for the radial wavefunction. Quantization of this series indeed gives the same quantization condition that was obtained using the Debye series (at least up to second order).

A scheme for quantization using the high-order WKB expansion is known, at least for an ordinary differential equation such as the equations found for separable Hamiltonians [4–6,14]. For one-dimensional systems the Schrödinger equation is

$$\left[-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}+V(x)\right]\psi(x)=E\psi(x). \tag{1}$$

The wavefunction is written in the form

$$\psi(x)=A\exp\left(\frac{\mathrm{i}}{\hbar}\sigma(x)\right) \tag{2}$$

and the phase is expanded in powers of $\hbar$

$$\sigma(x)=\sum_{k=0}^{\infty}\left(\frac{\hbar}{\mathrm{i}}\right)^k\sigma_k(x) \tag{3}$$

while A is a normalization constant. The Schrödinger equation can be solved order by order in $\hbar$ leading to a recursion relation for the expansion functions [4–6]

$$\begin{aligned}&\sigma'^2_0=2m(E-V(x))\\&\sum_{k=0}^{n}\sigma'_k\sigma'_{n-k}+\sigma''_{n-1}=0.\end{aligned} \tag{4}$$

The quantization condition is derived from the requirement that the wavefunction is single valued:

$$\sum_{k=0}^{\infty}\left(\frac{\hbar}{\mathrm{i}}\right)^k\oint\mathrm{d}\sigma_k=2\pi\hbar n. \tag{5}$$

The first odd term σ_1 has the form of a logarithmic derivative, $\mathrm{d}\sigma_1=-\frac{1}{4}\,\mathrm{d}(\ln\sigma_0'^2)$. Each turning point gives a simple zero of $\sigma_0'^2$, and the contour integral for σ_1 counts these zeros and results in the Maslov index. All of the other odd terms are real, and usually without cuts in the complex x plane. Thus, these terms do not contribute to the quantization condition [5]. Therefore, the quantization condition becomes

$$\sum_{k=0}^{\infty}\left(\frac{\hbar}{\mathrm{i}}\right)^{2k}\oint\mathrm{d}\sigma_{2k}=2\pi\hbar(n+m/4) \tag{6}$$

where m is the Maslov index to be evaluated later (for the simple problem with two turning points, m is just 2, the number of zeros of $\sigma_0'^2$) . The fact that only even terms contribute to the quantization makes this quantization method efficient since the correction to the eigenvalues will be smaller by a factor of $\hbar^2$ instead of $\hbar$. This motivates us to transform the radial differential equation to a form without a first derivative.

The specific problem that is studied in this work is the D-dimensional hyperspherical billiard, namely a free particle inside a D-dimensional ball ($R^2>\sum_{i=1}^{D}x_i^2$) with Dirichlet boundary conditions. Generalized spherical coordinates will be most convenient to solve the Schrödinger equation. The D-dimensional Hamiltonian reduces to the Laplacian operator

$$\mathcal{H}=-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2}+\frac{D-1}{r}\frac{\partial}{\partial r}+\frac{\Delta_s}{r^2}\right) \tag{7}$$

with the boundary condition $\psi(R) = 0$ on the wavefunctions. The generalized angular momentum operator is Δ_s and its eigenvalues are $-l(l + D - 2)$ [15]. The radial and angular variables can be separated as $\psi = R(r)\chi(\Omega)$. For the hyperspherical billiard the radial Schrödinger equation is

$$\mathcal{R}''(r) + \frac{D-1}{r}\mathcal{R}'(r) - \frac{l(l+D-2)}{r^2}\mathcal{R}(r) + \frac{2mE}{\hbar^2}\mathcal{R}(r) = 0. \tag{8}$$

The exact solution can be easily obtained using the fact that the radial equation (8) can be reduced to the Bessel equation of order ν, namely

$$u^2\mathcal{J}'' + u\mathcal{J}' + (u^2 - \nu^2)\mathcal{J} = 0 \tag{9}$$

where $R(u) = u^{\frac{2-D}{2}}\mathcal{J}(u)$, $\nu = l + \frac{D-2}{2}$ and $u = \sqrt{\frac{2mE}{\hbar^2}}r$. The solutions are $\mathcal{J}_\nu$, the Bessel functions of the first kind of order ν, and the quantization condition is

$$\mathcal{J}_\nu\left(\sqrt{\frac{2mE}{\hbar^2}}R\right) = 0. \tag{10}$$

This result is exact. The dimensionless variables

$$\begin{aligned} z &= \frac{\sqrt{2mE}R}{L_{sc}} \\ \nu &= \frac{L_{sc}}{\hbar} = l + \frac{D-2}{2} \end{aligned} \tag{11}$$

are introduced for simplicity. It is obvious that $z > 1$.

In order to make connection with the semiclassical expansion it is useful to introduce a large-order expansion of the Bessel function, since for small $\hbar$ the order ν is large. This is the Debye asymptotic expansion:

$$\begin{aligned} \mathcal{J}_\nu(\nu z)_{\nu\to\infty} \sim \left(\frac{2}{\pi\nu\sqrt{z^2-1}}\right)^{\frac{1}{2}} &\left[\cos\zeta\sum_{m=0}^{\infty}\frac{(-1)^m\Gamma(2m+\frac{1}{2})a_{2m}}{\Gamma(\frac{1}{2})}\left(\frac{2}{\nu\sqrt{z^2-1}}\right)^{2m}\right. \\ &\left. + \sin\zeta\sum_{m=0}^{\infty}\frac{(-1)^m\Gamma(2m+\frac{3}{2})a_{2m+1}}{\Gamma(\frac{1}{2})}\left(\frac{2}{\nu\sqrt{z^2-1}}\right)^{2m+1}\right] \end{aligned} \tag{12}$$

where $\zeta = \nu[\sqrt{z^2-1} - \arccos(\frac{1}{z})] - \frac{\pi}{4}$ and $a_0 = 1$, while $a_1 = \frac{1}{8} + \frac{5}{24}\frac{1}{z^2-1}$, and $a_2 = \frac{3}{128} + \frac{77}{576}\frac{1}{z^2-1} + \frac{385}{3456}\frac{1}{(z^2-1)^2}, \ldots$ [16].

Semiclassical quantization, using the Debye expansion, is performed in orders of $\hbar$, by requiring that the wavefunction has a zero at $r = R$, order by order in $\frac{1}{\nu}$. Thus, to second order the quantization condition is:

$$\cos\zeta + \frac{1}{\nu\sqrt{z^2-1}}\left(\frac{1}{8} + \frac{5}{24}\frac{1}{z^2-1}\right)\sin\zeta = 0. \tag{13}$$

First, we solve for the first-order condition and correct it perturbatively. Define $\zeta_0 = \zeta(z_0)$ as the leading-order solution. It satisfies

$$\cos\zeta_0 = 0. \tag{14}$$

The second-order solution can be expanded around the first-order one: $z = z_0 + \delta z$. The term $\delta\zeta = \zeta(z_0 + \delta z) - \zeta(z_0)$ is of the order $\frac{1}{\nu}$ and therefore small. Substituting in (13) one finds

$$\delta\zeta = \frac{1}{\nu\sqrt{z^2-1}}\left(\frac{1}{8} + \frac{5}{24}\frac{1}{z^2-1}\right). \tag{15}$$

This last expression can be given in terms of the first-order solutions z_0 or the second-order ones since the difference is of higher order in $\frac{1}{\nu}$. The last step is to rewrite the first-order condition as $\cos\zeta_0 = \cos(\zeta - \delta\zeta) = 0$. This results in

$$\nu\left(\sqrt{z^2-1} - \arccos\left(\frac{1}{z}\right)\right) - \frac{1}{\nu\sqrt{z^2-1}}\left(\frac{1}{8} + \frac{5}{24}\frac{1}{z^2-1}\right) = \pi\left(n + \frac{3}{4}\right). \tag{16}$$

This is the second-order semiclassical quantization condition. For every pair of quantum numbers (n, ν) one can solve for z and obtain $E_{sc}(n, \nu)$. Since the quantization condition is determined by only two quantum numbers, the problem behaves like a system of two degrees of freedom, if one chooses to ignore degeneracies. The reason for denoting this quantization condition as a second-order one will become clear shortly.

We turn now to apply the systematic semiclassical expansion to (8). Our goal is to show that the quantization condition that was obtained from the asymptotic expansion of Bessel functions coincides with the one obtained from a WKB expansion. This equation has a first-order derivative and, therefore, does not have the form of the one-dimensional Schrödinger equation (1). To exploit the formal WKB expansion described above, one has to eliminate the first-order derivative from the equation. Substitution of

$$\mathcal{R}(r) = r^{\frac{1-D}{2}}\phi(r) \tag{17}$$

in (8) leads to the following equation for $\phi(r)$:

$$-\frac{\hbar^2}{2m}\phi''(r) + \frac{\hbar^2}{2mr^2}\left[\left(l + \frac{D-2}{2}\right)^2 - \frac{1}{4}\right]\phi(r) = E\phi(r). \tag{18}$$

Thus, after this substitution the resulting Schrödinger equation is similar to that of a system with one degree of freedom and the WKB method will give better results. The angular momentum that appears in this equation is the semiclassical one (see (11) and appendix A), as opposed to the exact angular momentum $\hbar\sqrt{l(l+D-2)}$ as is explained in what follows. These differ by an extra term that vanishes in the limit $\hbar \to 0$. That gives one some freedom in defining the semiclassical variables. Thus, for example, we can define the limit as $\hbar \to 0$ while E and $L^2 = \hbar^2 l(l+D-2)$ are constants. This prescription for the semiclassical limit is problematic, since the form of the resulting leading-order wavefunction near zero and at infinity differs from the one of the exact wavefunction. This problem is known for the spherical case ($D = 3$), where in the leading order the exact angular momentum is replaced by the semiclassical one, a modification introduced by Langer [1, 17]. For the D-dimensional generalized angular momentum the analogue is the replacement of $(l + \frac{D-2}{2})^2 - \frac{1}{4}$ by $(l + \frac{D-2}{2})^2$. Therefore, we define the semiclassical limit as the limit where $\hbar \to 0$ while E and $L_{sc} = \hbar(l + \frac{D-2}{2})$ are constant. The difference between these definitions of the angular momentum vanishes in the limit $\hbar \to 0$. As a result, we apply the WKB approximation to the following equation:

$$-\hbar^2\phi''(r) = 2m\left(E - \frac{L_{sc}^2 - \frac{\hbar^2}{4}}{2mr^2}\right)\phi(r). \tag{19}$$

Using the expansion (3) for the wavefunction we find that the recursion relation (4) changes to

$$\begin{aligned} \sigma'^2_0(r) &= 2m\left(E - \frac{L_{sc}^2}{2mr^2}\right) \\ \sum_{k=0}^{n}\sigma'_k\sigma'_{n-k} + \sigma''_{n-1} &= -\frac{1}{4r^2}\delta_{n,2}. \end{aligned} \tag{20}$$

The first-order contribution to the quantization condition is obtained from the zeroth order of (20)

$$\oint \sigma_0' \,\mathrm{d}r = 2\int_{\sqrt{\frac{L_{sc}^2}{2mE}}}^{R} \frac{1}{r}\sqrt{2mEr^2 - L_{sc}^2}\,\mathrm{d}r = 2\hbar\nu\left[\sqrt{z^2-1} - \arccos\left(\frac{1}{z}\right)\right]. \tag{21}$$

The variable z (see equation (11)) is the ratio between the radius of the billiard and the minimal distance of the classical orbit from the origin, or the radius of the caustic. Therefore, if z is close to 1 then the state is more affected by caustics and the semiclassical approximation deteriorates. The reason is that the wavefunction of these states is close to both the caustic and to the hard wall where the pure semiclassical approximation fails. The next term gives us the Maslov index. The integration over σ_1' gives an extra phase of $\frac{\pi}{2}$ due to the turning point at $r = \sqrt{\frac{L_{sc}^2}{2mE}}$ (resulting in a zero of $\sigma_0'^2$ as discussed after (5)). We also have to include the hard wall at $r = R$. To do this correctly one has to build the wavefunction from the sum of two solutions in such a way that they cancel each other at the wall. The result is that the reflected wave acquires an extra phase of π, therefore the total Maslov index is just 3. Consequently, the quantization condition in the leading order is

$$\nu\left[\sqrt{z^2-1} - \arccos\left(\frac{1}{z}\right)\right] = \pi\left(n + \frac{3}{4}\right). \tag{22}$$

In appendix A it is derived in the framework of the 'EBK quantization' by direct action quantization.

Our goal is now to obtain the second-order semiclassical condition. A straightforward calculation leads to

$$\sigma_2'(r) = \frac{L_{sc}^2(L_{sc}^2 - 12mEr^2)}{8r(2mEr^2 - L_{sc}^2)^{5/2}} - \frac{1}{8r\sqrt{2mEr^2 - L_{sc}^2}}. \tag{23}$$

The contour integral over σ_2' is calculated in appendix B, and the result is

$$\oint \sigma_2' \,\mathrm{d}r = \frac{1}{4\hbar\nu\sqrt{z^2-1}} + \frac{5}{12\hbar\nu(z^2-1)^{3/2}}. \tag{24}$$

Using the quantization condition (6) up to the second order

$$\oint (\sigma_0' - \hbar^2\sigma_2')\,\mathrm{d}r = 2\pi\hbar\left(n + \frac{m}{4}\right) \tag{25}$$

and (21), one obtains the second-order quantization condition

$$\nu\left(\sqrt{z^2-1} - \arccos\left(\frac{1}{z}\right)\right) - \frac{1}{\nu\sqrt{z^2-1}}\left(\frac{1}{8} + \frac{5}{24}\frac{1}{z^2-1}\right) = \pi\left(n + \frac{3}{4}\right). \tag{26}$$

This condition is identical to (16), obtained from the Debye expansion. If L_{sc} is kept fixed in the semiclassical limit then the limit $\hbar \to 0$ is equivalent to $\nu \to \infty$. Note that if z is not too close to 1 the first term is much larger then the second one and dominates the result.

It was demonstrated explicitly that the Debye series and the WKB method lead to the same quantization condition up to the second order. Furthermore, these expansions are valid in the *same* limit. Therefore, we expect that these expansions give identical results in any order. This enables one to use the Debye asymptotic expansion, in this case, to obtain estimates for the semiclassical error. This is the subject of the next section.

Before we continue, it is worthwhile briefly discussing the semiclassical angular momentum L_{sc}. In appendix A we calculated the semiclassical eigenvalues of the generalized angular momentum using first-order WKB. One may ask whether it is possible to obtain the exact form of the angular momentum eigenvalues from a WKB expansion. It turns out that this is indeed the case. The WKB approximation for the three-dimensional angular momentum was treated by Robnik and Salasnich [18]. They computed several of the leading terms in the series for the angular momentum eigenvalues, and conjectured the general form of this series. This conjecture was later proved by Salasnich and Sattin [19]. The generalization for high-dimensional systems is not difficult and requires only minor changes in the differential equation and the WKB series. The details are presented in appendix C. The convergent series leads to the correct eigenvalues for the generalized angular momentum (namely, $\hbar\sqrt{l(l+D-2)}$), while the first order in the WKB expansion is $L_{sc} = \hbar(l + \frac{D-2}{2})$.

3. The semiclassical error for hyperspherical billiards

The leading semiclassical eigenvalues correspond to the zeros of $\mathcal{J}_\nu^{(0)}(\nu z)$, the leading term in the Debye asymptotic expansion. Here $\mathcal{J}_\nu^{(i)}(\nu z)$ denotes the ith-order term in this expansion. Let $\Delta z = z(E_{ex}) - z(E_{sc})$, then to the leading order in this asymptotic expansion $\Delta z = \frac{\mathcal{J}_\nu^{(0)}(\nu z) - \mathcal{J}_\nu(\nu z)}{\mathcal{J}_\nu^{'(0)}(\nu z)} \simeq -\frac{\mathcal{J}_\nu^{(1)}(\nu z)}{\mathcal{J}_\nu^{'(0)}(\nu z)}$ [12, 13], where $\mathcal{J}_\nu^{'(0)}(\nu z)$ is the first derivative of $\mathcal{J}_\nu^{(0)}(\nu z)$ with respect to z. From (12) one finds, $\Delta z = \frac{\delta\zeta}{(\frac{\mathrm{d}\zeta_0}{\mathrm{d}z_0})}$, where z_0 is the leading-order solution satisfying $\mathcal{J}_\nu^{(0)}(\nu z_0) = 0$ (see (14) and (15). The result can also be obtained directly from these equations).

If the difference Δz is small then $\frac{\Delta z}{z} = \frac{\Delta E}{2E}$. Using (11),

$$|\Delta E| \simeq \frac{\hbar^2}{mR^2}\frac{z^2}{z^2-1}\left[\frac{1}{8} + \frac{5}{24}\frac{1}{z^2-1}\right] \tag{27}$$

that is correct in the leading order in $\hbar$. Note that the error ΔE is independent of the number of degrees of freedom D. In the limit $z \to 1$ this expression diverges. This divergence is related to the fact that in this limit the caustic approaches the wall and the classical trajectories on the quantized torus are always adjacent to the caustic and to the hard wall. The approximation is best in the limit $z \to \infty$. In this limit the angular momentum contribution to the energy is negligible, and the problem is effectively one-dimensional.

To estimate the accuracy of the approximation it may be more meaningful to measure the error in units of the mean level spacing Δ. In the D-dimensional hyperspherical billiard the leading order in the mean level spacing is given by the Weyl formula

$$\Delta \simeq \frac{(2\pi)^D\hbar^D}{mR^2V_D^2DL_{sc}^{D-2}}\frac{1}{z^{D-2}} \tag{28}$$

where $V_D = \frac{\pi^{\frac{D}{2}}}{\Gamma(1+\frac{D}{2})}$ is the volume of the D-dimensional sphere of unit radius. With (27) and (28) the semiclassical error is

$$\frac{|\Delta E|}{\Delta} \simeq \frac{DL_{sc}^{D-2}}{\Gamma^2(1+\frac{D}{2})2^D}\frac{z^D}{z^2-1}\left[\frac{1}{8} + \frac{5}{24}\frac{1}{z^2-1}\right]\frac{1}{\hbar^{D-2}}. \tag{29}$$

In the calculation of the mean level spacing Δ, the levels were weighted with their degeneracy, leading to a large level density, resulting in a very small mean level spacing. The divergence of $\frac{|\Delta E|}{\Delta}$ for $D > 2$ in the limit $\hbar \to 0$ (L_{sc} and z fixed) and $z \to \infty$ (L_{sc} and $\hbar$ fixed) is a result of the rapid increase of the number of levels in these limits.

The hyperspherical billiard exhibits a high degree of symmetry. Therefore, there are only two quantum numbers, (n, l), that determine the quantization condition. As a result, if levels are not weighted by their degeneracies the density of the degenerate energy levels is quasi two dimensional. Consequently, if the number of states that are affected by caustics is small, then one can use the WKB method to determine single energy levels. Knowledge of the relative number of states that are badly approximated is crucial here. If such states are common than the semiclassical approximation will fail. In what follows the fraction of states that are badly approximated by the WKB method is estimated.

One can decompose the total spectrum using the angular momentum quantum number. Each sub-spectrum is a series of eigenvalues that depend on the quantum number n. The density of these states with respect to the energy can be approximated from the quantization condition (22)

$$\rho_n \simeq \left(\frac{\partial n}{\partial E}\right) = \frac{\nu}{2\pi E}\sqrt{\frac{E-\epsilon(\nu)}{\epsilon(\nu)}} \tag{30}$$

where $\epsilon(\nu) = \frac{\hbar^2\nu^2}{2mR^2}$. The decomposed spectrum is not very interesting, since our purpose is to find what is the total fraction of states that are badly approximated irrespective of the other quantum numbers. For this, the spectrum can be constructed by adding the contributions from different angular momenta. It is important to understand that when we sum over ν and the energy is kept fixed, we actually sum over the different quantum states (ν, n) with energy near E. If the sum is over all the possible values of ν then one is counting all the possible states and will get the total density of states. If one wants to sum only the states that are badly approximated one should sum only the states that satisfy the condition $1 \leqslant z \leqslant 1/\alpha$, where α is a measure for the maximally allowed error. From (27) it is clear that $|\Delta E|$ is monotonically decreasing with z. To find the density of badly approximated states one sums only values of ν satisfying this inequality. Replacing the restricted sum $\sum'$ by an integral and changing variables to ϵ, leads to

$$\rho \simeq {\sum_\nu}' \frac{\nu}{2\pi E}\sqrt{\frac{E-\epsilon(\nu)}{\epsilon(\nu)}} \simeq \frac{mR^2}{2\pi\hbar^2}\int_{\alpha^2 E}^{E}\sqrt{\frac{E-\epsilon}{\epsilon}}\frac{\mathrm{d}\epsilon}{E}. \tag{31}$$

The resulting density of badly approximated states is

$$\rho \simeq \frac{mR^2}{2\pi\hbar^2}\left[\arccos\alpha - \alpha\sqrt{1-\alpha^2}\right]. \tag{32}$$

The result depends only on α, which is a measure of the error but does not depend on energy. Thus, the probability that a state is badly approximated by the WKB method does not depend on the energy of the state. It is important to notice that this expression is useful only in the limit $\alpha \ll 1$. When $\alpha \simeq 1$ the connection between the allowed error and α is not accurate since the various terms in the Debye series are of comparable magnitude and the expansion cannot be terminated. Indeed, when all of the states are included, (for $\alpha = 0$ any state is considered to be badly approximated), the density of all the states is $\frac{mR^2}{4\hbar^2}$, as expected, since this is the total density of states according to the Weyl formula in two dimensions (the double degeneracy of states with positive and negative angular momentum quantum numbers is ignored here).

To verify these results we computed the first 125 336 exact and semiclassical levels in the $D = 4$ dimensional hyperspherical billiard numerically. A convenient set of units is $2m = \hbar = R = 1$. The error in each eigenvalue was computed directly from comparison between the exact energy levels computed from (10) and their semiclassical approximation computed from (22). A set of α values was chosen. Each value of α defines a semiclassical error by (27), with $z = \frac{1}{\alpha}$. Then, the density of states with error larger than this semiclassical error was computed by counting the number of such states in an energy interval which is much larger than the mean level spacing but small enough not to smear any possible energy dependence. This number is just the density of badly approximated states times the width of the

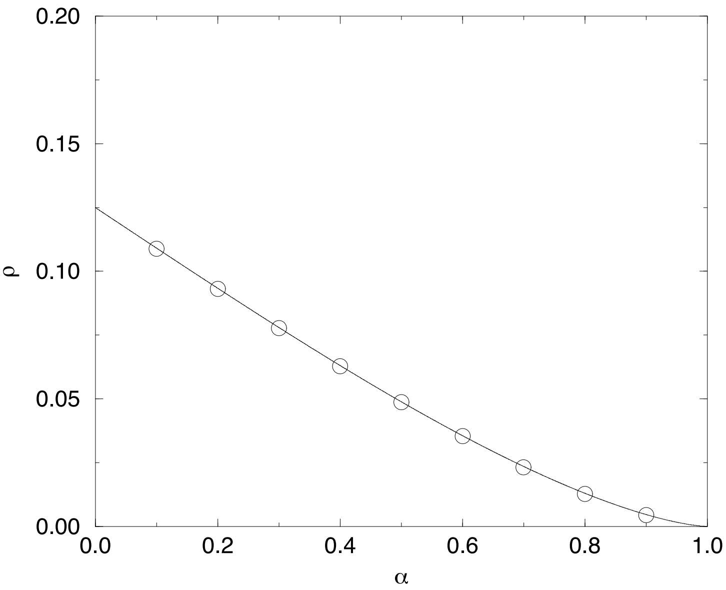

Figure 1. The density of badly approximated states (solid curve—the approximation, circles—numerical results).

energy interval. For each α the density of badly approximated states was found to be constant when the energy was varied, as expected from (32). The value of this density was compared with the density predicted by (32), and both are presented in figure 1. The approximation (32) was found to be excellent.

It was found that using the fact that the system is integrable and the knowledge of its degeneracy, we can treat the spectrum of the hyperspherical billiard as two dimensional. The density of badly approximated states was calculated and found to be energy independent, in contrast to a previous statement [12]. Only in the limit where the angular momentum is negligible there are no large errors in quantization, since the system is effectively one-dimensional.

4. Discussion and conclusions

The accuracy of the semiclassical approximation was studied for the hyperspherical billiard. The approximation was found to fail for energies corresponding to states that are localized on tori, such that the caustic is close to the wall. As the caustic approaches the wall the region in space where the semiclassical approximation for the wavefunction is justified shrinks, and the quality of this approximation deteriorates. The semiclassical approximation for eigenvalues can be arbitrarily bad (for $z \simeq 1$, in our case). For this reason the average semiclassical error is meaningless since it may be dominated by few large contributions. It is much more reasonable to calculate the fraction of badly approximated states, namely the fraction of states where the semiclassical error exceeds some value. The density of such states was found to depend only on one parameter that measures the ratio between the angular momentum and its maximal possible classical value for a given energy (the parameter was denoted by α, and the regime where the semiclassical approximation fails is $1 < z < \frac{1}{\alpha}$). The semiclassical error (27) depends only on z and not on the energy. Therefore, we concluded that the density of poorly approximated eigenvalues characterized by α is independent of energy. The semiclassical approximation does *not* improve as the energy increases, in contrast to common belief (stated, for example, in [12]). Lazutkin found that convex billiards have tori of the KAM type along the boundary. He also proved that it is possible to use a WKB-like method to obtain approximate solutions and energy levels on these tori [20]. For these states there is a caustic near a hard wall and we expect that the energy levels will be badly approximated.

The system that was studied in this work is somewhat special because of its high degree of degeneracy. Since the symmetries are respected by the semiclassical approximation, the levels calculated in this approximation have the same degeneracy as the exact ones. Therefore, for such a system, it is meaningless to compare the semiclassical error with the mean level spacing that is inversely proportional to the total number of energy levels. In such a situation it is more meaningful to consider the error within each group characterized by given constants of motion apart from the energy.

In the present work the badly approximated states were found within a finite energy range for values of angular momentum where $z \simeq 1$, that is when the caustic is close to the wall, and the classically allowed region is narrow. Such a situation can occur for many integrable systems in dimension $D > 1$. Fixing the action variables, except the energy, the classically allowed regions in space may be very narrow and they are bounded by caustics or boundaries (like the hard wall in the present work). Such regions may occur near extrema of the energy, subject to the constraint that the other quantum numbers are kept fixed. For wavefunctions localized in these narrow regions the semiclassical approximation is poor. Typically, such states are expected for various values of the quantum numbers, (excluding the energy), and these accumulate to the density of the poorly approximated energy levels. As in the present work, one expects a finite fraction of badly approximated states. The semiclassical approximation for several states may be extremely bad making the average error meaningless. In other words, it is expected that the semiclassical approximation will fail for well defined groups of states and the fraction of such states, rather than the mean semiclassical error, is a good measure of the quality of the semiclassical approximation. One can find such states in some rotationally invariant two-dimensional systems with some attractive potential (for example, the circle billiard with the hard wall replaced by a soft one that is sufficiently steep). The badly approximated states will be the lowest states in the radial potential well formed by the attractive potential and the angular momentum. To our understanding in general the density of badly approximated states may depend on energy, in contrast to the situation in the present work. The characterization of this dependence should be the subject of further studies.

The results of this work may be relevant for mixed systems, since some of the states are localized in the regular regions. For chaotic systems and for the chaotic component of mixed systems, there are no caustics and the wavefunctions usually spread over all the chaotic region. The energy is the only identity of an eigenstate, therefore, the results of this work may not be of direct relevance for such systems and the mechanism for the destruction of the semiclassical approximation is different there.

Alonso and Gaspard computed the correction to the Gutzwiller trace formula for billiards [21]. The correction is complicated but some of its parts have geometrical meaning. One term is proportional to the sum $\sum_i \frac{1}{C_i}$ where C_i is the chord length. Another contribution is proportional to $\sum_i \frac{1}{R\cos^3\phi}$ where R is the radius of curvature of the wall and ϕ is the angle between the orbit and the normal to the wall at the incident point . When a caustic is close to a hard wall the typical chord length will be small and so will $\cos\phi$. Thus, the correction to the leading-order contribution of periodic orbits will diverge and the semiclassical quantization may fail. Therefore, we expect that semiclassical methods will give poor results for contributions of orbits that are adjacent to a hard wall. For chaotic systems, because of ergodicity, a typical orbit will not have a large fraction of chords near the wall of a billiard, therefore, this correction will not be dominant. One can expect that in such systems the semiclassical error will fluctuate around some average without extreme deviations.

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Appendix A. The leading-order quantization condition

In this appendix we use the 'EBK quantization' in order to obtain the semiclassical quantization condition (22). The method uses the classical momenta for quantization of action integrals. This result is not new but it may help to clarify the form of the semiclassical limit that was used in the systematic WKB expansion. Our system is a D-dimensional spherical billiard and it is convenient to describe it using a hyperspherical coordinate system. The transformation between the hyperspherical and Cartesian coordinates is

$$\begin{aligned} x_D &= r\cos\xi_{D-1} \\ x_{D-1} &= r\sin\xi_{D-1}\cos\xi_{D-2} \\ x_{D-2} &= r\sin\xi_{D-1}\sin\xi_{D-2}\cos\xi_{D-3} \\ \vdots \quad & \quad \vdots \\ x_1 &= r\sin\xi_{D-1}\sin\xi_{D-2}\ldots\sin\xi_2\sin\xi_1. \end{aligned} \tag{A.1}$$

It is easy to show that the Hamiltonian of a free particle in spherical coordinates is

$$\mathcal{H}_D = \frac{1}{2m}\left(p_r^2 + \frac{p_{\xi_{D-1}}^2}{r^2} + \frac{p_{\xi_{D-2}}^2}{r^2\sin^2\xi_{D-1}} + \frac{p_{\xi_{D-3}}^2}{r^2\sin^2\xi_{D-1}\sin^2\xi_{D-2}} + \cdots + \frac{p_{\xi_1}^2}{r^2\prod_{i=2}^{D-1}\sin^2\xi_i}\right). \tag{A.2}$$

This Hamiltonian satisfies the Staeckel conditions [22], therefore Hamilton's characteristic function is completely separable, namely,

$$W(q) = \sum_i W_i(q_i). \tag{A.3}$$

The Hamilton–Jacobi equation in these coordinates is

$$\left(\frac{\partial W_r}{\partial r}\right)^2 + \frac{1}{r^2}\left[\left(\frac{\partial W_{\xi_{D-1}}}{\partial\xi_{D-1}}\right)^2 + \frac{1}{\sin^2\xi_{D-1}}\left[\left(\frac{\partial W_{\xi_{D-2}}}{\partial\xi_{D-2}}\right)^2 + \frac{1}{\sin^2\xi_{D-2}}\left[\cdots\left[\left(\frac{\partial W_{\xi_2}}{\partial\xi_2}\right)^2 + \frac{1}{\sin^2\xi_2}\left(\frac{\partial W_{\xi_1}}{\partial\xi_1}\right)^2\right]\cdots\right]\right]\right] = 2mE. \tag{A.4}$$

The brackets in this equation must be constants of motion since they depend upon different variables. Since the constants are positive we define α_i^2 as the value of the ith brackets. We can write the Hamiltonian as

$$\mathcal{H} = \frac{p_r^2}{2m} + \frac{L^2}{2mr^2} \tag{A.5}$$

where $L = \alpha_{D-1}$ is the generalized angular momentum. We calculate α_{D-1} by calculating the actions related to the angular variables. The first coordinate is cyclic, thus

$$\mathcal{S}_1 = 2\pi\alpha_1. \tag{A.6}$$

All the other actions are similar and are computed in [22]:

$$\mathcal{S}_i = \oint \frac{\partial W_{\xi_i}}{\partial \xi_i}\, \mathrm{d}\xi_i = \oint \sqrt{\alpha_i^2 - \frac{\alpha_{i-1}^2}{\sin^2 \xi_i}}\, \mathrm{d}\xi_i = 2\pi(\alpha_i - \alpha_{i-1}). \tag{A.7}$$

The WKB quantization is done by quantization of the actions $\mathcal{S}_i = 2\pi\hbar(l_i + \gamma_i/4)$ where γ_i is the Maslov index of the action. Now the angular momentum is given by

$$L = \alpha_{D-1} = \frac{1}{2\pi}\sum_i \mathcal{S}_i = \hbar\left(\sum_{i=2}^{D-1}\left(l_i + \frac{1}{2}\right) + l_1\right) = \hbar\left(l + \frac{D-2}{2}\right). \tag{A.8}$$

This is just the semiclassical angular momentum L_{sc}.

One additional quantization is needed in order to obtain the energy levels

$$\mathcal{S}_r = \oint p_r\, \mathrm{d}r = 2\int_{\sqrt{\frac{L^2}{2mE}}}^{R} \sqrt{2mE - \frac{L^2}{r^2}}\, \mathrm{d}r \tag{A.9}$$

where R is the radius of the hyperspherical billiard. Here the Maslov index is 3, since the contribution from the turning point is 1 and the hard wall contributes 2. A straightforward calculation leads to the quantization condition:

$$\mathcal{S}_r = 2\left[\sqrt{2mER^2 - L^2} - L \arccos\sqrt{\frac{L^2}{2mER^2}}\right] = 2\pi\hbar\left(n + \frac{3}{4}\right). \tag{A.10}$$

Introducing ν and z, and identifying $L \equiv L_{sc}$, the equation takes the form

$$\nu\left[\sqrt{z^2 - 1} - \arccos\left(\frac{1}{z}\right)\right] - \frac{\pi}{4} = \pi\left(n + \frac{1}{2}\right) \tag{A.11}$$

which is simply (22).

Appendix B. Calculation of the second-order contribution to the quantization condition

The objective of this appendix is to calculate the contour integral (24). The contour must encircle the turning point at r_{min} and also the point $r = R$ that represents the hard wall. It is convenient to compute this integral by taking the contour infinitesimally close to the real line. The parts of the contour that are parallel to the real r-axis give the same real contribution, which can be computed directly. Calculation of this integral reveals that the classical turning point gives an infinite contribution. The part of the contour that encircles the turning point also gives an infinite contribution, and the sum of all the terms is finite.

The standard way to deal with integrals of this kind is to integrate and differentiate using a suitable parameter as a variable (usually the energy). Here, one first integrates with respect to the energy. The number of integrations is such that the contribution from the turning point to the contour integral in the complex r plane converges. Then the contour integral is computed.

The last step is to differentiate with respect to the energy to obtain the desired result. For this purpose (23) is written in the form

$$\sigma_2' = \frac{3L_{sc}^2}{4mr^3}\frac{\partial}{\partial E}\frac{1}{(2mEr^2 - L_{sc}^2)^{1/2}} - \frac{5L_{sc}^4}{24m^2r^5}\frac{\partial^2}{\partial E^2}\frac{1}{(2mEr^2 - L_{sc}^2)^{1/2}} - \frac{1}{8r\sqrt{2mEr^2 - L_{sc}^2}}. \tag{B.1}$$

Now each term will be treated separately. Integration of the first one results in

$$I_1 = \int_{\sqrt{\frac{L_{sc}^2}{2mE}}}^{R} \frac{3L_{sc}^2}{2mr^3}\frac{\mathrm{d}r}{\sqrt{2mEr^2 - L_{sc}^2}}$$
$$= \frac{3}{4mR^2}\sqrt{2mER^2 - L_{sc}^2} - \frac{3E}{2L_{sc}}\arcsin\left(\sqrt{\frac{L_{sc}^2}{2mER^2}}\right) + \frac{3E}{2L_{sc}}\frac{\pi}{2}. \tag{B.2}$$

Differentiation with respect to E and change of variable from E to z gives

$$\frac{\partial I_1}{\partial E} = \frac{3}{2L_{sc}}\frac{1}{\sqrt{\frac{2mER^2}{L_{sc}^2} - 1}} + \frac{3}{2L_{sc}}\arccos\left(\sqrt{\frac{L_{sc}^2}{2mER^2}}\right)$$
$$= \frac{3}{2L_{sc}}\left(\frac{1}{\sqrt{z^2 - 1}} + \arccos\left(\frac{1}{z}\right)\right). \tag{B.3}$$

The next term can be treated in a similar manner,

$$I_2 = \int_{\sqrt{\frac{L_{sc}^2}{2mE}}}^{R} \frac{5L_{sc}^4}{12m^2r^5}\frac{\mathrm{d}r}{\sqrt{2mEr^2 - L_{sc}^2}}. \tag{B.4}$$

Substitution of $y = \frac{1}{r}$ helps to perform the integral and to obtain

$$I_2 = \frac{5L_{sc}^2}{12m^2}\sqrt{2mER^2 - L_{sc}^2}\left(\frac{3mE}{4L_{sc}^2R^2} + \frac{1}{4R^4}\right) + \frac{5E^2}{8L_{sc}}\left(\frac{\pi}{2} - \arctan\left[\frac{1}{\sqrt{\frac{2mER^2}{L_{sc}^2} - 1}}\right]\right). \tag{B.5}$$

This term has to be differentiated twice with respect to E, and then the variable E should be replaced by z. After some manipulations the contribution of this term is found to be

$$\frac{\partial^2 I_2}{\partial E^2} = \frac{5}{4L_{sc}}\frac{1}{\sqrt{z^2 - 1}} - \frac{5}{12L_{sc}}\frac{1}{(z^2 - 1)^{3/2}} + \frac{5}{4L_{sc}}\arccos\left(\frac{1}{z}\right). \tag{B.6}$$

The third term is simply

$$I_3 = \int_{\sqrt{\frac{L_{sc}^2}{2mE}}}^{R} \frac{\mathrm{d}r}{4r\sqrt{2mEr^2 - L_{sc}^2}} = \frac{1}{4L_{sc}}\arccos\left(\frac{1}{z}\right). \tag{B.7}$$

And the final result is

$$\oint \sigma_2'\,\mathrm{d}r = \frac{\partial I_1}{\partial E} - \frac{\partial^2 I_2}{\partial E^2} - I_3 = \frac{1}{4L_{sc}}\frac{1}{\sqrt{z^2 - 1}} + \frac{5}{12L_{sc}}\frac{1}{(z^2 - 1)^{3/2}} \tag{B.8}$$

which reduces to (24).

Appendix C. Exact generalized angular momentum eigenvalues in WKB

The WKB series for the angular momentum in $D = 3$ dimensions were constructed by Salasnich and Sattin [19]. Summation of this series leads to the correct form of the quantum angular eigenvalues, namely, $(l+1)l$. Here this result is generalized to the angular momentum in arbitrary dimension D.

The first step is to compute the form of the Laplacian in hyperspherical coordinates. Then, by separation of variables an equation relating the generalized angular momentum operator to its projection on a $D-1$ dimensional space is found. We assume that the Laplacian is of the form

$$\Delta = \frac{\partial^2}{\partial^2 r} + \frac{D-1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\Delta^s_D \tag{C.1}$$

where Δ^s_D is the angular part that does not depend on the radial variable. We use induction in the number of degrees of freedom to prove that the Laplacian indeed has this form. First, one should note that for $D = 2$ and 3 this assumption holds. Assume it holds for a $D-1$ dimensional system and add an additional Cartesian coordinate x_D. The Laplacian is now

$$\Delta = \frac{\partial^2}{\partial^2 x_D} + \Delta_{D-1} \tag{C.2}$$

where Δ_{D-1} is the Laplacian in the space of the coordinates $x_1, x_2, \ldots, x_{D-1}$. Transforming $x_1, x_2, \ldots, x_{D-1}$ to hyperspherical coordinates and using the induction assumption we obtain

$$\Delta = \frac{\partial^2}{\partial^2 x_D} + \frac{\partial^2}{\partial^2 r} + \frac{D-2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\Delta^s_{D-1}. \tag{C.3}$$

The transformation to hyperspherical coordinates involves only the two coordinates r and x_D. All of the angular coordinates will not change and, therefore, neither will Δ^s_{D-1}. To transform to the D-dimensional hyperspherical coordinates one substitutes

$$\begin{aligned} x_D &= R\cos\theta \\ r &= R\sin\theta. \end{aligned} \tag{C.4}$$

The computation of the Laplacian is straightforward and leads to

$$\Delta = \frac{\partial^2}{\partial^2 R} + \frac{D-1}{R}\frac{\partial}{\partial R} + \frac{1}{R^2}\Delta^s_D \tag{C.5}$$

where

$$\Delta^s_D = \frac{\partial^2}{\partial^2\theta} + (D-2)\cot\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\Delta^s_{D-1} \tag{C.6}$$

is the D-dimensional angular momentum operator. Since the systematic high-order WKB expansion works only for ordinary differential equations we assume that the exact form of the eigenvalues of the angular momentum in lower dimensions is known. The equation connecting eigenvalues of angular momentum in D and $D-1$ dimensions is obtained by separation of variables

$$T''(\theta) + (D-2)\cot(\theta)T'(\theta) - \frac{(m+D-3)m}{\sin^2(\theta)}T(\theta) = -\lambda^2 T(\theta) \tag{C.7}$$

where $T(\theta)$ is the eigenfunction for the eigenvalue λ^2, while $m(m+D-3)$ is the eigenvalue of Δ^s_{D-1}. It is justified by induction in what follows (see (C.11)). This is the generalization of equation (4) in [19]. The computation follows [19] with only minor changes. Instead of (5) in [19] one substitutes

$$T(\theta) = \frac{F(\theta)}{(\sin\theta)^\eta} \tag{C.8}$$

where $\eta = \frac{D-2}{2}$. After some manipulations and substitution of $x = \theta + \frac{\pi}{2}$ one obtains

$$-F''(x) + \frac{U}{\cos^2(x)} F(x) = EF(x) \tag{C.9}$$

that is (7) of [19]. However, the values of the parameters are different. Here $E = \lambda^2 + \eta^2$ and $U = m(m + D - 3) - \eta(1 - \eta)$. The WKB expansion of (C.9) is developed in [14, 19] for any order. The quantization condition is given by a series which is then summed. This results in

$$\sqrt{E} - \tfrac{1}{2}\sqrt{1 + 4U^2} = n + \tfrac{1}{2} \tag{C.10}$$

but here $\sqrt{1 + 4U^2} = 2(m + \frac{D-3}{2})$. Substitution of U and E leads to

$$\lambda^2 = (n + m)(n + m + D - 2). \tag{C.11}$$

This is indeed the correct result for the generalized angular momentum eigenvalues. The semiclassical eigenvalue is found from (C.10) assuming $E \simeq \lambda^2$, leading to $\lambda \simeq n + m + \frac{D-2}{2}$. Identifying $l = n + m$ results in (A.8).

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