

First-Order \hbar Corrections to Gutzwiller's Trace Formula for Systems with Discrete Symmetries

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In the reference [B. Grémaud, Phys. Rev. E 65, 056207 (2002)] first-order \hbar corrections to Gutzwiller's trace formula for systems with a smooth potential were presented. Here we present an extension of that theory to systems with discrete symmetries. We apply the method to the two-dimensional hydrogen atom in a uniform magnetic field and exploit the C_{4v} -symmetry in the calculation of the correction terms. The numerical results for the semiclassical values are compared with values extracted from exact quantum mechanical calculations. The comparison shows a very good agreement.

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1. Introduction

Gutzwiller's trace formula [1] provides a semiclassical approximation of the quantum level density in terms of classical periodic orbits. In a systematic expansion of the level density in powers of \hbar it can be considered as the leading order. Higher orders of this asymptotic expansion have been developed in several studies [2–4], but for a long time were only tested for billiard systems, i.e., systems with hard walls instead of smooth potentials. By extending an expansion which was derived by Gaspard et al. [3, 4], Grémaud [5] obtained \hbar corrections to Gutzwiller's trace formula for quantum systems with a smooth potential. However, in [5] no symmetries of the Hamiltonian were considered. Preliminary results for the diamagnetic hydrogen atom, which has discrete and continuous symmetries were published in [6] but the influence of the symmetries on the numerical calculations which are required to obtain the correction terms was not discussed.

In this paper we extend the theory presented in [5] and investigate systems with discrete symmetries. The main focus will be on the classical Green's function, which is an essential part of the correction terms and has the most complicated symmetry properties. If there are discrete symmetries, the eigenstates of the quantum system split up into several subspaces. In these subspaces, classical orbits which are not periodic without a symmetry transformation contribute to the level density. We will show how discrete symmetries of the Hamiltonian have to be taken into account for the calculation of the first-order \hbar corrections, and apply the method to the two-dimensional diamagnetic hydrogen atom, which has a C_{4v} symmetry but no continuous symmetry. A continuous symmetry would require a further study. The \hbar corrections will be calculated for selected periodic orbits taking into account that discrete symmetry. The semiclassical values will be compared with the analysis of exact quantum calculations. The agreement between the results of both methods turns out to be very good.

The outline of the paper is as follows. In section 2 we will briefly present the most important

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terms of the \hbar corrections for systems without discrete symmetries. In section 3, we will introduce the hydrogen atom in a uniform magnetic field with the aspects relevant for the calculation of the correction terms. Then we will give an introduction to the extension to discrete symmetries, calculate results for the two-dimensional hydrogen atom and compare them with exact quantum mechanical calculations in section 4.

2. Semiclassical approximation of the quantum level density

Grémaud presented a semiclassical approximation of the quantum Green's function, which included the first-order \hbar correction. The result reads [5]:

$$G_\ell(E) = \frac{1}{i\hbar} \frac{T_{0p} \exp \left[\frac{i}{\hbar} S_\ell^{(cl)}(T_0) - \frac{i\pi}{2} \mu_\ell \right]}{\sqrt{|\det(\mathbf{m}_\ell(T_0) - \mathbf{1})|}} \{ 1 + i\hbar (C_{1\ell}(T_0) + C_{1\ell}^{T \rightarrow E}(T_0)) + O(\hbar^2) \}, \quad (1)$$

where the leading order, belonging to the 1 in the curly brackets, is known from Gutzwiller's trace formula [1]. In this expression, $S_\ell^{(cl)}(T_0)$ is the reduced action and μ_ℓ represents the Maslov index. The stability matrix is denoted by \mathbf{m}_ℓ and T_0

stands for the time period with T_{0p} for the primitive periodic orbit. The first-order \hbar correction consists of two terms. The first has the explicit form

$$C_{1\ell}(T, t_0) = \frac{1}{8} \int_0^T dt V_{,i_1 i_2 i_3 i_4} \mathcal{G}_{i_1 i_2}(t, t; t_0) \mathcal{G}_{i_3 i_4}(t, t; t_0) + \frac{1}{24} \int_0^T dt \int_0^T dt' V_{,i_1 i_2 i_3} V_{,j_1 j_2 j_3} \\ \times (3\mathcal{G}_{i_1 i_2}(t, t; t_0) \mathcal{G}_{i_3 j_1}(t, t'; t_0) \mathcal{G}_{j_2 j_3}(t', t'; t_0) + 2\mathcal{G}_{i_1 j_1}(t, t'; t_0) \mathcal{G}_{i_2 j_2}(t, t'; t_0) \mathcal{G}_{i_3 j_3}(t, t'; t_0)) \\ + \frac{V_{,j}(t_0)}{2|\dot{\mathbf{q}}_\ell^{(cl)}(t_0)|^2} \int_0^T dt V_{,i_1 i_2 i_3} \mathcal{G}_{j i_1}(0, t; t_0) \mathcal{G}_{i_2 i_3}(t, t; t_0), \quad (2)$$

where the $V_{,i_1 \dots i_n}$ are derivatives of the potential evaluated at the point $\mathbf{q}_\ell^{(cl)}(t)$ on the classical orbit. \mathcal{G}_{ij} are the components of the classical Green's function, which is a solution of the linearized equation of motion

$$\left(-\mathbf{1} \frac{d^2}{dt^2} - \frac{\partial^2 V}{\partial \mathbf{q} \partial \mathbf{q}} \left(\mathbf{q}^{(cl)}(t) \right) \right) \mathcal{G}(t, t') = \mathbf{1} \delta(t - t') \quad (3)$$

and fulfils the boundary conditions

$$\begin{aligned} \mathcal{G}(0, t') &= \mathcal{G}(T, t'), \\ \mathcal{P}_{t_0} \mathcal{G}(0, t') &= \mathcal{P}_{t_0} \mathcal{G}(T, t') = 0, \\ \mathcal{Q}_{t_0} \dot{\mathcal{G}}(0, t') &= \mathcal{Q}_{t_0} \dot{\mathcal{G}}(T, t'), \end{aligned} \quad (4)$$

with the projection operators

$$(\mathcal{P}_{t_0})_{ij} = \left(\frac{\dot{\mathbf{q}}(t_0) \otimes \dot{\mathbf{q}}(t_0)}{|\dot{\mathbf{q}}(t_0)|^2} \right)_{ij} = \frac{\dot{q}_i(t_0) \dot{q}_j(t_0)}{|\dot{\mathbf{q}}(t_0)|^2}, \quad (5)$$

and $\mathcal{Q}_{t_0} = \mathbf{1} - \mathcal{P}_{t_0}$, where $\mathbf{1}$ is the f -dimensional unity matrix. At time $t = t'$, the additional condition

$$\begin{pmatrix} \mathcal{G}_-(t', t') \\ \dot{\mathcal{G}}_-(t', t') \end{pmatrix} = \begin{pmatrix} \mathcal{G}_+(t', t') \\ \dot{\mathcal{G}}_+(t', t') \end{pmatrix} + \begin{pmatrix} \mathbf{0} \\ \mathbf{1} \end{pmatrix}, \quad (6)$$

with $\mathcal{G}_-(t, t') = \mathcal{G}(t, t')$ for $0 \leq t \leq t'$, and $\mathcal{G}_+(t, t') = \mathcal{G}(t, t')$ for $t' \leq t \leq T$ has to be fulfilled.

The second contribution to the \hbar correction is given by:

$$C_{1\ell}^{T \rightarrow E}(T_0) = \frac{1}{2W_\ell^{(2)}(T_0)} \left(C_{0\ell}^{(1)}(T_0)^2 + C_{0\ell}^{(2)}(T_0) \right) - \frac{1}{2} \frac{W_\ell^{(3)}(T_0)C_{0\ell}^{(1)}(T_0)}{W_\ell^{(2)}(T_0)^2} - \frac{1}{8} \frac{W_\ell^{(4)}(T_0)}{W_\ell^{(2)}(T_0)^2} + \frac{5}{24} \frac{W_\ell^{(3)}(T_0)^2}{W_\ell^{(2)}(T_0)^3}, \quad (7)$$

where $W_\ell^{(n)}$ and $C_{0\ell}^{(n)}$ are the derivatives

$$W_\ell^{(n)}(T) = \frac{\partial^n W_\ell^{(\text{cl})}(T)}{\partial T^n}, \quad C_{0\ell}^{(n)}(T) = \frac{\partial^n C_{0\ell}^{(\text{cl})}(T)}{\partial T^n}$$

of the action $W_\ell^{(\text{cl})}(T)$ and of the logarithm of the amplitude of the trace of the propagator

$$C_{0\ell}(T) = \ln \left(\frac{T_p}{\sqrt{|\partial_E T \det(\mathbf{m}_\ell(T) - \mathbf{1})|}} \right), \quad (8)$$

respectively.

All quantities required for the \hbar corrections can be obtained by the solution of ordinary differential equations as is discussed in [5] in detail. The number of the differential equations can become very large. For example, in a two-dimensional system the correction term $C_{1\ell}$ leads to 97 ordinary differential equations.

3. The hydrogen atom in a uniform magnetic field

The diamagnetic hydrogen atom was often used as an example of a quantum system whose classical dynamics is chaotic (see e.g. [7] or [8] for an overview). As a real physical system it was the

topic of studies in experimental physics [9, 10]. It has even been used for the numerical test of the \hbar correction terms C_1 and $C_1^{T \rightarrow E}$ [5]. Because of its simple scaling property, which is also fulfilled for the \hbar corrections, it is possible to compare the semiclassical results for individual orbits with exact quantum mechanical calculations.

3.1. The two-dimensional hydrogen atom

The hydrogen atom with three degrees of freedom in a uniform magnetic field has a continuous symmetry, namely the rotational invariance around the magnetic field axis, which can be used to formulate the dynamics in a two-dimensional coordinate system. The calculation of the classical values in the two-dimensional coordinate system works very well for the leading order but it leads to new difficulties for the first-order \hbar correction [6, 11]. In the following sections we only look at the two-dimensional hydrogen atom for the calculation of the first-order \hbar corrections where no continuous symmetry does exist.

For a uniform magnetic field represented by γ , the classical Hamiltonian of the two-

dimensional diamagnetic hydrogen atom in atomic units and semiparabolic coordinates [7, 12] is given by

$$\mathcal{H} = \frac{1}{2}p_\mu^2 + \frac{1}{2}p_\nu^2 - \epsilon(\mu^2 + \nu^2) + \frac{1}{8}\mu^2\nu^2(\mu^2 + \nu^2) = 2, \quad (9)$$

where ϵ is the scaled energy $\epsilon = \gamma^{-2/3}E$ and (μ, ν) are treated as Cartesian coordinates which can also be negative contrary to the regularization of the three-dimensional hydrogen atom.

The Schrödinger equation associated with the classical Hamiltonian (9) is given by:

$$\left\{ 2 + \epsilon(\mu^2 + \nu^2) - \frac{1}{8}\mu^2\nu^2(\mu^2 + \nu^2) \right\} \psi(\mu, \nu) = \gamma^{2/3} \left\{ -\frac{1}{2} \left(\frac{\partial^2}{\partial \mu^2} + \frac{\partial^2}{\partial \nu^2} \right) \right\} \psi(\mu, \nu). \quad (10)$$

Note that $\gamma^{1/3}$ takes the place of \hbar , which is equal to one in atomic units. It is often called “effective \hbar ”.

The “potential” of the two-dimensional diamagnetic hydrogen atom in semiparabolic coordinates (see equation (9))

$$V(\mu, \nu) = -\epsilon(\mu^2 + \nu^2) + \frac{1}{8}\mu^2\nu^2(\mu^2 + \nu^2) \quad (11)$$

has a C_{4v} -symmetry. This symmetry can be seen in figure 1 (a), in which a few equipotential contours of the potential (11) are plotted.

One has to integrate differential equations along the periodic orbits of the classical system in order to calculate the required classical values. It is known that, because of the symmetry, the classical calculations can be reduced to a fundamental domain [13], which is shown in figure 1 (b). It consists of one eighth of the full coordinate plane.

The restriction to the fundamental domain and the introduction of symmetry operations lead to new periodic orbits, which are only periodic if

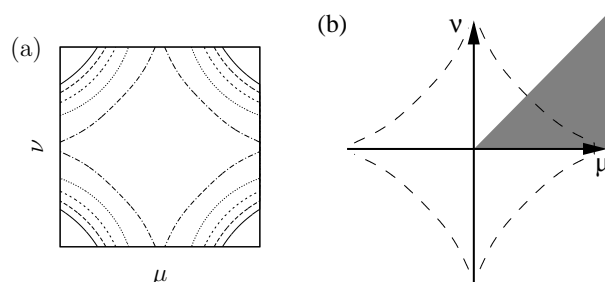


FIG. 1. (a) Equipotential contours of the potential (11) for different scaled energies ϵ . (b) The shadowed area in the coordinate system marks the fundamental domain.

one exploits the symmetry properties of the system. The periodic continuation can be achieved by reflections at the borders of the fundamental domain. An example is the orbit $+$, which is shown in figure 2 (a). Starting for example on the μ -axis the orbit has to be reflected at the angle bisector. After returning to the μ -axis a second reflection (this time at the μ -axis) is necessary such that the momenta at the initial and final points agree. For practical purposes it is often easier not to restrict the calculation to the fundamental domain but to find a periodic continuation of the orbit by mapping the final point of the orbit on its initial point via a symmetry transformation from C_{4v} , namely rotations by multiples of 90 degrees, reflections at the coordinate axes, and reflections at the angle bisectors. For example, figure 2 (b) shows the orbit from figure 2 (a) in the case where it is not restricted to the fundamental domain. The periodic continuation is done by a clockwise rotation by 90 degrees. This method requires only one symmetry operation to render an orbit periodic, and is in general easier to implement as the restriction to the fundamental domain.

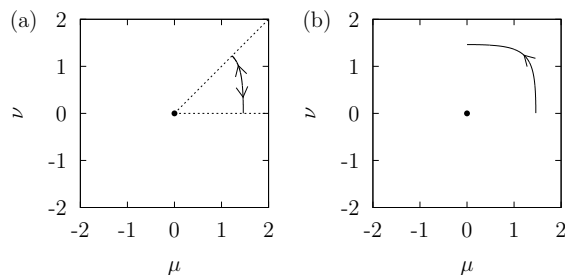


FIG. 2. The periodic orbit + in semiparabolic coordinates for a scaled energy of $\epsilon = -0.1$. The dot marks the nucleus at the origin. Both orbits shown correspond to the single repetition in the fundamental domain.

3.2. Symmetry properties of the wave functions and calculation of the quantum spectra

Because of the C_{4v} -symmetry of the Hamiltonian (10), the eigenfunctions of the system split up into subspaces belonging to a representation of the symmetry group. The symmetry group C_{4v} has four one-dimensional representations, namely A_1 , A_2 , B_1 and B_2 , and a two-dimensional representation, which is called E . Applying a symmetry element from C_{4v} to a wave function with symmetry E leads in general to a linear combination of two (energetically degenerate) wave functions.

At fixed scaled energy ϵ , equation (10) can be considered as a generalized eigenvalue problem in the variable $\gamma^{2/3}$. The eigenvalues can be calculated by diagonalizing a matrix representation of the Hamiltonian in a complete basis set with the Lanczos algorithm [5, 14]. Using only the wave functions of one of the subspaces, which means that the block diagonal form of the Hamiltonian is exploited, reduces the dimension of the eigenvalue problem and leads to separate spectra for each of the subspaces, which is necessary for the analysis of the influence of the symmetry.

The analysis of the quantum spectra can be

performed with the harmonic inversion method [8, 15]. It provides an efficient possibility to extract the amplitude of Gutzwiller's trace formula, the action $S_\ell^{(\text{cl})}(T_0)$ and the sum

$$C_{\hbar\ell} = C_{1\ell} + C_{1\ell}^{T \rightarrow E} \quad (12)$$

of the two first-order \hbar correction terms for individual orbits. Details can be found in [5] or [11].

4. Discrete symmetries and the correction terms

4.1. Symmetry transformations in the calculation of the correction terms

The classical quantities which contribute to the semiclassical level density have to be calculated for periodic orbits and, as we have seen in section 3, some orbits are only periodic after the application of a symmetry operation during or at the end of the integration along the classical orbit. It is well known which symmetry operations (reflections or rotations of vectors) have to be implemented for the calculation of the phase space coordinates but, as was mentioned in section 2, one has to solve a large number of additional differential equations for a "new" set of coordinates if one wants to calculate the first-order \hbar correction. These quantities are the monodromy matrix $\mathbf{M}(t, T_0)$, which can be obtained from the linearized Hamiltonian equations of motion

$$\dot{\mathbf{M}}(t, T_0) = \Sigma \frac{\partial^2 H}{\partial \mathbf{X} \partial \mathbf{X}} \mathbf{M}(t, T_0), \quad (13)$$

the derivatives of the phase space coordinates of the orbit $\mathbf{X}^{(1)}(t, T_0)$, $\mathbf{X}^{(2)}(t, T_0)$, $\mathbf{X}^{(3)}(t, T_0)$ with respect to the time period T , and the derivatives $\mathbf{M}^{(1)}(t, T_0)$ and $\mathbf{M}^{(2)}(t, T_0)$. One has to search for the correct transformations of the additional coordinates.

In particular, the classical Green's function, which in our case is a 2×2 matrix, has compli-

cated symmetry properties, as one can see in figure 3. The function plotted in figure 3 belongs to the orbit which corresponds in the fundamental domain to four repetitions of the orbit shown in figure 2. The symmetry of the orbit is not obvious in the elements of the Green's function. This behaviour is due to the boundary conditions (see equations (4) and (6)) which are different for an orbit and its multiple repetitions and affect the whole Green's function.

The symmetry transformations have to be applied during the integration of the linearized equations of motion (13). Each component of the monodromy matrix transforms the same way as the corresponding element of the phase space vector [11]. If one applies the symmetry operations to the elements of the monodromy matrix at every time when one transforms the coordinates of the orbit during the integration, all boundary conditions of the classical Green's function are fulfilled because the monodromy matrix is the only part that follows from the solution of a differential equation. All other values follow from formulas which include already the boundary conditions and are not affected by the symmetry transformations during the integration.

In order to illustrate the influence of the symmetry transformation, the elements of the classical Green's function of the orbit in the fundamental domain is shown in figure 4 (a). The Green's function was rotated in such a way that the $\mathcal{G}_{1j}(\tau, \tau')$ components represent the direction along the classical orbit at the initial point, which is marked by a cross in the figure. One recognizes the discontinuities at the positions of the reflection which appear due to the change in the meaning of the components accordingly to the change of the variables by using the symmetry transformation. In figure 4 (a), all boundary conditions which were mentioned in section 2 are fulfilled. At the final point of the orbit, all components have the same values as at the initial point. The

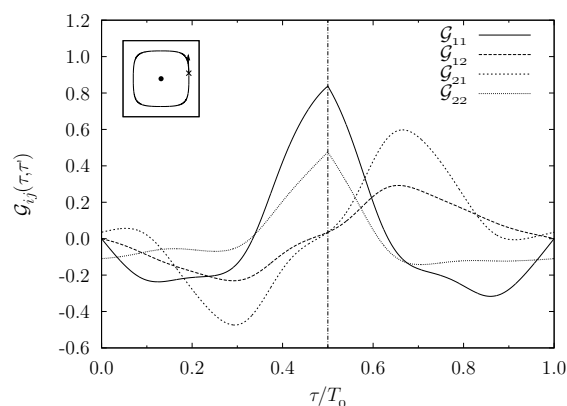


FIG. 3. The picture shows the classical Green's function of the orbit + + + +, which corresponds to four repetitions of the orbit + in the fundamental domain, for $\tau' = 0.5 \cdot T_0$. In the elements of the Green's function, no obvious symmetry is visible. The elements of the Green's function are chosen in such a way that the components \mathcal{G}_{1j} correspond to the direction along the orbit at the initial point, which is marked by a cross.

condition $\mathcal{G}_{1j}(0, \tau') = \mathcal{G}_{1j}(T_0, \tau') = 0$, which is expected from equation (4), is also fulfilled. The discontinuities in the elements $\dot{\mathcal{G}}_{2j}$, which appear due to equation (6), are clearly visible.

Figure 4 (b) shows the classical Green's function for the same orbit, which is not restricted to the fundamental domain but closed by a rotation of its final point. Therefore, the only discontinuity appears at the end point of the orbit. To show this, the first and the last point (after the symmetry transformation) of each component are marked with the same symbol. Again, the boundary conditions are fulfilled.

Under symmetry operations even all further variables of the differential equations which contribute to the first-order \hbar correction transform in the same way as the corresponding phase space coordinates of the orbit [11]. With this knowledge it is possible to calculate the correction terms for orbits which require a symmetry operation to become periodic.

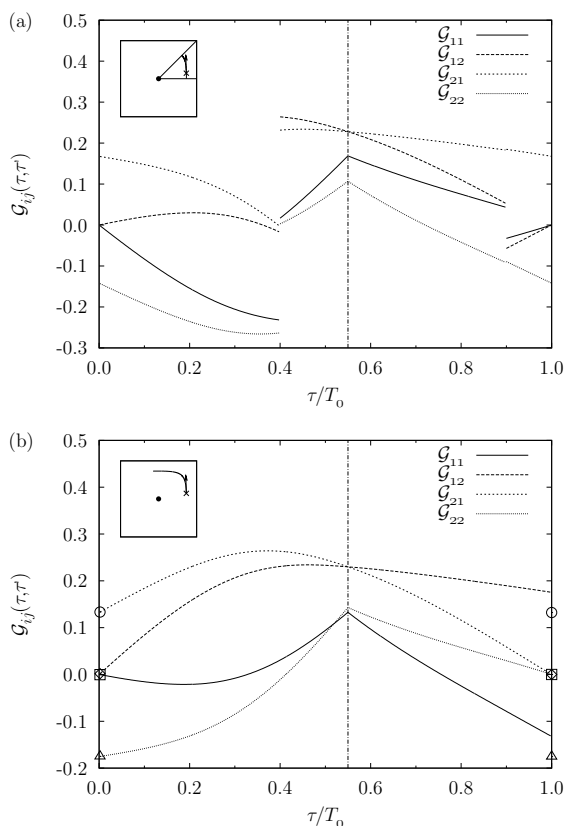


FIG. 4. The classical Green's function of the orbit + is shown in two cases for $\tau' = 0.55 \cdot T_0$. (a) Orbit in the fundamental domain. (b) The same orbit in the full plane of semiparabolic coordinates, which becomes periodic by the application of a rotation of the final point. The elements of the Green's function are chosen as described in the text of figure 3.

4.2. Examples for some orbits

In the different subspaces of the quantum wave functions, the individual amplitudes A_ℓ of Gutzwiller's trace formula can be found with a prefactor. This prefactor is given by the character of the element from C_{4v} which provides the periodic continuation of the orbit in the representation of the corresponding subspace [13]. As an example one can see the Fourier transformation of the quantum spectrum which includes all eigenvalues from the subspace A_1 in figure 5 (a). In

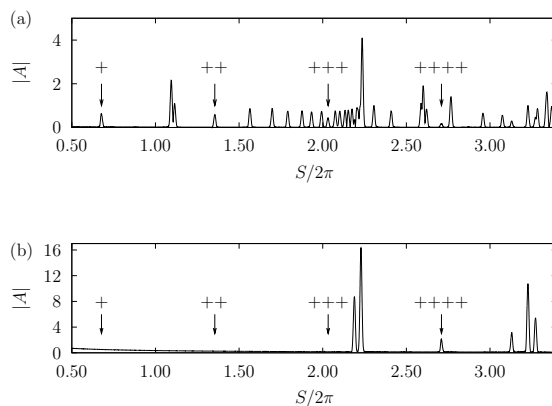


FIG. 5. (a) The Fourier transform of the eigenvalues from subspace A_1 includes all orbits which are periodic after the application of a symmetry transformation. S : action, A : amplitude of Gutzwiller's trace formula. (b) If one looks at the Fourier transformation of the spectrum which includes the eigenvalues of all subspaces, one can only find the orbits which are periodic in the full plane of semiparabolic coordinates.

this subspace all orbits contribute with a prefactor of 1 independently of the symmetry element required to find the periodic continuation. The orbit + and some of its multiple repetitions are marked. If one uses the quantum spectrum which consists of the eigenvalues of all subspaces, only the orbits which are periodic in the full plane of the semiparabolic coordinates appear (see figure 5 (b)). For example, the orbit +++++ is periodic.

One possibility to obtain the first-order terms from the quantum spectrum is to subtract the leading order of the individual orbits from the whole spectrum. If one uses A_ℓ with its prefactor for this method, the harmonic inversion of the quantum spectrum leads to the correct first-order terms $C_{\hbar\ell}$. Table 1 shows the results for the orbit + in all one-dimensional subspaces of C_{4v} , which are compared with the classically calculated value.

The classical results for the correction terms of a few orbits which require a symmetry opera-

Table 1. Modulus $|C_{\hbar\ell}^{(\text{qm})}|$ and phase $\arg(C_{\hbar\ell}^{(\text{qm})})$ of the sum $C_{\hbar\ell}$ of the correction terms (see equation (12)) of the orbit + in different subspaces obtained by the analysis of the quantum spectrum. They are in good agreement with the classical value $C_{\hbar\ell}^{(\text{cl})} = -0.0944300$ as is shown in the last column.

Subspace	$ C_{\hbar\ell}^{(\text{qm})} $	$\arg(C_{\hbar\ell}^{(\text{qm})})$	$\frac{ C_{\hbar\ell}^{(\text{qm})} }{ C_{\hbar\ell}^{(\text{cl})} } - 1$
A_1	0.09455	$1.0006 \cdot \pi$	0.0013
A_2	0.09396	$0.9999 \cdot \pi$	-0.0050
B_1	0.09456	$1.0006 \cdot \pi$	0.0013
B_2	0.09452	$1.0003 \cdot \pi$	0.0010

tion to become periodic, are given in table 2. Figure 6 shows the comparison of these results with values $C_{\hbar\ell}^{(\text{qm})}$ extracted from exact quantum calculations. Only the eigenvalues of the subspace belonging to the representation A_1 were used for the harmonic inversion of the quantum spectrum. As one can see, the agreement of the amplitudes from classical and quantum calculations is very good. In most cases the differences are only of the order 10^{-3} . If one compares the phases of the (complex) quantum mechanically calculated correction terms, one sees that they reproduce the correct signs of the classical values. The differences are typically of the order 10^{-2} .

5. Conclusion and Outlook

In this paper we have studied the influence of discrete symmetries on the \hbar correction terms to Gutzwiller's trace formula. The main focus was on the symmetry properties of the classical Green's function. A complete analysis of all parts of the correction terms can be found in [11]. We applied symmetry transformations which made possible the calculation of the correction terms for a number of orbits which could not be included without symmetry operations. Nevertheless, these orbits contribute to some of the sub-

Table 2. The first-order \hbar corrections $C_{\hbar\ell}$ (see equation (12)) for some orbits which are only periodic with a symmetry transformation obtained by classical calculations.

Orbit	$C_{1\ell}$	$C_{1\ell}^{T \rightarrow E}$	$C_{\hbar\ell}^{(\text{cl})}$
+	-0.0900370	-0.0043931	-0.0944300
++	-0.3916524	0.0299638	-0.3616886
0-	0.0184174	0.0309192	0.0493366
++--	-0.578572	0.063221	-0.515351
0---	0.25147	0.08191	0.33338
++++	-0.92396	0.16120	-0.76277
0-+	-0.444747	0.063019	-0.381729
00+	2.56347	0.27548	2.83895
+++--	-2.97331	0.25335	-2.71997
0-++	-0.319617	0.036473	-0.283144

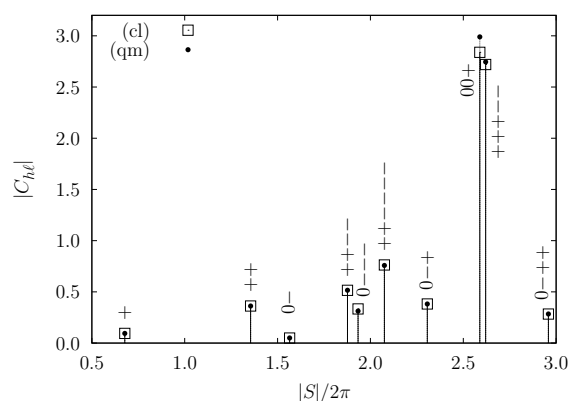


FIG. 6. The modulus $|C_{\hbar\ell}^{(\text{qm})}|$ of the first-order \hbar corrections obtained by harmonic inversion of the quantum spectrum (filled circles) is compared with the classical value $|C_{\hbar\ell}^{(\text{cl})}|$ (open squares). One can see that the agreement is very good.

spaces of the quantum spectrum. The classical results for the correction terms could be compared with values which were extracted from exact quantum calculations. An excellent agreement between the results of both methods was found.

In spite of this success, it must be noted that before semiclassical spectra including first-order \hbar corrections can be calculated over the complete

spectrum a number of problems still remain to be solved.

On the one hand, as was already mentioned in [5], the correction term C_1 cannot be calculated in the form presented for orbits which have a turning point, but the inclusion of these orbits is essential for the \hbar correction of the level density. The correction term C_1 diverges for orbits with turning points.

On the other hand, besides the successfully implemented discrete symmetries, physical systems often have a continuous symmetry. For ex-

ample, it is necessary to take into account the rotational invariance around the magnetic field axis for the complete calculation of all first-order \hbar corrections to the semiclassical level density of the three-dimensional diamagnetic hydrogen atom. The problem can be considered as an additional centrifugal term in the potential. This term leads to diverging integrals if the course of the orbit is not changed. A regularization of these integrals suggested in [6] leads to good results for a few individual orbits, however, a mathematical justification is lacking.

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