

\hbar expansions in semiclassical theories for systems with smooth potentials and discrete symmetries

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Abstract

We extend a theory of first order \hbar corrections to Gutzwiller's trace formula for systems with a smooth potential to systems with discrete symmetries and, as an example, apply the method to the two-dimensional hydrogen atom in a uniform magnetic field. We exploit the C_{4v} -symmetry of the system in the calculation of the correction terms. The numerical results for the semiclassical values will be compared with values extracted from exact quantum mechanical calculations. The comparison shows an excellent agreement and demonstrates the power of the \hbar expansion method.

Key words: semiclassical theories, Gutzwiller's trace formula, \hbar expansions, discrete symmetries, diamagnetic hydrogen atom

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1 Introduction

Semiclassical theories have become very important for a deeper understanding of quantum systems, and Gutzwiller's trace formula [1] has become a powerful tool for classically chaotic systems. It 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 [2,3,4], 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] developed \hbar corrections to Gutzwiller's trace formula for quantum systems with a smooth potential. He presented a first-order \hbar correction term to Gutzwiller's trace

formula and obtained numerical results for the diamagnetic hydrogen atom. Comparisons with values extracted from exact quantum calculations showed that the semiclassical results can be computed with very high accuracy.

However, in the theory presented in [5] some important topics have not yet been considered. For example, the \hbar corrections cannot be calculated for classical orbits which have a turning point (i.e., the velocity vanishes completely at this point). Furthermore, discrete and continuous symmetries have not been included.

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. Preliminary results for the diamagnetic hydrogen atom, which is an example system with discrete symmetries, were published in [6] without explaining which modifications in the numerical calculations the introduction of discrete symmetries entails. In particular, an analysis of the differential equations which have to be solved to obtain the correction terms is not presented. In this paper we want to give a transparent derivation of the modifications necessary for the calculation of the correction terms in systems with discrete symmetries. We will show in detail how such symmetries of the Hamiltonian have to be taken into account. It will be explained in which equations it is necessary to introduce symmetry operations and which transformations lead to the correct boundary conditions of the classical Greens function, which is an essential part of the correction terms. Furthermore, we want to give a deeper understanding of the significance of the symmetry of the system for the quantum spectrum and the connection to periodic orbits.

We will apply the method to the diamagnetic hydrogen atom. The three-dimensional hydrogen atom in a uniform magnetic field has a continuous symmetry, namely the rotational invariance around the magnetic field axis. Continuous symmetries have a substantial influence on the correction terms. Actually one cannot obtain the correct results for the first-order \hbar correction for the three-dimensional hydrogen atom with the formulas presented because the rotational invariance leads to additional contributions to the first-order corrections. Therefore, we will consider the hydrogen atom as a pure two-dimensional system as it was done before in [5]. If one uses semiparabolic coordinates, the potential of the two-dimensional diamagnetic hydrogen atom exhibits a discrete C_{4v} -symmetry. The \hbar corrections will be calculated for selected periodic orbits taking into account that discrete symmetry. The semiclassical results 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 first give a summary

of the derivation of the \hbar corrections without taking into account discrete symmetries. In section 3, we will introduce the hydrogen atom in a uniform magnetic field with all aspects relevant for the calculation of the correction terms. We will also discuss the influence of the rotational invariance of the three-dimensional hydrogen atom. Then we will extend the \hbar corrections 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

As mentioned in the introduction the \hbar corrections to Gutzwiller's trace formula for systems with a smooth potential were derived by Grémaud [5] based on earlier work by Gaspard et al. [3,4]. In this section, for the reader's convenience we will briefly summarize all major steps of this derivation by following the way described in [5] in order to be able to include discrete symmetries in section 4.

2.1 The trace of the propagator and the first part of the \hbar correction

The starting point for the derivation of the semiclassical level density which is used in this theory is a discrete version of Feynman's path integral representation of the propagator

$$K(\vec{q}, \vec{q}_0, T) = \frac{1}{(2\pi i \hbar \Delta t)^{\frac{Nf}{2}}} \int d\vec{q}_1 d\vec{q}_2 \cdots d\vec{q}_{N-1} \times \exp \left[\frac{i}{\hbar} \sum_{n=0}^{N-1} L \left(\frac{\vec{q}_{n+1} - \vec{q}_n}{\Delta t}, \vec{q}_n \right) \Delta t + O(\Delta t) \right], \quad (1)$$

for a system with f degrees of freedom and a time independent Hamiltonian:

$$H = \frac{\vec{p}^2}{2} + V(\vec{q}). \quad (2)$$

$K(\vec{q}, \vec{q}_0, T)$ represents the propagation of a particle going from \vec{q}_0 to $\vec{q}_N = \vec{q}$ in time T with $\Delta t = T/N$. $L(\vec{q}, \dot{\vec{q}})$ denotes the classical Lagrangian of the system.

For the calculation of the level density one has to know the trace of the propagator, which can be obtained by setting $\vec{q}_0 = \vec{q}$ in (1) and by integrating over

this variable:

$$K(T) = \int K(\vec{q}_0, \vec{q}_0, T) d\vec{q}_0 = \frac{1}{(2\pi i \hbar \Delta t)^{\frac{Nf}{2}}} \int d\vec{q}_0 d\vec{q}_1 d\vec{q}_2 \cdots d\vec{q}_{N-1} \\ \times \exp \left[\frac{i}{\hbar} \sum_{n=0}^{N-1} L \left(\frac{\vec{q}_{n+1} - \vec{q}_n}{\Delta t}, \vec{q}_n \right) \Delta t + O(\Delta t) \right]. \quad (3)$$

After expanding the exponential function and including all terms which produce contributions to the leading order in \hbar and to the first-order correction, the integral is evaluated as described in [4]. The result in the limit $\Delta t \rightarrow 0$ is given by:

$$K(T) = \sum_{\ell} K_{\ell}^{(0)}(T) \left\{ 1 + \frac{i\hbar}{T_p} \int_0^{T_p} dt_0 C_{1\ell}(T, t_0) + O(\hbar^2) \right\}. \quad (4)$$

In this formula the sum runs over all periodic orbits of the classical system described by the Hamiltonian (2) with period T . T_p represents the time period of the primitive periodic orbit, i.e., if the orbit consists of multiple repetitions of a periodic orbit, one considers only the basic traversal in this case. $K_{\ell}^{(0)}(T)$ stands for the leading order of the semiclassical approximation. It is identical with Gutzwiller's [1] result, and is given by:

$$K_{\ell}^{(0)}(T) = \frac{1}{\sqrt{2\pi\hbar}} \frac{T_p}{\sqrt{|\partial_E T \det(\mathbf{m}_{\ell}(T) - \mathbf{1})|}} \\ \times \exp \left[\frac{i}{\hbar} W_{\ell}^{(\text{cl})}(T) - \frac{i\pi}{2} \mu_{\ell} + \frac{i\pi}{4} \text{sign}(\partial_E T) \right]. \quad (5)$$

In this expression one can find the $(2f - 2) \times (2f - 2)$ -dimensional stability matrix \mathbf{m} , which represents the stability properties of the periodic orbit. The determinant $\det(\mathbf{m}_{\ell}(T) - \mathbf{1})$ is related to the $2f \times 2f$ -dimensional monodromy matrix. This relation is shown in section 2.4.2. A further term is the classical action

$$W_{\ell}^{(\text{cl})}(T) = \int_0^T L(\vec{q}, \vec{q}) dt, \quad (6)$$

μ_{ℓ} is the Maslov index, and $\partial_E T$ is the derivative of the time period with respect to the energy E . In equation (4) $C_{1\ell}$ is the abbreviation of the first-order correction in \hbar . As one can see in (4) one has to use the average of $C_{1\ell}(T, t_0)$, where t_0 parametrizes the periodic orbit. The integral over t_0 runs from 0 to T_p , i.e., one has to integrate over the whole primitive periodic orbit. The explicit expression of $C_{1\ell}(T, t_0)$ needs lengthy calculations, which are

discussed in [3,4,5] in detail. The result reads:

$$\begin{aligned}
C_{1\ell}(T, t_0) &= \frac{1}{8} \int_0^T dt V_{,i_1 i_2 i_3 i_4}(\vec{q}_\ell^{(\text{cl})}(t)) \mathcal{G}_{i_1 i_2}(t, t; t_0) \mathcal{G}_{i_3 i_4}(t, t; t_0) \\
&+ \frac{1}{24} \int_0^T dt \int_0^T dt' V_{,i_1 i_2 i_3}(\vec{q}_\ell^{(\text{cl})}(t)) V_{,j_1 j_2 j_3}(\vec{q}_\ell^{(\text{cl})}(t')) \left(3\mathcal{G}_{i_1 i_2}(t, t; t_0) \right. \\
&\times \mathcal{G}_{i_3 j_1}(t, t'; t_0) \mathcal{G}_{j_2 j_3}(t', t'; t_0) + 2\mathcal{G}_{i_1 j_1}(t, t'; t_0) \mathcal{G}_{i_2 j_2}(t, t'; t_0) \mathcal{G}_{i_3 j_3}(t, t'; t_0) \Big) \\
&+ \frac{V_{,j}(t_0)}{2|\vec{q}_\ell^{(\text{cl})}(t_0)|^2} \int_0^T dt V_{,i_1 i_2 i_3}(\vec{q}_\ell^{(\text{cl})}(t)) \mathcal{G}_{j i_1}(0, t; t_0) \mathcal{G}_{i_2 i_3}(t, t; t_0), \quad (7)
\end{aligned}$$

where

$$V_{,i_1 \dots i_n}(\vec{q}_\ell^{(\text{cl})}(t)) = \frac{\partial^n V(\vec{q}_\ell^{(\text{cl})}(t))}{\partial q_{i_1} \dots \partial q_{i_n}} \quad (8)$$

are derivatives of the potential evaluated at the point $\vec{q}_\ell^{(\text{cl})}(t)$ 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:

$$\left(-\mathbf{1} \frac{d^2}{dt^2} - \frac{\partial^2 V}{\partial \vec{q} \partial \vec{q}}(\vec{q}_\ell^{(\text{cl})}(t)) \right) \mathcal{G}(t, t') = \mathbf{1} \delta(t - t'). \quad (9)$$

Due to the factor $1/|\vec{q}_\ell^{(\text{cl})}|^2$ in equation (7), the correction term is singular for vanishing velocities, and because of the integral over t_0 in equation (4), the \hbar correction term diverges for orbits with a turning point.

2.2 The classical Green's function for the trace of the propagator

The classical Green's function is an essential part of the first-order \hbar correction to the trace of the propagator. In order to be able to look at the symmetry transformations of $C_{1\ell}$ in equation (7), one has to know its structure. In this section we discuss all important parts of this structure.

From the derivation of the correction term $C_{1\ell}$, it follows that the classical Green's function has to fulfil the boundary conditions [5]

$$\begin{aligned}
\mathcal{G}(0, t') &= \mathcal{G}(T, t'), \\
\mathcal{P}_{t_0} \mathcal{G}(0, t') &= \mathcal{P}_{t_0} \mathcal{G}(T, t') = 0, \\
\mathcal{Q}_{t_0} \dot{\mathcal{G}}(0, t') &= \mathcal{Q}_{t_0} \dot{\mathcal{G}}(T, t'),
\end{aligned} \quad (10)$$

with the projection operator \mathcal{P}_{t_0} along the direction of the classical orbit at time t_0 , which has the form

$$(\mathcal{P}_{t_0})_{ij} = \left(\frac{\vec{q}(t_0) \otimes \vec{q}(t_0)}{|\vec{q}(t_0)|^2} \right)_{ij} = \frac{\dot{q}_i(t_0) \dot{q}_j(t_0)}{|\dot{\vec{q}}(t_0)|^2}, \quad (11)$$

furthermore, $\mathcal{Q}_{t_0} = \mathbf{1} - \mathcal{P}_{t_0}$, with the f -dimensional unity matrix $\mathbf{1}$. If we use the notation

$$\begin{aligned}\mathcal{G}_-(t, t') &= \mathcal{G}(t, t') \quad \text{for } 0 \leq t \leq t', \\ \mathcal{G}_+(t, t') &= \mathcal{G}(t, t') \quad \text{for } t' \leq t \leq T,\end{aligned}\tag{12}$$

it is possible to write the classical Green's function as a product [5]

$$\begin{pmatrix} \mathcal{G}_\pm(t, t') \\ \dot{\mathcal{G}}_\pm(t, t') \end{pmatrix} = \mathbf{M}(t) \begin{pmatrix} \mathbf{A}_\pm(t') \\ \mathbf{B}_\pm(t') \end{pmatrix}\tag{13}$$

with the $2f \times 2f$ monodromy matrix $\mathbf{M}(t)$ and the four $f \times f$ matrices \mathbf{A}_\pm and \mathbf{B}_\pm . The monodromy matrix is a symplectic matrix, which can be obtained by solving the linearized Hamiltonian equations of motion

$$\dot{\mathbf{M}}(t, T) = \Sigma \frac{\partial^2 H}{\partial \vec{X} \partial \vec{X}} \mathbf{M}(t, T).\tag{14}$$

Here, Σ is the matrix

$$\Sigma = \begin{pmatrix} \mathbf{0} & \mathbf{1} \\ -\mathbf{1} & \mathbf{0} \end{pmatrix}$$

and $\mathbf{1}$ is the $f \times f$ unity matrix. For a Hamiltonian of the form (2) it has the structure:

$$\mathbf{M}(t) = \begin{pmatrix} \mathbf{J}_2(t) & \mathbf{J}_1(t) \\ \dot{\mathbf{J}}_2(t) & \dot{\mathbf{J}}_1(t) \end{pmatrix},\tag{15}$$

where \mathbf{J}_1 and \mathbf{J}_2 are $f \times f$ matrices. The boundary conditions at time $t = t'$ are

$$\begin{pmatrix} \mathcal{G}_-(t', t') \\ \dot{\mathcal{G}}_-(t', t') \end{pmatrix} = \begin{pmatrix} \mathcal{G}_+(t', t') \\ \dot{\mathcal{G}}_+(t', t') \end{pmatrix} + \begin{pmatrix} \mathbf{0} \\ \mathbf{1} \end{pmatrix}.\tag{16}$$

Exploiting the formulation (13) of the classical Green's function and the symplecticity of the monodromy matrix $\mathbf{M}(t)$, one can formulate the boundary condition (16) as follows:

$$\begin{pmatrix} \mathbf{A}_+(t') \\ \mathbf{B}_+(t') \end{pmatrix} = \begin{pmatrix} \mathbf{A}_-(t') \\ \mathbf{B}_-(t') \end{pmatrix} - \mathbf{M}(t')^{-1} \begin{pmatrix} \mathbf{0} \\ \mathbf{1} \end{pmatrix} = \begin{pmatrix} \mathbf{A}_-(t') \\ \mathbf{B}_-(t') \end{pmatrix} - \begin{pmatrix} -\mathbf{J}_1(t')^\top \\ \mathbf{J}_2(t')^\top \end{pmatrix}.\tag{17}$$

If this expression is combined with the condition

$$\begin{pmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & \mathcal{Q}_{t_0} \end{pmatrix} \begin{pmatrix} \mathbf{A}_-(t') \\ \mathbf{B}_-(t') \end{pmatrix} = \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & \mathcal{Q}_{t_0} \end{pmatrix} \mathbf{M}(T) \begin{pmatrix} \mathbf{A}_+(t') \\ \mathbf{B}_+(t') \end{pmatrix},\tag{18}$$

which is identical with the first and third condition of (10), it leads to the matrix equation:

$$\begin{pmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & \mathcal{Q}_{t_0} \end{pmatrix} [\mathbf{M}(T) - \mathbf{1}] \begin{pmatrix} \mathbf{A}_-(t') \\ \mathbf{B}_-(t') \end{pmatrix} = \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & \mathcal{Q}_{t_0} \end{pmatrix} \mathbf{M}(T) \begin{pmatrix} -\mathbf{J}_1(t')^\top \\ \mathbf{J}_2(t')^\top \end{pmatrix}. \quad (19)$$

This equation has to be solved in order to obtain the matrices \mathbf{A}_- and \mathbf{B}_- . When \mathbf{A}_- and \mathbf{B}_- are known one has the solution for the classical Green's function (13). Unfortunately, the matrix

$$\begin{pmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & \mathcal{Q}_{t_0} \end{pmatrix} [\mathbf{M}(T) - \mathbf{1}]$$

is singular but, as was shown in [5], there is a solution for classical trajectories which have no turning point (i.e. the velocity $\vec{q}(t)$ never vanishes completely along the orbit), viz.

$$\begin{pmatrix} \mathbf{A}_-(t'; t_0) \\ \mathbf{B}_-(t'; t_0) \end{pmatrix} = \mathcal{X} = \mathcal{X}_0 + \frac{1}{|\vec{q}(t_0)|^2} \begin{pmatrix} \vec{q}(t_0) \otimes \vec{q}(t_0) & \mathbf{0} \\ \vec{p}(t_0) \otimes \vec{q}(t_0) & \mathbf{0} \end{pmatrix} \mathcal{X}_0, \quad (20)$$

where \mathcal{X}_0 represents a particular solution of equation (19), which can be determined by a singular value decomposition (see e.g. [7]). The second condition of equation (10) has been used to derive this result.

In summary, it is possible to obtain the classical Green's function by solving the linearized equation of motion (14) of the monodromy matrix and by calculating \mathbf{A}_- and \mathbf{B}_- from equation (20). Then the correction term $C_{1\ell}(T, t_0)$ follows from equation (7). In equation (20), the factor $1/|\vec{q}^{(\text{cl})}|^2$ appears in the construction of $C_{1\ell}(T, t_0)$ a second time. The reason for this lies in the application of the projection operator \mathcal{P}_{t_0} in the second condition of (10).

The integrals and double integrals in equation (7) can be transformed into a set of ordinary differential equations, which can be computed effectively. The transformation of the integrals is discussed in [5] in detail.

2.3 The trace of the quantum Green's function and the second part of the \hbar corrections

The next step on the way to the level density is the trace of the quantum Green's function, which can be obtained from the trace of the propagator via

the semi-sided Fourier transform

$$G(E) = \sum_{\ell} G_{\ell}(E) = \sum_{\ell} \frac{1}{i\hbar} \int_0^{\infty} dT \exp\left[\frac{i}{\hbar}ET\right] K_{\ell}(T). \quad (21)$$

One has to include all contributions to the leading order as well as the first-order \hbar correction in the semiclassical approximation of the integral. The methods which are used to evaluate this integral are discussed in [4]. We do not want to repeat the calculation but present the results obtained in [4] and [5], which can be summarized as follows:

$$G_{\ell}(E) = \frac{1}{i\hbar} \frac{T_{0p}}{\sqrt{|\det(\mathbf{m}_{\ell}(T_0) - \mathbf{1})|}} \exp\left[\frac{i}{\hbar}S_{\ell}^{(\text{cl})}(T_0) - \frac{i\pi}{2}\mu_{\ell}\right] \times \left\{1 + i\hbar\left(C_{1\ell}(T_0) + C_{1\ell}^{T \rightarrow E}(T_0)\right) + O(\hbar^2)\right\}, \quad (22)$$

where the leading order, belonging to the 1 in the curly brackets, is known from Gutzwiller's trace formula [1]. The reduced action

$$S_{\ell}^{(\text{cl})}(T_0) = W_{\ell}^{(\text{cl})}(T_0) + ET_0 \quad (23)$$

is used in this expression, and μ_{ℓ} represents the Maslov index. The first-order \hbar correction consists of two terms. The first,

$$C_{1\ell}(T_0) = \frac{1}{T_{0p}} \int_0^{T_{0p}} C_{1\ell}(T_0, t_0) dt_0, \quad (24)$$

is the same as in equation (7) but now with fixed period T_0 , and the second is the contribution from integral (21) to the \hbar correction, and is given by:

$$C_{1\ell}^{T \rightarrow E}(T_0) = \frac{1}{2W_{\ell}^{(2)}(T_0)} \left(C_{0\ell}^{(1)}(T_0)^2 + C_{0\ell}^{(2)}(T_0)\right) - \frac{1}{2} \frac{W_{\ell}^{(3)}(T_0)C_{0\ell}^{(1)}(T_0)}{W_{\ell}^{(2)}(T_0)^2} - \frac{1}{8} \frac{W_{\ell}^{(4)}(T_0)}{W_{\ell}^{(2)}(T_0)^2} + \frac{5}{24} \frac{W_{\ell}^{(3)}(T_0)^2}{W_{\ell}^{(2)}(T_0)^3}. \quad (25)$$

$W_{\ell}^{(n)}$ 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

$$C_{0\ell}(T) = \ln \left(\frac{T_p}{\sqrt{|\partial_E T \det(\mathbf{m}_{\ell}(T) - \mathbf{1})|}} \right), \quad (26)$$

respectively.

2.4 Contributions to the correction terms of the trace of the semiclassical Green's function

In this section we want to summarize the contributions to the second correction term $C_t^{T \rightarrow E}$ which are important for the understanding of the symmetry properties of this term. As we will see, all parts of equation (25) can be obtained as numerical solutions of differential equations of some “new” coordinates.

2.4.1 Derivatives of $W_\ell^{(\text{cl})}(T)$

Because of the relation

$$W_\ell^{(1)}(T_0) = \left. \frac{\partial W_\ell^{(\text{cl})}(T)}{\partial T} \right|_{T=T_0} = -E(T_0) = -H(\vec{X}(t, T_0)) \quad (27)$$

all higher derivatives of the action $W_\ell^{(\text{cl})}(T_0)$ with respect to the time period of the orbit can be expressed as derivatives of the classical Hamiltonian, where $\vec{X}(t, T_0) = (\vec{q}(t, T_0), \vec{p}(t, T_0))$ represents the phase space vector of the orbit. Introducing the derivatives

$$\vec{X}^{(n)}(t, T_0) = \left. \frac{\partial^n \vec{X}(t, T)}{\partial T^n} \right|_{T=T_0}, \quad (28)$$

which appear as coefficients of the Taylor expansion

$$\vec{X}(t, T) = \vec{X}(t, T_0 + \delta T) = \sum_{n=0}^{\infty} \frac{1}{n!} \vec{X}^{(n)}(t, T_0) (\delta T)^n \quad (29)$$

of the orbit $\vec{X}(t, T)$ around a reference orbit $\vec{X}(t, T_0)$ with period T_0 , the higher derivatives of $W_\ell^{(\text{cl})}(T_0)$ are:

$$\begin{aligned} W_\ell^{(2)}(T_0) &= -H_{,i}(\vec{X}(t, T_0)) X_i^{(1)}(t, T_0), \\ W_\ell^{(3)}(T_0) &= -H_{,ij}(\vec{X}(t, T_0)) X_i^{(1)}(t, T_0) X_j^{(1)}(t, T_0) - H_{,i}(\vec{X}(t, T_0)) X_i^{(2)}(t, T_0), \\ W_\ell^{(4)}(T_0) &= -H_{,ijk}(\vec{X}(t, T_0)) X_i^{(1)}(t, T_0) X_j^{(1)}(t, T_0) X_k^{(1)}(t, T_0) \\ &\quad - 3H_{,ij}(\vec{X}(t, T_0)) X_i^{(1)}(t, T_0) X_j^{(2)}(t, T_0) - H_{,i}(\vec{X}(t, T_0)) X_i^{(3)}(t, T_0). \end{aligned} \quad (30)$$

From Hamilton's equations of motion for the phase space coordinates

$$\dot{\vec{X}}(t, T_0) = \Sigma \frac{\partial H(\vec{X}(t, T_0))}{\partial \vec{X}},$$

one can infer the equations which govern the motion of the derivatives $\vec{X}^{(n)}(t, T_0)$:

$$\begin{aligned}
\dot{X}_i^{(1)}(t, T_0) &= \Sigma_{ij} H_{,jk}(\vec{X}(t, T_0)) X_k^{(1)}(t, T_0), \\
\dot{X}_i^{(2)}(t, T_0) &= \Sigma_{ij} H_{,jkl}(\vec{X}(t, T_0)) X_k^{(1)}(t, T_0) X_l^{(1)}(t, T_0) \\
&\quad + \Sigma_{ij} H_{,jk}(\vec{X}(t, T_0)) X_k^{(2)}(t, T_0), \\
\dot{X}_i^{(3)}(t, T_0) &= \Sigma_{ij} H_{,jklm}(\vec{X}(t, T_0)) X_k^{(1)}(t, T_0) X_l^{(1)}(t, T_0) X_m^{(1)}(t, T_0) \\
&\quad + 3\Sigma_{ij} H_{,jkl}(\vec{X}(t, T_0)) X_k^{(1)}(t, T_0) X_l^{(2)}(t, T_0) \\
&\quad + \Sigma_{ij} H_{,jk}(\vec{X}(t, T_0)) X_k^{(3)}(t, T_0).
\end{aligned} \tag{31}$$

These equations are inhomogeneous differential equations. Their solutions are of the type

$$\begin{aligned}
\vec{X}^{(1)}(t, T_0) &= \mathbf{M}(t, T_0) \vec{X}^{(1)}(0, T_0), \\
\vec{X}^{(2)}(t, T_0) &= \mathbf{M}(t, T_0) \vec{X}^{(2)}(0, T_0) + \vec{F}^{(2)}(t, T_0), \\
\vec{X}^{(3)}(t, T_0) &= \mathbf{M}(t, T_0) \vec{X}^{(3)}(0, T_0) + \vec{F}^{(3)}(t, T_0),
\end{aligned} \tag{32}$$

where $\mathbf{M}(t, T_0)$ is the monodromy matrix, which was introduced in section 2.2. Together with the condition

$$\vec{X}(t = 0, T_0) = \vec{X}(t = T_0, T_0) \tag{33}$$

for periodic orbits, the solutions (32) lead to the following equations for the initial values:

$$\begin{aligned}
[\mathbf{1} - \mathbf{M}(T_0, T_0)] \vec{X}^{(1)}(0, T_0) &= \vec{X}(T_0, T_0), \\
[\mathbf{1} - \mathbf{M}(T_0, T_0)] \vec{X}^{(2)}(0, T_0) &= 2\vec{X}^{(1)}(T_0, T_0) + \vec{X}(T_0, T_0) + \vec{F}^{(2)}(T_0, T_0), \\
[\mathbf{1} - \mathbf{M}(T_0, T_0)] \vec{X}^{(3)}(0, T_0) &= 3\vec{X}^{(2)}(T_0, T_0) + 3\vec{X}^{(1)}(T_0, T_0) + \vec{X}(T_0, T_0) \\
&\quad + \vec{F}^{(3)}(T_0, T_0).
\end{aligned} \tag{34}$$

The matrix $[\mathbf{1} - \mathbf{M}(T_0, T_0)]$ is singular. A particular solution can be found via a singular value decomposition. For a general unstable orbit the kernel is one-dimensional, i.e., the solution space is in general one-dimensional (see [5]) but, as also shown in [5], $W_\ell^{(2)}(T_0)$ can directly be computed if a particular solution $\vec{X}_0^{(1)}(0, T_0)$ from (34) is known:

$$W_\ell^{(2)}(T_0) = -\vec{\nabla} H(\vec{X}(T_0, T_0)) \cdot \vec{X}_0^{(1)}(0, T_0). \tag{35}$$

Similar relations can be found for $W_\ell^{(3)}(T_0)$ and $W_\ell^{(4)}(T_0)$, in which also only a particular solution of equation (34) is required.

2.4.2 Derivatives of $C_{0\ell}(T)$

If one looks at the definition of $C_{0\ell}(T)$ in equation (26), one can easily convince oneself that

$$\begin{aligned} C_{0\ell}^{(1)}(T_0) &= \frac{1}{T_0} + \frac{1}{2} \frac{W_\ell^{(3)}(T_0)}{W_\ell^{(2)}(T_0)} - \frac{1}{2} \frac{d}{dT} \ln |\det(\mathbf{m}(T) - \mathbf{1})| \Big|_{T=T_0}, \\ C_{0\ell}^{(2)}(T_0) &= -\frac{1}{T_0^2} + \frac{1}{2} \frac{W_\ell^{(4)}(T_0)}{W_\ell^{(2)}(T_0)} - \frac{1}{2} \left(\frac{W_\ell^{(3)}(T_0)}{W_\ell^{(2)}(T_0)} \right)^2 \\ &\quad - \frac{1}{2} \frac{d^2}{dT^2} \ln |\det(\mathbf{m}(T) - \mathbf{1})| \Big|_{T=T_0}. \end{aligned} \quad (36)$$

The derivatives of the action are already known from section 2.4.1. In the next step one has to find an expression for the derivatives of $\ln |\det(\mathbf{m}(T) - \mathbf{1})|$. Following again the method presented in [5] we can introduce a new matrix $\mathbf{N}(T)$ whose determinant is identical with $\det(\mathbf{m}(T) - \mathbf{1})$. It is given by

$$\mathbf{N}(T) = \mathbf{M}(T) - (\mathbf{1} - \mathcal{P}_\parallel(T) - \mathcal{P}_\perp(T)), \quad (37)$$

where

$$\mathcal{P}_\parallel(T) = \vec{e}_\parallel \otimes \vec{e}_\parallel = \frac{\vec{X}(0, T) \otimes \vec{X}(0, T)}{|\vec{X}(0, T)|^2} \quad (38)$$

and

$$\mathcal{P}_\perp(T) = \vec{e}_\perp \otimes \vec{e}_\perp = \frac{\boldsymbol{\Sigma} \vec{X}(0, T) \otimes \boldsymbol{\Sigma} \vec{X}(0, T)}{|\vec{X}(0, T)|^2} = -\boldsymbol{\Sigma} \mathcal{P}_\parallel(T) \boldsymbol{\Sigma} \quad (39)$$

are the projection operators parallel to the flow of the classical orbit and perpendicular to the energy shell, respectively. These relations lead to the expressions

$$\frac{d}{dT} \ln |\det(\mathbf{m}(T) - \mathbf{1})| \Big|_{T=T_0} = \text{Tr} \left(\mathbf{N}(T_0)^{-1} \frac{d\mathbf{N}(T)}{dT} \Big|_{T=T_0} \right), \quad (40)$$

$$\begin{aligned} \frac{d^2}{dT^2} \ln |\det(\mathbf{m}_\ell(T) - \mathbf{1})| \Big|_{T=T_0} &= \text{Tr} \left(\mathbf{N}(T_0)^{-1} \frac{d^2 \mathbf{N}(T)}{dT^2} \Big|_{T=T_0} \right. \\ &\quad \left. - \mathbf{N}(T_0)^{-1} \frac{d\mathbf{N}(T)}{dT} \Big|_{T=T_0} \mathbf{N}(T_0)^{-1} \frac{d\mathbf{N}(T)}{dT} \Big|_{T=T_0} \right), \end{aligned} \quad (41)$$

with

$$\frac{d\mathbf{N}(T)}{dT} = \frac{d\mathbf{M}(T, T)}{dT} + \frac{d\mathcal{P}_{\parallel}(T)}{dT} - \Sigma \frac{d\mathcal{P}_{\parallel}(T)}{dT} \Sigma, \quad (42)$$

$$\frac{d^2\mathbf{N}(T)}{dT^2} = \frac{d^2\mathbf{M}(T, T)}{dT^2} + \frac{d^2\mathcal{P}_{\parallel}(T)}{dT^2} - \Sigma \frac{d^2\mathcal{P}_{\parallel}(T)}{dT^2} \Sigma. \quad (43)$$

By using the derivatives $\vec{X}^{(n)}(t, T_0)$ and the definition of the projection operator $\mathcal{P}_{\parallel}(T)$, one obtains:

$$\begin{aligned} \frac{d\mathcal{P}_{\parallel}(T)}{dT} &= \frac{1}{|\vec{X}(0, T)|^2} \left(\vec{X}^{(1)}(0, T) \otimes \vec{X}(0, T) + \vec{X}(0, T) \otimes \vec{X}^{(1)}(0, T) \right) \\ &\quad - 2 \frac{\vec{X}(0, T) \cdot \vec{X}^{(1)}(0, T)}{|\vec{X}(0, T)|^2} \mathcal{P}_{\parallel}(T), \\ \frac{d^2\mathcal{P}_{\parallel}(T)}{dT^2} &= \frac{1}{|\vec{X}(0, T)|^2} \left(\vec{X}^{(2)}(0, T) \otimes \vec{X}(0, T) + \vec{X}(0, T) \otimes \vec{X}^{(2)}(0, T) \right. \\ &\quad + 2\vec{X}^{(1)}(0, T) \otimes \vec{X}^{(1)}(0, T) \left. + \left(8 \frac{(\vec{X}(0, T) \cdot \vec{X}^{(1)}(0, T))^2}{|\vec{X}(0, T)|^4} \right. \right. \\ &\quad \left. \left. - 2 \frac{\vec{X}(0, T) \cdot \vec{X}^{(2)}(0, T)}{|\vec{X}(0, T)|^2} - 2 \frac{\vec{X}^{(1)}(0, T) \cdot \vec{X}^{(1)}(0, T)}{|\vec{X}(0, T)|^2} \right) \mathcal{P}_{\parallel}(T) \right. \\ &\quad \left. - 4 \frac{\vec{X}(0, T) \cdot \vec{X}^{(1)}(0, T)}{|\vec{X}(0, T)|^2} (\vec{X}^{(1)}(0, T) \otimes \vec{X}(0, T) \right. \\ &\quad \left. + \vec{X}(0, T) \otimes \vec{X}^{(1)}(0, T) \right). \end{aligned}$$

The last pieces which are needed for calculating $C_{0\ell}(T)$ are the first and the second derivative of the monodromy matrix $\mathbf{M}(T, T)$ with respect to the period T :

$$\begin{aligned} \frac{d\mathbf{M}(T, T)}{dT} &= \frac{\partial \mathbf{M}(t = T, T)}{\partial t} \frac{dt}{dT} + \frac{\partial \mathbf{M}(t = T, T)}{\partial T} \\ &= \dot{\mathbf{M}}(T, T) + \mathbf{M}^{(1)}(T, T), \\ \frac{d^2\mathbf{M}(T, T)}{dT^2} &= \ddot{\mathbf{M}}(T, T) + 2\dot{\mathbf{M}}^{(1)}(T, T) + \mathbf{M}^{(2)}(T, T). \end{aligned} \quad (44)$$

Similar to the procedure which was used in section 2.4.1 to arrive at the equations of motion for the $\vec{X}^{(n)}(t, T_0)$, it is possible to obtain the differential equations governing the evolution of the derivatives $M^{(n)}(T, T)$ from differen-

tial equation (14) of the monodromy matrix. The equations read

$$\begin{aligned}
\dot{M}_{ij}^{(1)}(t, T) &= \Sigma_{ik} \left(H_{,klm}(\vec{X}(t, T)) M_{lj}(t, T) X_m^{(1)}(t, T) + H_{,kl}(\vec{X}(t, T)) M_{lj}^{(1)}(t, T) \right), \\
\dot{M}_{ij}^{(2)}(t, T) &= \Sigma_{ik} \left(H_{,klmn}(\vec{X}(t, T)) M_{lj}(t, T) X_m^{(1)}(t, T) X_n^{(1)}(t, T) \right. \\
&\quad + 2H_{,klm}(\vec{X}(t, T)) M_{lj}^{(1)}(t, T) X_m^{(1)}(t, T) \\
&\quad \left. + H_{,klm}(\vec{X}(t, T)) M_{lj}(t, T) X_m^{(2)}(t, T) + H_{,kl}(\vec{X}(t, T)) M_{lj}^{(2)}(t, T) \right),
\end{aligned} \tag{45}$$

with initial values

$$\mathbf{M}^{(n)}(t = 0, T) = \mathbf{0}. \tag{46}$$

Now we have obtained all results necessary for the calculation of the first-order \hbar corrections to Gutzwiller's trace formula without taking into account symmetries. In the next sections we will apply this theory to the diamagnetic hydrogen atom.

3 The hydrogen atom in a uniform magnetic field

The diamagnetic hydrogen atom was often used as an example for a quantum system whose classical dynamics is chaotic (see e.g. [8] or [9] for an overview). As a real physical system it was the topic of studies in experimental physics [10,11]. It has even been used for the numerical test of the \hbar correction terms C_1 and $C_1^{T \rightarrow E}$ [5,6]. 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.

The hydrogen atom in a uniform magnetic field has a continuous symmetry, namely the rotational invariance around the magnetic field axis. This symmetry can be used to formulate the dynamics in a two-dimensional coordinate system. This method works very well for the leading order but it leads to new difficulties for the first-order \hbar correction. This aspect is discussed in section 3.1 before we will look at the "two-dimensional hydrogen atom" with its discrete symmetries.

3.1 The rotational invariance and correction terms

Written in the cylindrical coordinates $\varrho = \sqrt{x^2 + y^2}$, φ and z and atomic units, the classical Hamiltonian of the hydrogen atom in a uniform magnetic

field in z -direction has the form:

$$H = \frac{p_\rho^2}{2} + \frac{p_z^2}{2} + \frac{l_z^2}{2\rho^2} - \frac{1}{r} + \frac{1}{8}\gamma^2\rho^2, \quad (47)$$

where

$$r = \sqrt{\rho^2 + z^2}, \quad (48)$$

$$\gamma = \frac{B}{B_0}, \quad B_0 \approx 2.35 \cdot 10^5 \text{ T}. \quad (49)$$

In this expression l_z is the z component of the angular momentum, which is a constant of motion. The paramagnetic term is not considered in equation (47) because it is constant. If one exploits the classical scaling property

$$\vec{r} = \gamma^{2/3}\vec{r}, \quad \vec{p} = \gamma^{-1/3}\vec{p}, \quad \tilde{t} = \gamma t, \quad (50)$$

the scaled Hamiltonian

$$\gamma^{-2/3}H = \tilde{H} = \frac{\tilde{p}_\rho^2}{2} + \frac{\tilde{p}_z^2}{2} + \frac{\tilde{l}_z^2}{2\tilde{\rho}^2} - \frac{1}{\tilde{r}} + \frac{1}{8}\tilde{\rho}^2 \quad (51)$$

only depends on the scaled energy $\epsilon = \gamma^{-2/3}E$, but not on the energy E or the magnetic field strength γ separately. The regularization of the Coulomb singularity can be achieved by introducing semiparabolic coordinates [8]

$$\mu = \sqrt{\tilde{r} + \tilde{z}}, \quad \nu = \sqrt{\tilde{r} - \tilde{z}} \quad (52)$$

and the scaled time τ

$$d\tilde{t} = 2\tilde{r} d\tau = (\mu^2 + \nu^2) d\tau. \quad (53)$$

This transformation leads to the new Hamiltonian

$$\mathcal{H} = \frac{1}{2}p_\mu^2 + \frac{1}{2}p_\nu^2 + \frac{l_z^2}{2} \left(\frac{1}{\mu^2} + \frac{1}{\nu^2} \right) - \epsilon (\mu^2 + \nu^2) + \frac{1}{8}\mu^2\nu^2 (\mu^2 + \nu^2) = 2, \quad (54)$$

where the momenta are defined by

$$p_\mu = \frac{d\mu}{d\tau}, \quad p_\nu = \frac{d\nu}{d\tau}. \quad (55)$$

The scaled time τ is the parameter for the integration of the differential equations of the classical values. In the case $l_z = 0$, the μ and ν coordinates, which are only defined as positive coordinates in equation (52), can be extended to negative values. Then, p_μ and p_ν have the same structure as the momenta of Cartesian coordinates. This structure of the momenta is very important because it is often used in the derivation of the \hbar corrections (see e.g. equation (15) for the monodromy matrix). However, it cannot be found in the quantum

mechanical analogue of equation (54). Starting again with the Hamiltonian in cylindrical coordinates

$$H = \frac{1}{2} \left(-\frac{1}{\varrho} \frac{\partial}{\partial \varrho} \varrho \frac{\partial}{\partial \varrho} - \frac{\partial^2}{\partial z^2} + \frac{m^2}{\varrho^2} \right) - \frac{1}{r} + \frac{1}{8} \gamma^2 \varrho^2 \quad (56)$$

and using the transformations (50) and (52), one arrives at the Schrödinger equation for the (μ, ν) -part of the wave function:

$$\left\{ -\frac{\gamma^{2/3}}{2} \left(\frac{1}{\mu} \frac{\partial}{\partial \mu} \mu \frac{\partial}{\partial \mu} + \frac{1}{\nu} \frac{\partial}{\partial \nu} \nu \frac{\partial}{\partial \nu} - \frac{m^2}{\mu^2} - \frac{m^2}{\nu^2} \right) - \epsilon(\mu^2 + \nu^2) + \frac{1}{8} \mu^2 \nu^2 (\mu^2 + \nu^2) \right\} \psi(\mu, \nu) = 2\psi(\mu, \nu). \quad (57)$$

In this quantum mechanical expression, the momentum operators for μ and ν differ from those in Cartesian coordinates even for $m = 0$, which is the quantum analogue of $l_z = 0$. As was mentioned above, this difference does not have any effect on the leading order of the semiclassical level density. The results of the classical calculations agree very well with values which were extracted from quantum calculations. But there is no agreement at all between the classically evaluated correction terms C_1 and $C_1^{T \rightarrow E}$ and quantum mechanical calculations. This behaviour can be understood, when one introduces the new wave function

$$\psi(\mu, \nu) = \frac{u(\mu, \nu)}{\sqrt{\mu\nu}}, \quad (58)$$

which leads to the following Schrödinger equation:

$$\left\{ -\frac{\gamma^{2/3}}{2} \left(\frac{\partial^2}{\partial \mu^2} + \frac{\partial^2}{\partial \nu^2} \right) + \gamma^{2/3} \frac{m^2 - \frac{1}{4}}{2} \left(\frac{1}{\mu^2} + \frac{1}{\nu^2} \right) - \epsilon(\mu^2 + \nu^2) + \frac{1}{8} \mu^2 \nu^2 (\mu^2 + \nu^2) \right\} u(\mu, \nu) = 2u(\mu, \nu). \quad (59)$$

Now, the momentum operators agree with the structure in the classical case but an additional term $-\frac{1}{8} \gamma^{2/3} (1/\mu^2 + 1/\nu^2)$ appears, which leads to a non-vanishing centrifugal part of the potential even for $m = 0$. The additional term has also to be inserted in the classical Hamiltonian:

$$\mathcal{H} = \frac{1}{2} p_\mu^2 + \frac{1}{2} p_\nu^2 + \frac{l_z^2 - \frac{\gamma^{2/3}}{4}}{2} \left(\frac{1}{\mu^2} + \frac{1}{\nu^2} \right) - \epsilon(\mu^2 + \nu^2) + \frac{1}{8} \mu^2 \nu^2 (\mu^2 + \nu^2) = 2. \quad (60)$$

Since the new centrifugal part is proportional to \hbar^2 , which was set to one when atomic units were introduced, it contributes to the first-order \hbar correction in the expansion of the level density as one can easily see when one repeats the calculations from section 2. That is the reason why the influence of the continuous symmetry does not appear in the leading order but in the first-order corrections.

The centrifugal term consists of an integral over the classical periodic orbit with the kernel $1/\mu^2 + 1/\nu^2$, which diverges at the coordinate axes. This problem does not arise if one regards the hydrogen atom as a purely two-dimensional system because in this case there is no centrifugal term. The momenta have the structure of the momenta of Cartesian coordinates in the classical dynamics as well as in the quantum case. Therefore, in the following sections we only look at this *two-dimensional hydrogen atom* for the calculation of the first-order \hbar corrections, as it was done in [5] before.

3.2 Classical dynamics and Schrödinger equation of the two-dimensional hydrogen atom

The two-dimensional diamagnetic hydrogen atom can be formulated similar to the three-dimensional one. For a magnetic field $\vec{B} = B\vec{e}_x$, the classical Hamiltonian is given by:

$$H = \frac{p_x^2}{2} + \frac{p_y^2}{2} - \frac{1}{\varrho} + \frac{1}{8}\gamma^2 y^2. \quad (61)$$

If one uses the classical scaling property (50) and semiparabolic coordinates for the two-dimensional case [12]

$$\mu = \sqrt{\tilde{\varrho} + \tilde{x}}, \quad \nu = \sqrt{\tilde{\varrho} - \tilde{x}}, \quad (62)$$

the transformed Hamiltonian reads:

$$\mathcal{H} = \frac{1}{2}p_\mu^2 + \frac{1}{2}p_\nu^2 - \epsilon(\mu^2 + \nu^2) + \frac{1}{8}\mu^2\nu^2(\mu^2 + \nu^2) = 2. \quad (63)$$

The Schrödinger equation associated with the classical Hamiltonian (63) can be obtained by the same procedure as in the three-dimensional case. The result is:

$$\begin{aligned} & \left\{ 2 + \epsilon(\mu^2 + \nu^2) - \frac{1}{8}\mu^2\nu^2(\mu^2 + \nu^2) \right\} \psi(\mu, \nu) \\ & = \gamma^{2/3} \left\{ -\frac{1}{2} \left(\frac{\partial^2}{\partial \mu^2} + \frac{\partial^2}{\partial \nu^2} \right) \right\} \psi(\mu, \nu). \end{aligned} \quad (64)$$

In this case, the momentum operators have exactly the same structure as for Cartesian coordinates. Note that $\gamma^{1/3}$ takes the place of \hbar , which is equal to one in atomic units and which is often called “effective \hbar ”.

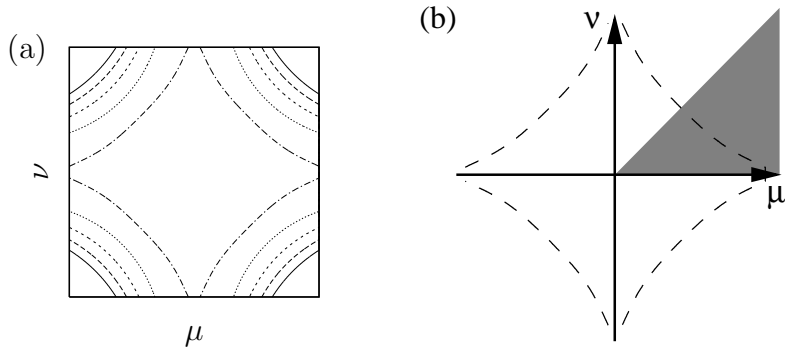


Fig. 1. Equipotential contours of the potential (65) for different scaled energies ϵ are plotted in figure (a). The shadowed area in the coordinate system of figure (b) marks the fundamental domain.

3.3 The symmetry of the potential

The “potential” of the two-dimensional diamagnetic hydrogen atom in semiparabolic coordinates (see equation (63))

$$V(\mu, \nu) = -\epsilon (\mu^2 + \nu^2) + \frac{1}{8} \mu^2 \nu^2 (\mu^2 + \nu^2) \quad (65)$$

has a C_{4v} -symmetry. This symmetry can be seen in figure 1 (a), in which a few equipotential contours of the potential (65) are plotted. For the leading order (Gutzwiller’s trace formula), it is known, how the symmetry of the system can be exploited in the calculation of the classical values. In section 4 we look at the influence of the discrete C_{4v} -symmetry on classical values which contribute to the first-order \hbar correction terms C_1 and $C_1^{T \rightarrow E}$.

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. If during the integration along an orbit one arrives at one of the borders of the fundamental domain, one reflects the orbit at the border. This is possible because the borders of the fundamental domain are reflection planes of the potential.

In addition, the symmetry of the potential allows of a compact labelling of the unstable classical periodic orbits. In the symmetry reduced fundamental domain, the orbits are described by a ternary code, which was introduced by Eckhardt and Wintgen [14]. It uses the symbols “0”, “+” and “-” and has its origin in the description of the orbits of the four disk scattering system, which has the same symmetry as the diamagnetic hydrogen atom in semiparabolic coordinates.

The restriction to the fundamental domain and the introduction of symmetry operations lead to new periodic orbits, which are only periodic if 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 ($c_4, c_4^2 = c_2, c_4^3$), reflections at the coordinate axes (σ_v), and reflections at the angle bisectors (σ_d). Then one can obtain the same new periodic orbits as described above. 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.

Figure 2 (c) shows the orbit which corresponds to the double repetition of the orbit $+$ in the fundamental domain and figure 2 (d) shows the orbit which consists of four times the same repetition in the fundamental domain and which is periodic in the plane of semiparabolic coordinates.

3.4 *Symmetry properties of the wave functions and calculation of the quantum spectra*

Because of the C_{4v} -symmetry of the Hamiltonian (64), 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 (64) 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 [15,5]. 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

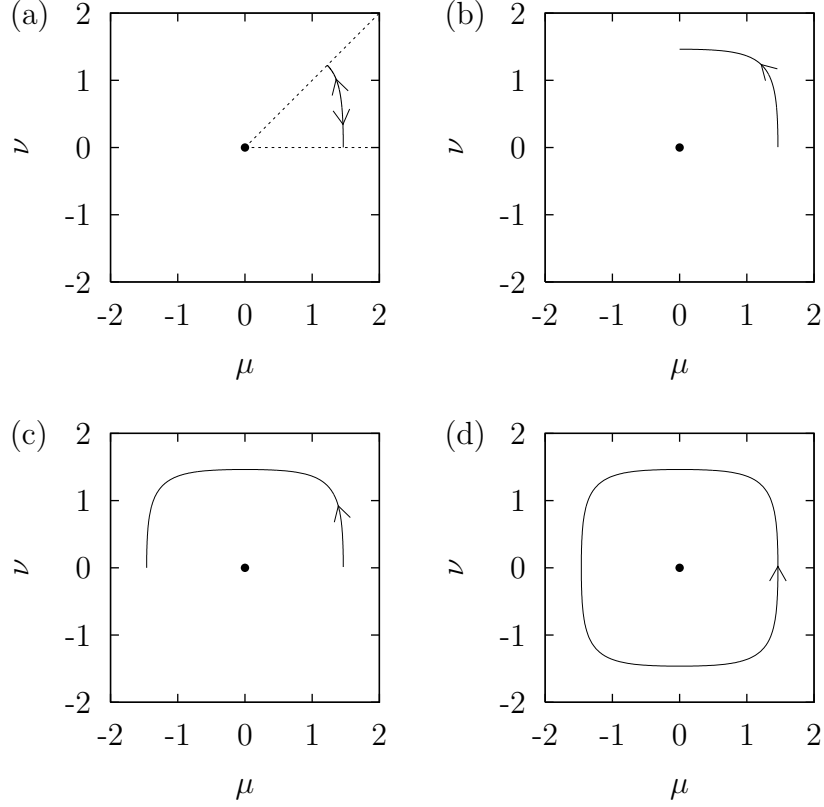


Fig. 2. The periodic orbit + in semiparabolic coordinates for a scaled energy of $\epsilon = -0.1$. The dot marks the nucleus at the origin. The orbits shown correspond to the single (see figures (a) and (b)), the double (c) and the quadruple (d) repetition in the fundamental domain.

of the influence of the symmetry.

Up to a maximum $\gamma^{-1/3}$ (the eigenvalues are needed in this form) of about 156 one obtains circa 12,000 eigenvalues in each of the one-dimensional subspaces A_1 , A_2 , B_1 , and B_2 . In the subspace which belongs to the two-dimensional representation E one finds roughly 19,000 eigenvalues up to a maximum $\gamma^{-1/3}$ of about 140.

3.5 Analysis of the quantum spectrum by harmonic inversion

If one looks at the semiclassical level density

$$g_{\text{osc}}(E) = \sum_{\ell} \frac{1}{\pi \hbar} \frac{T_{0p}}{\sqrt{|\det(\mathbf{m}_{\ell}(T_0) - \mathbf{1})|}} \left\{ \cos \left(\frac{1}{\hbar} S_{\ell}^{(\text{cl})}(T_0) - \frac{\pi}{2} \mu_{\ell} \right) - \hbar C_{\hbar \ell} \sin \left(\frac{1}{\hbar} S_{\ell}^{(\text{cl})}(T_0) - \frac{\pi}{2} \mu_{\ell} \right) + O(\hbar^2) \right\}, \quad (66)$$

which one obtains from the semiclassical approximation of the quantum Green's function (22) via the relation

$$-\frac{1}{\pi} \text{Im} (\text{Tr } G(E)) = g(E) = \sum_n \delta(E - E_n), \quad (67)$$

one recognizes that it should be possible to extract the amplitude of the leading order (Gutzwiller's trace formula),

$$A_\ell = \frac{T_{0p}}{|\det(\mathbf{m}_\ell(T_0) - \mathbf{1})|}, \quad (68)$$

and the reduced action $S_\ell^{(\text{cl})}$ from a Fourier transformation of the quantum level density. A higher precision in both the amplitude and the action can be achieved with the harmonic inversion method (see e.g. [9]), where the solution of the nonlinear set of equations

$$g_{\text{osc}}(w_n) = \sum_\ell \bar{A}_\ell e^{i w_n \bar{S}_\ell} \quad (69)$$

yields the parameters \bar{A}_ℓ and \bar{S}_ℓ . The w_n are chosen on an equidistant grid. For a spectrum which consists of δ -functions such as that in equation (67), one has to modify it in order to obtain non-vanishing contributions on the grid, e.g., by a convolution of the δ -functions with a Gaussian or by applying a filter to the signal. We used the latter method, which is described in [16]. Using the harmonic inversion method makes it possible to gain the classical values from an analysis of the quantum eigenvalues and to compare these results with those from classical calculations.

The harmonic inversion method can also be applied to extract higher-order \hbar corrections

$$C_{\hbar\ell} = C_{1\ell} + C_{1\ell}^{T \rightarrow E} \quad (70)$$

for individual orbits in the following way [5]. The quantum level density formulated in semiparabolic coordinates depends on the variable $w \equiv \gamma^{-1/3}$:

$$\delta(\mathcal{H} - 2) = \sum_n \frac{w_n}{2} \frac{1}{\left| \langle \psi_n(\mu, \nu) \left| -\frac{1}{2w_n^2} \left(\frac{\partial^2}{\partial \mu^2} + \frac{\partial^2}{\partial \nu^2} \right) \right| \psi_n(\mu, \nu) \rangle \right|} \delta(w - w_n), \quad (71)$$

where \mathcal{H} is the quantum Hamiltonian which belongs to the classical Hamiltonian (63). Using the classical scaling property (63) of the system, the semiclassical approximation of the quantum Green's function and the relation (67)

lead to the level density

$$g_{\text{osc}}(E) = \sum_{\ell} \frac{w}{\pi} \frac{T_{0\text{p}}}{\sqrt{|\det(\mathbf{m}_{\ell}(T_0) - \mathbf{1})|}} \left\{ \cos\left(wS_{\ell}^{(\text{cl})}(T_0) - \frac{\pi}{2}\mu_{\ell}\right) - \frac{1}{w}C_{\hbar\ell} \sin\left(wS_{\ell}^{(\text{cl})}(T_0) - \frac{\pi}{2}\mu_{\ell}\right) + \mathcal{O}\left(\left(\frac{1}{w}\right)^2\right) \right\}. \quad (72)$$

Combining the formulas for the quantum level density (71) and for its semi-classical approximation (72) shows that the harmonic inversion of

$$g(w) = \sum_n \frac{\pi}{2} \frac{1}{\left| \left\langle \psi_n(\mu, \nu) \left| -\frac{1}{2w_n^2} \left(\frac{\partial^2}{\partial \mu^2} + \frac{\partial^2}{\partial \nu^2} \right) \right| \psi_n(\mu, \nu) \right\rangle \right|} \delta(w - w_n) \quad (73)$$

leads to an expansion of the form (69), where

$$\bar{A}_{\ell} = \frac{1}{2}A_{\ell} \exp\left[-\frac{i\pi}{2}\mu_{\ell}\right], \quad \bar{S}_{\ell} = S_{\ell}^{(\text{cl})}(T_0) \quad (74)$$

with A_{ℓ} from equation (68). This method can provide access to the first-order \hbar correction, if one subtracts the leading order and multiplies the result by w . The final expression is

$$\sum_n -\frac{\pi w_n}{2} \frac{1}{\left| \left\langle \psi_n(\mu, \nu) \left| -\frac{1}{2w_n^2} \left(\frac{\partial^2}{\partial \mu^2} + \frac{\partial^2}{\partial \nu^2} \right) \right| \psi_n(\mu, \nu) \right\rangle \right|} \delta(w - w_n) + w \sum_{\ell} \frac{T_{0\text{p}}}{\sqrt{|\det(\mathbf{m}_{\ell}(T_0) - \mathbf{1})|}} \cos\left(wS_{\ell}^{(\text{cl})}(T_0) - \frac{\pi}{2}\mu_{\ell}\right), \quad (75)$$

and the harmonic inversion leads to the amplitude

$$\bar{A}_{\ell} = \frac{1}{2i} A_{\ell} \exp\left[-\frac{i\pi}{2}\mu_{\ell}\right] C_{\hbar\ell}, \quad (76)$$

from which one can easily extract the first-order \hbar correction $C_{\hbar\ell}$ because all other values are known.

4 Influence of discrete symmetries on the correction terms

In this section we investigate the influence of the discrete C_{4v} -symmetry on the correction terms C_1 and $C_1^{T \rightarrow E}$. The \hbar corrections are computed for some orbits which are not periodic without a symmetry transformation from C_{4v} .

4.1 Symmetry transformations in the calculations of the correction terms

The classical quantities 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. For example the linearized equation of motion (14) has to be solved in order to obtain the monodromy matrix. In addition, the derivatives of the coordinates of the orbit and of the monodromy matrix with respect to the period are required. Thus we face the question of how the symmetry has to be implemented into the correction terms. What are the correct transformations for the additional coordinates? What is the transformation of the boundary conditions of the classical Green’s function?

4.1.1 Correction term C_1

The solution of the linearized equation of motion (14) for the monodromy matrix is essential for the calculation of the classical Green’s function by using the formulation (13) and by solving equation (19). The monodromy matrix is one of the classical values which contribute to Gutzwiller’s trace formula, and its symmetry behaviour has often been used. However, we look at the transformations of its elements because it is an example for all other variables which are necessary for the first-order \hbar corrections. All further elements follow the same scheme.

The monodromy matrix can be obtained by solving equation (14) for four linear independent column vectors

$$\vec{X}_M = \begin{pmatrix} \mu_M \\ \nu_M \\ p_{\mu M} \\ p_{\nu M} \end{pmatrix}$$

with initial values which match the condition $M(0) = \mathbf{1}$. In our system, the monodromy matrix has the dimensions 4×4 and the linearized equations of

motion in semiparabolic coordinates are:

$$\begin{aligned}
\dot{\mu}_{\mathbf{M}} &= p_{\mu\mathbf{M}}, \\
\dot{\nu}_{\mathbf{M}} &= p_{\nu\mathbf{M}}, \\
\dot{p}_{\mu\mathbf{M}} &= \left(2\epsilon - \frac{3}{2}\mu^2\nu^2 - \frac{1}{4}\nu^4\right)\mu_{\mathbf{M}} - (\mu^3\nu + \mu\nu^3)\nu_{\mathbf{M}}, \\
\dot{p}_{\nu\mathbf{M}} &= \left(2\epsilon - \frac{3}{2}\mu^2\nu^2 - \frac{1}{4}\mu^4\right)\nu_{\mathbf{M}} - (\mu^3\nu + \mu\nu^3)\mu_{\mathbf{M}}.
\end{aligned} \tag{77}$$

As an example, we look at the anticlockwise rotation by an angle of 90 degrees. In this case the symmetry transformation for the coordinates and momenta of the orbit leads to

$$\begin{aligned}
\dot{\mu}_{\mathbf{M}} &= p_{\mu\mathbf{M}}, \\
\dot{\nu}_{\mathbf{M}} &= p_{\nu\mathbf{M}}, \\
\dot{p}_{\mu\mathbf{M}} &= \left(2\epsilon - \frac{3}{2}\bar{\nu}^2\bar{\mu}^2 - \frac{1}{4}\bar{\mu}^4\right)\mu_{\mathbf{M}} + (\bar{\nu}^3\bar{\mu} + \bar{\nu}\bar{\mu}^3)\nu_{\mathbf{M}}, \\
\dot{p}_{\nu\mathbf{M}} &= \left(2\epsilon - \frac{3}{2}\bar{\nu}^2\bar{\mu}^2 - \frac{1}{4}\bar{\nu}^4\right)\nu_{\mathbf{M}} + (\bar{\nu}^3\bar{\mu} + \bar{\nu}\bar{\mu}^3)\mu_{\mathbf{M}},
\end{aligned} \tag{78}$$

where $\bar{\mu}$ and $\bar{\nu}$ are the new variables in the rotated system. Because of the symmetry invariance of the Hamiltonian, one has to find a transformation in such a way that

$$\begin{aligned}
\dot{\bar{\mu}}_{\mathbf{M}} &= \bar{p}_{\mu\mathbf{M}}, \\
\dot{\bar{\nu}}_{\mathbf{M}} &= \bar{p}_{\nu\mathbf{M}}, \\
\dot{\bar{p}}_{\mu\mathbf{M}} &= \left(2\epsilon - \frac{3}{2}\bar{\mu}^2\bar{\nu}^2 - \frac{1}{4}\bar{\nu}^4\right)\bar{\mu}_{\mathbf{M}} - (\bar{\mu}^3\bar{\nu} + \bar{\mu}\bar{\nu}^3)\bar{\nu}_{\mathbf{M}}, \\
\dot{\bar{p}}_{\nu\mathbf{M}} &= \left(2\epsilon - \frac{3}{2}\bar{\mu}^2\bar{\nu}^2 - \frac{1}{4}\bar{\mu}^4\right)\bar{\nu}_{\mathbf{M}} - (\bar{\mu}^3\bar{\nu} + \bar{\mu}\bar{\nu}^3)\bar{\mu}_{\mathbf{M}}.
\end{aligned} \tag{79}$$

In our example this condition leads to the results:

$$\bar{\mu}_{\mathbf{M}} = -\nu_{\mathbf{M}}, \quad \bar{\nu}_{\mathbf{M}} = \mu_{\mathbf{M}}, \quad \bar{p}_{\mu\mathbf{M}} = -p_{\nu\mathbf{M}}, \quad \bar{p}_{\nu\mathbf{M}} = p_{\mu\mathbf{M}}. \tag{80}$$

The condition is always fulfilled if one uses for the elements of $\vec{X}_{\mathbf{M}}$ the same transformations as for the corresponding phase space coordinates of the orbit.

Since the matrices \vec{A}_- and \vec{B}_- can directly be determined from equation (20), there is no need for further symmetry operations in order to obtain the right values for these two matrices if the monodromy matrix was calculated with all symmetry transformations. The same is true for the matrices \vec{A}_+ and \vec{B}_+ , which follow from equation (17), and for the classical Green's function, which follows from (13). This is evident if one recalls the calculations from section 2.2. Furthermore, if one applies the correct symmetry transformation 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.

4.1.2 Correction term $C_1^{T \rightarrow E}$

In addition to the coordinates considered until now, one has to obtain the values of the derivatives $\vec{X}^{(n)}$ and $\mathbf{M}^{(n)}$ for the second correction term $C_1^{T \rightarrow E}$.

The equations of motion of the components of $\vec{X}^{(1)}$

$$\dot{X}_i^{(1)}(t, T_0) = \Sigma_{ij} H_{,jk}(\vec{X}(t, T_0)) X_k^{(1)}(t, T_0) \quad (81)$$

have exactly the same structure as the differential equations for the monodromy matrix, i.e., we already know the symmetry operations which have to be implemented here.

Looking at the differential equations of $\vec{X}^{(2)}$ and $\vec{X}^{(3)}$, namely

$$\begin{aligned} \dot{X}_i^{(2)}(t, T_0) &= \Sigma_{ij} H_{,jkl}(\vec{X}(t, T_0)) X_k^{(1)}(t, T_0) X_l^{(1)}(t, T_0) \\ &\quad + \Sigma_{ij} H_{,jk}(\vec{X}(t, T_0)) X_k^{(2)}(t, T_0), \\ \dot{X}_i^{(3)}(t, T_0) &= \Sigma_{ij} H_{,jklm}(\vec{X}(t, T_0)) X_k^{(1)}(t, T_0) X_l^{(1)}(t, T_0) X_m^{(1)}(t, T_0) \\ &\quad + 3\Sigma_{ij} H_{,jkl}(\vec{X}(t, T_0)) X_k^{(1)}(t, T_0) X_l^{(2)}(t, T_0) \\ &\quad + \Sigma_{ij} H_{,jk}(\vec{X}(t, T_0)) X_k^{(3)}(t, T_0), \end{aligned} \quad (82)$$

one recognizes that the terms which contain the $X_k^{(2)}$ and the $X_k^{(3)}$, respectively, have the same form as the equation of motion of the monodromy matrix. Therefore, we have to use the same transformation.

The differential equations of the elements of $\mathbf{M}^{(1)}$ and $\mathbf{M}^{(2)}$,

$$\begin{aligned} \dot{M}_{ij}^{(1)}(t, T) &= \Sigma_{ik} \left(H_{,klm}(\vec{X}(t, T)) M_{lj}(t, T) X_m^{(1)}(t, T) + H_{,kl}(\vec{X}(t, T)) M_{lj}^{(1)}(t, T) \right), \\ \dot{M}_{ij}^{(2)}(t, T) &= \Sigma_{ik} \left(H_{,klmn}(\vec{X}(t, T)) M_{lj}(t, T) X_m^{(1)}(t, T) X_n^{(1)}(t, T) \right. \\ &\quad + 2H_{,klm}(\vec{X}(t, T)) M_{lj}^{(1)}(t, T) X_m^{(1)}(t, T) + H_{,klm}(\vec{X}(t, T)) \\ &\quad \left. \times M_{lj}(t, T) X_m^{(2)}(t, T) + H_{,kl}(\vec{X}(t, T)) M_{lj}^{(2)}(t, T) \right) \end{aligned} \quad (83)$$

are derived in the same way as those for, e.g., the $X_k^{(2)}$ by differentiating Hamilton's equations of motion, and have the same structure. One can easily see that the elements of the derivatives $\mathbf{M}^{(1)}$ and $\mathbf{M}^{(2)}$ obey the same symmetry transformation as the elements of the monodromy matrix.

We can summarize the results of this section as follows: Under symmetry operations all variables which contribute to the first-order \hbar correction transform in the same way as the corresponding phase space coordinates of the orbit. Whenever a symmetry transformation of the phase space coordinates of the orbit is necessary during the integration of a set of differential equations in order to obtain a periodic orbit, one has to transform the variables which were discussed in this section simultaneously.

4.2 An example for a symmetry reduced orbit

As an example for an orbit which is periodic only when a symmetry transformation is applied, we look at the orbit $+$, which has been introduced in section 3.3 and is shown in figures 2 (a) and (b) in the fundamental domain and in the full (μ, ν) -plane, respectively.

As a first test for the correct implementation of the symmetry in the correction term C_1 , the classical Green's function $\mathcal{G}(\tau, \tau')$ is considered. 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 (figure 2 (a)) is shown in figure 3 (a). The Green's function, which in our case is a 2×2 matrix, 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 figure 3 (b). One recognizes the discontinuities at the positions of the reflection which appear due to the change in the meaning of the components according to the change of the variables by using the symmetry transformation. All boundary conditions, which were mentioned in the sections 2.1 and 2.2, are fulfilled. At the final point of the orbit, all components have the same values as at the initial point. The condition $\mathcal{G}_{1j}(0, \tau') = \mathcal{G}_{1j}(T_0, \tau')$, which is expected from equation (10), is also fulfilled. The discontinuities in the elements $\dot{\mathcal{G}}_{2j}$, which appear due to equation (16), are clearly visible.

Figure 3 (c) 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 (see figure 3 (d)). Therefore, the only discontinuity appears at the end 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.

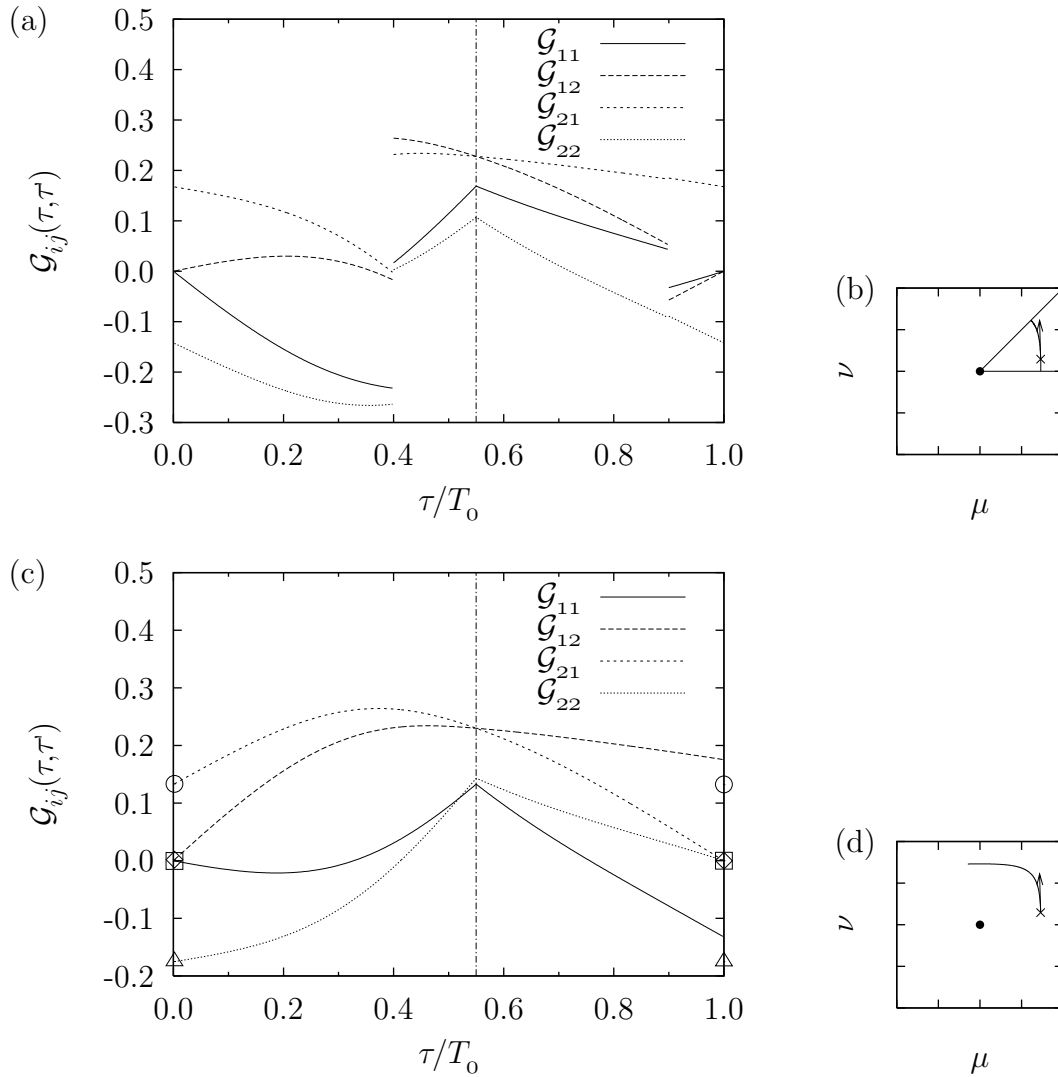


Fig. 3. The classical Green's function of the orbit + is shown in two cases for $\tau' = 0.55 \cdot T_0$. The upper two pictures (a) and (b) represent the orbit in the fundamental domain, whereas, the two lower ones (c) and (d) stand for the same orbit in the full plane of semiparabolic coordinates, which becomes periodic by the application of a rotation of the final point. In both cases 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 in figures (b) and (d). In the fundamental domain (figure (a)), where two reflections are required, one can clearly see the discontinuities in the elements of the Green's function at the two positions at which the orbit is reflected. The discontinuities correspond to the change of the meaning of the components. In figure (b) only the last point is affected by the symmetry operation (clockwise rotation by 90 degrees). This effect has been visualized by marking the last point of each component with the same symbol as the first point of the same component. The last point was plotted after the rotation has been carried out. In both cases the boundary conditions are fulfilled.

Table 1

Character table of the symmetry group C_{4v}

representation	e	c_4, c_4^3	$c_4^2 = c_2$	$2\sigma_v$	$2\sigma_d$
A_1	1	1	1	1	1
A_2	1	1	1	-1	-1
B_1	1	-1	1	1	-1
B_2	1	-1	1	-1	1
E	2	0	-2	0	0

4.3 Influence of the symmetry behaviour of the quantum wave functions and comparison of semiclassical and quantum results for the correction terms

In the different subspaces, which belong to a representation of the symmetry group, the individual amplitudes A_ℓ of the orbits can be found with a prefactor, which is given by the character χ (see table 1) of the element from C_{4v} which provides the periodic continuation of the orbit in the representation of the corresponding subspace. The cause of the prefactor is the projection [13] of the level density on the subspace belonging to the representation α of the group G (in our case $G = C_{4v}$) with the projection operator

$$P_\alpha = \frac{d_\alpha}{|G|} \sum_{X \in G} \chi_\alpha(X) D_\alpha(X). \quad (84)$$

Here, $|G|$ stands for the order of the group ($|C_{4v}| = 8$) and d_α for the dimension of the representation D_α . The element $D_\alpha(X)$ operates on the final point of the orbit with the matrix representation $\mathbf{M}(X^{-1})$. Only if the symmetry element X^{-1} leads to a periodic continuation of the orbit, it will contribute to the level density. For the weight of the orbit, one has to take into account that the fundamental domain appears eight times in the complete coordinate plane and that always eight “identical” orbits appear in the full (μ, ν) -plane.

As a consequence of the symmetry (eq. (84)), the orbit $+$, which requires the rotation c_4^3 in order to become periodic, should appear in the subspaces A_1 and A_2 with the prefactor $p_\alpha = 1$, in B_1 and B_2 with $p_\alpha = -1$, and in the subspace belonging to the representation E it should not appear at all. Table 2 shows the results of the harmonic inversion of the level density which consists only of the eigenvalues of one of the one-dimensional subspaces. The quantum values are compared with classical calculations. The action is independent of the subspace, and its classical value is $S_\ell^{(cl)} = 0.67746283$. The quantum amplitudes $A_\ell^{(qm)}$ include information from the Maslov index μ_ℓ (see equation (74)). Therefore, they have complex values, and the modulus and phase are

Table 2

The actions $S_\ell^{(\text{qm})}$ and the amplitudes $A_\ell^{(\text{qm})}$ of the orbit $+$ which were extracted from the quantum spectrum are compared with their classical counterparts. The classical value of the action is $S_\ell^{(\text{cl})} = 0.67746283$, independently of the subspace. Because of the projection to the individual subspaces the modulus of the quantum mechanical amplitudes corresponds to $|A_\ell^{(\text{qm})}| = |p_\alpha|A_\ell \equiv |A_\ell^{(\text{cl})}|$ and the phase is given by $\arg(A_\ell^{(\text{qm})}) = -\frac{\pi}{2}\mu_\ell + \arg(p_\alpha) \equiv \arg(A_\ell^{(\text{cl})})$. Since the quantum mechanical phases are only determined modulo 2π , all arguments are shifted into the standard interval $(-\pi, \pi]$. The orbit $+$ has a vanishing amplitude in subspace E .

subspace	$S_\ell^{(\text{qm})}$	$ A_\ell^{(\text{qm})} $	$ A_\ell^{(\text{cl})} $	$\arg(A_\ell^{(\text{qm})})$	$\arg(A_\ell^{(\text{cl})})$
A_1	0.67746323	0.685264	0.68523409	$-0.5003 \cdot \pi$	$-\pi/2$
A_2	0.67746335	0.685487	0.68523409	$-0.5003 \cdot \pi$	$-\pi/2$
B_1	0.67746326	0.685174	0.68523409	$0.4997 \cdot \pi$	$\pi/2$
B_2	0.67746325	0.685091	0.68523409	$0.4997 \cdot \pi$	$\pi/2$

Table 3

Amplitude of the orbit $++$ in different subspaces. See table 2 for an explanation.

subspace	$S_\ell^{(\text{qm})}$	$ A_\ell^{(\text{qm})} $	$ A_\ell^{(\text{cl})} $	$\arg(A_\ell^{(\text{qm})})$	$\arg(A_\ell^{(\text{cl})})$
A_1	1.35492668	0.64643	0.64647361	$0.9991 \cdot \pi$	π
A_2	1.35492857	0.64638	0.64647361	$0.9985 \cdot \pi$	π
B_1	1.35492697	0.64652	0.64647361	$0.9990 \cdot \pi$	π
B_2	1.35492700	0.64639	0.64647361	$0.9990 \cdot \pi$	π
E	1.35492730	2.58530	2.58589444	$-0.0012 \cdot \pi$	0

given by

$$\begin{aligned} |A_\ell^{(\text{qm})}| &= |p_\alpha| A_\ell \equiv |A_\ell^{(\text{cl})}|, \\ \arg(A_\ell^{(\text{qm})}) &= -\frac{\pi}{2}\mu_\ell + \arg(p_\alpha) \equiv \arg(A_\ell^{(\text{cl})}), \end{aligned}$$

where p_α is the prefactor which appears due to the projection operator P_α . In table 2 all amplitudes and phases have the expected values. The agreement is very good. All arguments are shifted into the standard interval $(-\pi, \pi]$.

Table 3 shows the same comparison for two repetitions (counted in the fundamental domain) of the orbit $+$, which are labelled with the symbol $++$. While the orbit $+$ vanishes in subspace E , the orbit $++$ can be found in this subspace with the expected amplitude prefactor $p_\alpha = -4$.

It is important to use the amplitude with the correct prefactor in equation (75) for the extraction of the sum $C_{\hbar\ell}$ of the two first-order correction terms.

Table 4

Correction term $C_{\hbar\ell}$ of the orbit + in different subspaces. The modulus $|C_{\hbar\ell}^{(\text{qm})}|$ and phase $\arg(C_{\hbar\ell}^{(\text{qm})})$ of the analysis of the quantum spectra are compared with the classically calculated value $C_{\hbar\ell}^{(\text{cl})}$.

subspace	$C_{\hbar\ell}^{(\text{cl})}$	$ 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	-0.09443001	0.09455	$1.0006 \cdot \pi$	0.0013
A_2	-0.09443001	0.09396	$0.9999 \cdot \pi$	-0.0050
B_1	-0.09443001	0.09456	$1.0006 \cdot \pi$	0.0013
B_2	-0.09443001	0.09452	$1.0003 \cdot \pi$	0.0010

If this condition is taken into account, one obtains the correction terms in every subspace in which the orbit appears. Table 4 shows the results for the orbit + in all one-dimensional subspaces of C_{4v} , which are compared with the classically calculated value.

In tables 5 and 6, the semiclassical results for the correction terms are compared with values which were 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. In this subspace all orbits contribute with a prefactor of 1 independently of the symmetry element which is required to find the periodic continuation. Quantum mechanical eigenvalues up to a maximum w of about 156 were used for the analysis.

In table 5, classically calculated correction terms are given for some orbits which are only periodic with a symmetry transformation. The orbits $0-+-$ and $0--+$ have the same shape but are traversed in opposite directions. In all other cases mentioned in the tables, the symbol is independent of the direction because the orbit is identical with its time reversed counterpart. The classical values are compared with the results from the analysis of the quantum spectrum in table 6. The agreement of the amplitudes from classical and quantum calculations is again very good. In most cases the differences are only of the order 10^{-3} . In all three cases in which the difference is larger, the actions of these orbits lie close to those of other orbits. This makes the analysis of the quantum spectrum difficult. The phases of the quantum mechanically calculated correction terms reproduce the correct signs of the classical values but the differences are of the order 10^{-2} . A similar behaviour was found in [5] for orbits which are periodic without any symmetry transformation.

Table 5

The first-order \hbar corrections for some orbits which are only periodic with a symmetry transformation obtained by classical calculations. $C_{\hbar\ell}^{(\text{cl})}$ is the sum of the correction terms $C_{1\ell}$ and $C_{1\ell}^{T \rightarrow E}$ (see equation (70)).

Symbol	$C_{1\ell}$	$C_{1\ell}^{T \rightarrow E}$	$C_{\hbar\ell}^{(\text{cl})}$
+	-0.09003695	-0.00439305	-0.09443001
++	-0.3916016	0.0299637	-0.3616379
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
0-+-, 0---+	-1.93292	0.29321	-1.63971
+++--	-2.97331	0.25335	-2.71997
0-++	-0.319617	0.036473	-0.283144

Table 6

Modulus $|C_{\hbar\ell}^{(\text{qm})}|$ and phase $\arg(C_{\hbar\ell}^{(\text{qm})})$ of first-order \hbar corrections obtained by harmonic inversion of the quantum spectrum. In the last column the relative difference between the classical $C_{\hbar\ell}^{(\text{cl})}$ and quantum results for the modulus is given.

Symbol	$C_{\hbar\ell}^{(\text{cl})}$	$ C_{\hbar\ell}^{(\text{qm})} $	$\arg(C_{\hbar\ell}^{(\text{qm})})$	$\frac{ C_{\hbar\ell}^{(\text{qm})} }{ C_{\hbar\ell}^{(\text{cl})} } - 1$
+	-0.09443001	0.09455	$1.0006 \cdot \pi$	-0.0013
++	-0.3616379	0.36155	$0.9963 \cdot \pi$	-0.0002
0-	0.0493366	0.04974	$0.0293 \cdot \pi$	0.0082
++--	-0.515351	0.51564	$0.9883 \cdot \pi$	0.0006
0---	0.33338	0.31303	$0.0168 \cdot \pi$	-0.0610
++++	-0.76277	0.75772	$0.9731 \cdot \pi$	-0.0066
0-+	-0.381729	0.38192	$0.9861 \cdot \pi$	0.0005
00+	2.83895	2.9894	$0.0529 \cdot \pi$	0.0530
0-+-, 0---+	-1.63971	1.6622	$0.8646 \cdot \pi$	0.0137
+++--	-2.71997	2.7453	$0.9726 \cdot \pi$	0.0093
0-++	-0.283144	0.28428	$0.9867 \cdot \pi$	0.0040

5 Conclusion and Outlook

In this paper we extended the theory presented in [5] to systems with discrete symmetries and the influence of these symmetries on the correction terms was discussed in detail. The symmetry transformations presented in this paper made possible the calculation of the correction terms for a number of orbits which could not be included without symmetry operations. Nevertheless, these orbits, which are not periodic in the plane of semiparabolic coordinates without a symmetry operation, contribute to some of the subspaces 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], and was pointed out in section 2, 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. However, the extraction of the \hbar correction terms from quantum spectra with the method presented in section 3.4 leads to results which are on the same order of magnitude as the values of orbits without turning points. Thus we can assume that the reason lies in an insufficiency of the theory, and is not a physical property.

On the other hand, besides the successfully implemented discrete symmetries, physical systems often have a continuous symmetry. For example, 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. As was mentioned in section 3.1, 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.

Furthermore, for the hydrogen atom it would be interesting to look at the w level density, $g(w) = \sum_n \delta(w - w_n)$, where w is the scaling parameter introduced in section 3.5, in contrast to the “energy” level density (73). In this case, there is no need to calculate the quantum mechanical matrix elements which in our case are required in equations (73) and (75). This was already done before for the leading order (see e.g. [9]). This means that one has to find

a semiclassical expression for a level density with weighting factors, $g_A(E) = \sum_n \langle \psi_n | \frac{1}{2} (p_\mu^2 + p_\nu^2) | \psi_n \rangle \delta(E - E_n)$. Eckhardt et al. [17] presented an extension of Gutzwiller's theory which allows the calculation of the leading order of the level density $g_A(E)$. It would be desirable to include higher orders of the \hbar expansion in that theory.

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