Semiclassical treatment of diffraction in billiard systems with a flux line

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(Received 6 April 1999)

In billiard systems with a flux line, semiclassical approximations for the density of states contain contributions from periodic orbits as well as from diffractive orbits that are scattered on the flux line. We derive a semiclassical approximation for diffractive orbits that are scattered once on a flux line. This approximation is uniformly valid for all scattering angles. The diffractive contributions are necessary in order that semiclassical approximations are continuous if the position of the flux line is changed. [S1063-651X(99)11710-0]

PACS number(s): 05.45.Mt, 03.65.Sq

I. INTRODUCTION

Billiard systems with flux lines are simple dynamical systems that can model the typical behavior of low-dimensional quantum systems. One main application has been in the investigation of universal properties of quantum systems that are chaotic in the classical limit [1]. The high lying states of these systems have statistical properties that depend only on the symmetries of the system, and can be described by random matrix theory [2–4]. Ordinary billiards are used to model systems that are invariant under time inversion and are described by the Gaussian orthogonal ensemble (GOE). The introduction of an additional flux line allows us to study a further universality class since the flux line breaks the time-reversal symmetry. If the flux strength is sufficiently large (when considering levels in a fixed energy range) the corresponding universality class is that of the Gaussian unitary ensemble (GUE), but by varying the flux strength one can investigate also the GOE-GUE transition or parametric correlations in the GUE regime. Another application is for integrable billiard systems where the introduction of a flux line can break the integrability of the quantum billiard [5], or to use billiards with a flux line to model the properties of quantum dots (see e.g., [6]).

A major advantage in all these applications is that the classical trajectories are not changed by the presence of a flux line, except for the set of orbits of measure zero that hit the flux line. In a semiclassical analysis the same set of periodic orbits appears independent of the flux strength, and only the semiclassical contributions of these orbits are changed. For example, in approximations to the density of states the periodic orbit contributions have an additional phase $2\pi m\alpha$, where α is related to the flux strength and m is the number of times the orbit winds around the flux line. However, this is not the only semiclassical effect of a flux line. Its presence also leads to wave diffraction, that can be semiclassically described by an additional set of trajectories that are closed but not periodic, and which start and end on the flux line. In semiclassical arguments these so-called diffractive orbits are often neglected since their semiclassical contribution is estimated to be of order $\sqrt{\hbar}$ smaller than the contributions of periodic orbits. Such an estimate is, however, only valid if the scattering angle is not too close to the forward direction. In the forward direction, diffractive orbits contribute in the same order as periodic orbits.

In this paper we investigate the semiclassical contributions of diffractive orbits to the density of states. We derive an approximation for orbits that are scattered once on a flux line. This approximation is valid for all scattering angles, also in the forward scattering direction. We show that these contributions are necessary in order to cancel discontinuities in periodic orbit contributions that occur when the position of the flux line is changed and crosses a periodic orbit. We also discuss the importance of diffractive orbits in the semiclassical limit.

This paper is organized as follows. In Sec. II we consider the scattering on a flux line in a plane, and derive a uniform approximation for the Green function. With this input, in Sec. III we derive a uniform approximation for semiclassical contributions to the density of states from isolated diffractive orbits that are scattered once on a flux line. As an example of a system with nonisolated diffractive orbits, in Sec. IV we consider the integrable circular billiard with a flux line in its center. The results are discussed in Sec. V.

II. A FLUX LINE IN A PLANE

The scattering of a wave function on a flux line in a plane without boundaries has been studied in great detail since the problem was first treated by Aharonov and Bohm [7]. There exists, for example, an exact integral representation for the propagator. A review on the quantum effects of electromagnetic fluxes is given in Ref. [8]. In this section we review some of the results and derive a uniform approximation for the Green function that will be used in Sec. III.

The Schrödinger equation for a particle with mass M and charge q in a magnetic field in two dimensions is given in Gaussian units by

$$\frac{1}{2M}\left[\frac{\hbar}{i}\nabla - \frac{q}{c}\mathbf{A}\right]^2 \Psi(\mathbf{r}) = E\Psi(\mathbf{r}), \qquad (1)$$

and for a flux line the vector potential can be chosen as

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$$\mathbf{A}=\frac{\Phi}{2\pi r}\hat{\boldsymbol{\phi}}, \quad \nabla\times\mathbf{A}=\Phi\,\delta(\mathbf{r})\hat{\mathbf{z}}, \quad \nabla\cdot\mathbf{A}=0, \tag{2}$$

which describes a magnetic field with flux Φ that is concentrated in form of a delta-function in the origin.

In polar coordinates the Schrödinger equation with vector potential (2) has the form

$$-\left[\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}+\frac{1}{r^2}\left(\frac{\partial}{\partial\phi}-i\alpha\right)^2\right]\Psi(r,\phi)=k^2\Psi(r,\phi), \tag{3}$$

where $\alpha=q\Phi/(2\pi\hbar c)$ and $k=\sqrt{2ME}/\hbar$. The solutions that are regular in the origin are given by ($m\in\mathbb{Z}$, $k\in\mathbb{R}_+$)

$$\Psi_{m,k}(r,\phi)=\sqrt{\frac{k}{2\pi}}J_{|m-\alpha|}(kr)\exp\{im\phi\}, \tag{4}$$

where the normalization is chosen such that

$$\int_0^{2\pi}d\phi\int_0^{\infty}dr\,r\,\Psi_{m,k}(r,\phi)\Psi^*_{m',k'}(r,\phi)=\delta_{m,m'}\delta(k-k'), \tag{5}$$

as follows from the orthogonality relations of the exponential and the Bessel functions [9]. It is sufficient to consider only values $0\leqslant\alpha\leqslant0.5$, since the solutions for other values of α can be obtained by a multiplication of a (ϕ-dependent) phase factor and possibly a complex conjugation.

With the normalized solution [Eq. (4)] the propagator can be written down directly:

$$\begin{aligned}K_\alpha(\mathbf{r},\mathbf{r}_0,t)&=\sum_{m=-\infty}^{\infty}\int_0^{\infty}dk\,\Psi_{m,k}(r,\phi)\Psi^*_{m,k}(r_0,\phi_0)\\&\quad\times\exp\left\{-\frac{i}{\hbar}\frac{\hbar^2k^2}{2M}t\right\}\\&=\sum_{m=-\infty}^{\infty}\frac{M}{2\pi i\hbar t}J_{|m-\alpha|}\left(\frac{rr_0M}{\hbar t}\right)\exp\left\{im(\phi-\phi_0)\right.\\&\quad\left.-\frac{M(r^2+r_0^2)}{2i\hbar t}-i\frac{\pi}{2}|m-\alpha|\right\},\end{aligned} \tag{6}$$

and in the same way one obtains an exact representation for the Green function,

$$\begin{aligned}G_\alpha(\mathbf{r},\mathbf{r}_0,E)&=\lim_{\varepsilon\to0}\frac{1}{i\hbar}\int_0^{\infty}dt\,K_\alpha(\mathbf{r},\mathbf{r}_0,t)\exp\left\{\frac{i}{\hbar}t(E+i\varepsilon)\right\}\\&=\lim_{\varepsilon\to0}\sum_{m=-\infty}^{\infty}\int_0^{\infty}dk'\,\Psi_{m,k'}(r,\phi)\\&\quad\times\Psi^*_{m,k'}(r_0,\phi_0)\frac{1}{E+i\varepsilon-\frac{\hbar^2k'^2}{2M}}\\&=\sum_{m=-\infty}^{\infty}\frac{M}{2i\hbar^2}e^{im(\phi-\phi_0)}J_{|m-\alpha|}(kr_<)H^{(1)}_{|m-\alpha|}(kr_>),\end{aligned} \tag{7}$$

where $r_<$ and $r_>$ are the smaller and larger values of r and r_0, respectively.

For further evaluations the representation in the basis of the angular momentum eigenstates is not convenient. However from the sum in Eq. (6), one can derive an exact integral representation for the propagator (see Ref. [8]). It involves an integral over Hankel functions. In the following we use an approximation to this integral representation that is obtained after replacing the Hankel functions by their leading asymptotic form. This gives a semiclassical approximation for the propagator that is valid if $0<\alpha<1$ and $Mrr_0/t\gg\hbar$, i.e., for times that are not too long or distances that are not too close to the flux line:

$$\begin{aligned}K_\alpha(\mathbf{r},\mathbf{r}_0,t)&\approx\frac{M}{2\pi i\hbar t}\exp\left\{\frac{iM}{2\hbar t}(\mathbf{r}-\mathbf{r}_0)^2+i\alpha(\phi-\phi_0)\right\}\\&\quad-\frac{M\sin(\alpha\pi)}{\pi i\hbar t}\exp\left\{\frac{iM}{2\hbar t}(r+r_0)^2\right.\\&\quad\left.+\frac{i}{2}(\phi-\phi_0)\right\}K\left(\sqrt{\frac{2Mrr_0}{\hbar t}}\cos\left(\frac{\phi-\phi_0}{2}\right)\right).\end{aligned} \tag{8}$$

The angles in Eq. (8) have to be chosen such that $|\phi-\phi_0|\leqslant\pi$, and the function $K(z)$ is described below. The semiclassical propagator in Eq. (8) (and also the exact propagator) consists of two parts. The first part is almost identical to the propagator in a free plane with the difference of an additional phase proportional to α. Semiclassically it can be interpreted as the contribution from the direct path from $\mathbf{r}_0$ to $\mathbf{r}$. The additional phase results from the dependence of the Lagrangian on the vector potential. The second term in Eq. (8) describes the scattering on the flux line, and is discussed in more detail in connection with the Green function. Both terms are discontinuous in the forward direction, $|\phi-\phi_0|=\pi$, but the sum is continuous and uniformly valid for all values of ϕ and ϕ_0.

The function $K(z)$ in Eq. (8) is a modified Fresnel function that is defined by

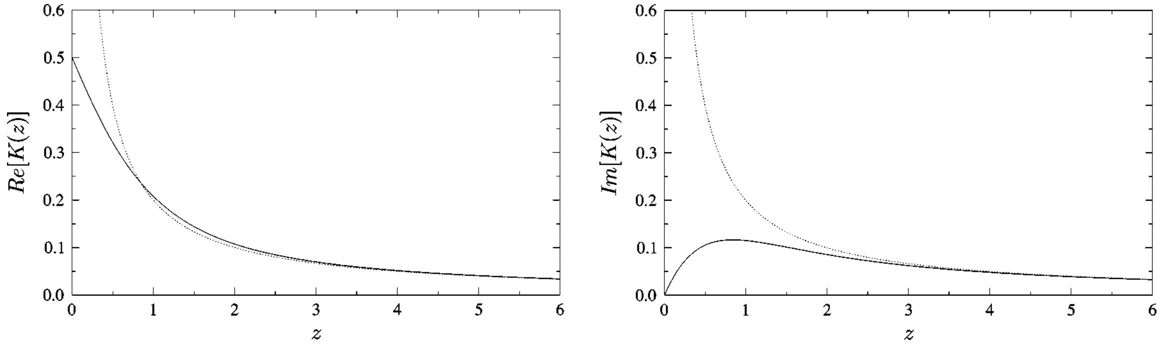

FIG. 1. Real and imaginary parts of the modified Fresnel function $K(z)$ (full line) and its asymptotic approximation (dotted line).

$$K(z)=\frac{1}{\sqrt{\pi}}\exp\left\{-iz^2-i\frac{\pi}{4}\right\}\int_z^\infty dy\, e^{iy^2}$$

$$=\frac{1}{2}e^{-iz^2}\operatorname{erfc}(e^{-i\pi/4}z), \tag{9}$$

and it has the following properties

$$K(0)=\frac{1}{2},\quad K(z)\sim\frac{e^{i\pi/4}}{2z\sqrt{\pi}},\quad |z|\to\infty,$$

$$-\frac{\pi}{4}<\arg(z)<\frac{3\pi}{4}. \tag{10}$$

An important alternative representation of $K(z)$ is given by the integral (β, $z>0$)

$$K(\sqrt{\beta}z)=\frac{1}{2\pi i}\int_{-i\infty}^{i\infty}dx\,\frac{e^{-i\beta x^2}}{x+z}. \tag{11}$$

Due to this form, the function K arises in semiclassical evaluations of oscillatory integrals in which a pole of the integrand is close to a stationary point. In Fig. 1 we show the real and imaginary parts of the function $K(z)$ for positive z. The function has its largest absolute value at $z=0$, and from approximately $z=3$ on it agrees well with its asymptotic approximation [Eq. (10)].

With the relation between the propagator and the Green function in Eq. (7), one can obtain a uniform approximation for the Green function. We consider the contributions from the two parts of the propagator separately. These parts are called the geometrical and the diffractive part in the following:

$$G_\alpha(\mathbf{r},\mathbf{r}_0,E)=G_g(\mathbf{r},\mathbf{r}_0,E)+G_d(\mathbf{r},\mathbf{r}_0,E). \tag{12}$$

For the first part in Eq. (8), one can evaluate the integral in Eq. (7) by stationary phase approximation, and one obtains, analogously to the propagator, the free semiclassical Green function modified by a phase

$$G_g(\mathbf{r},\mathbf{r}_0,E)\approx\frac{M}{\hbar^2\sqrt{2\pi k|\mathbf{r}-\mathbf{r}_0|}}\exp\left\{ik|\mathbf{r}-\mathbf{r}_0|+i\alpha(\phi-\phi_0)-i\frac{3\pi}{4}\right\}. \tag{13}$$

For the second part we express the Fresnel function by integral (11), and arrive at

$$G_d(\mathbf{r},\mathbf{r}_0,E)\approx-\frac{iM\sin(\alpha\pi)}{2\pi^2\hbar^2}\lim_{\varepsilon\to0}\int_0^\infty dt\times\int_{-i\infty}^{i\infty}dz\frac{1}{t}\,\frac{1}{z+\cos\frac{\phi-\phi}{2}}\exp\left\{\frac{iM}{2\hbar t}(r+r_0)^2+\frac{i}{2}(\phi-\phi_0)-i\frac{2Mrr_0z^2}{\hbar t}+\frac{i}{\hbar}t(E+i\varepsilon)\right\}. \tag{14}$$

This double integral has a stationary point at $(z,t)=(0,t_{\mathrm{cl}})$ where $t_{\mathrm{cl}}=\sqrt{M/(2E)}(r+r_0)$ is the classical time for the path from $\mathbf{r}$ to $\mathbf{r}_0$ via the origin at energy E. In order to evaluate the integral we expand the exponent in Eq. (14) up to second order around the stationary point. Then the integral over t can be evaluated by stationary phase approximation, since the stationary point at $t=t_{cl}$ is well separated from the pole at $t=0$. In the integral over z, however, the z dependence of the denominator has to be taken into account, and this again yields a modified Fresnel function. In this way a uniform approximation for the diffractive part of the Green function is obtained,

$$G_d(\mathbf{r},\mathbf{r}_0,E)\approx\frac{M\sin(\alpha\pi)\sqrt{2\pi i}}{\pi\hbar^2\sqrt{k(r+r_0)}}\exp\left\{ik(r+r_0)+\frac{i}{2}(\phi-\phi_0)\right\}K\left[\sqrt{\frac{2krr_0}{r+r_0}}\cos\left(\frac{\phi-\phi_0}{2}\right)\right], \tag{15}$$

where again the angular coordinates have to be chosen such that $|\phi-\phi_0|\leqslant\pi$. This approximation for the Green function will be the ingredient for the derivation of semiclassical contributions of diffractive orbits in trace formulas in Sec. III. It is valid as long as $kr,\ kr_0\gg1$.

We now consider an approximation to this expression that is valid if $|\phi-\phi_0|$ is not too close to π. Then the argument of the Fresnel function can be replaced by its leading asymptotic term (10), and yields

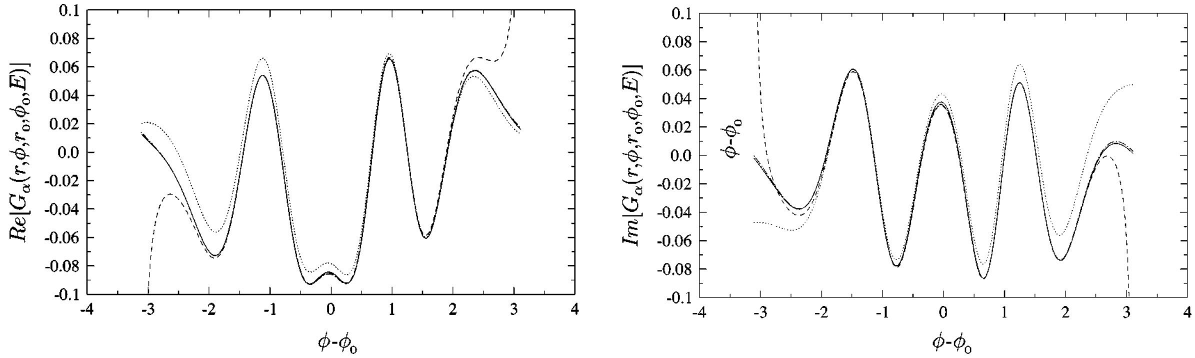

FIG. 2. Real and imaginary parts for different approximations of the Green function $G_\alpha(\mathbf{r},\mathbf{r}_0,E)$ (in dimensionless units $\hbar=2M=1$) with $r=1$, $r_0=2$, $k=5$, and $\alpha=0.4$. Full line: exact result; dotted line: $G_g(\mathbf{r},\mathbf{r}_0,E)$; dashed line: GTD approximation; and dash-dotted line: uniform approximation.

$$G_d(\mathbf{r},\mathbf{r}_0,E)\approx\frac{M\sin(\alpha\pi)}{2\pi k\hbar^2\sqrt{rr_0}\cos\left(\frac{\phi-\phi_0}{2}\right)}\exp\left\{ik(r+r_0)+\frac{i}{2}(\phi-\phi_0)+i\frac{\pi}{2}\right\}. \tag{16}$$

This approximation is of the general form that is obtained within the geometrical theory of diffraction (GTD) (see, e.g., Ref. [10])

$$G_d(\mathbf{r},\mathbf{r}_0,E)\approx\frac{\hbar^2}{2M}G_0(\mathbf{r},0,E)\mathcal{D}(\phi,\phi_0)G_0(0,\mathbf{r}_0,E). \tag{17}$$

In this theory the scattering is described by a free Green function from $\mathbf{r}_0$ to the scattering source at the origin, multiplied by a diffraction coefficient $\mathcal{D}(\phi,\phi_0)$ that contains the information about the particular scattering process and a further free Green function from the origin to the point $\mathbf{r}$. A comparison with Eq. (16) shows that the diffraction coefficient for the present case is given by

$$\mathcal{D}(\phi,\phi_0)=\frac{2\sin(\alpha\pi)}{\cos\left(\frac{\phi-\phi_0}{2}\right)}\exp\left\{i\frac{\phi-\phi_0}{2}\right\}. \tag{18}$$

Term (16) can be interpreted as the contribution of a trajectory that runs from $\mathbf{r}_0$ to the origin and then to $\mathbf{r}$. It is of order $k^{-1/2}$ smaller than the contribution of the direct trajectory from $\mathbf{r}_0$ to $\mathbf{r}$ in Eq. (13). However, the GTD approximation breaks down in the forward direction $|\phi-\phi_0|=\pi$, where the diffraction coefficient (18) diverges. This reflects the fact that the diffractive part of the Green function has a different leading asymptotic term in the forward direction. Here the diffractive trajectory contributes in the same order in k as the direct trajectory. The uniform approximation (15) interpolates between these two different asymptotic regimes.

In Fig. 2 we compare the different approximations to the Green function with the exact result (7). The dotted line is the geometrical part (13). The approximation is already reasonably good, but one can still see a clear deviation from the exact curve. By adding the diffractive part in the GTD approximation (dashed line), the difference becomes much smaller for most values of $\phi-\phi_0$, except near the end points $\phi-\phi_0=\pm\pi$ where it diverges. This divergence is removed by the uniform approximation in Eq. (15) (dash-dotted line) for which the difference with the exact line can hardly be seen, even though we chose relatively small values of kr and kr_0.

III. SEMICLASSICAL CONTRIBUTIONS OF ISOLATED DIFFRACTIVE ORBITS

For the derivation of semiclassical approximations in billiard systems it is convenient to apply the boundary integral method. It provides an alternative formulation of the quantum mechanical eigenvalue problem in terms of an integral equation along the billiard boundary. All semiclassical contributions due to diffraction in billiard systems that go beyond the GTD approximation have so far been derived by this method [11,12].

The boundary integral method has been developed for billiard systems without internal fields (see, e.g., Refs. [13,14]), but it can be extended to more general situations. In Ref. [15] Tiago *et al.*, derived an integral equation for billiard systems with magnetic field which is described by a vector potential in the Coulomb gauge. The resulting integral equation has the same form as for billiards without field. For a billiard system with a flux line and Dirichlet boundary conditions, one obtains

$$-2\int_{\partial\mathcal{D}}ds'\,\partial_{\hat{n}}G_\alpha(\mathbf{r}',\mathbf{r},E)u(\mathbf{r}')=u(\mathbf{r}), \tag{19}$$

where from here on we use units in which $\hbar=2M=1$. The difference from the field free case is that the Green function in Eq. (19) is the one for a flux line in a plane and the solutions $u(\mathbf{r})$ are the complex conjugate of the normal derivatives of the wave functions. The form of the integral equation in Eq. (19) is different from that in Ref. [15] since we applied an additional normal derivative to the equation in order to obtain a nondivergent integral kernel. Also the Green function differs by a factor (-8π) from that in Ref. [15].

In Eq. (19) the points $\mathbf{r}$ and $\mathbf{r}'$ lie on the boundary, the position of $\mathbf{r}'$ is parametrized by s', and $\partial_{\hat{n}}$ denotes the outward normal derivative at $\mathbf{r}$. The integral is evaluated along the boundary $\partial\mathcal{D}$ of the billiard system. The left-hand side of

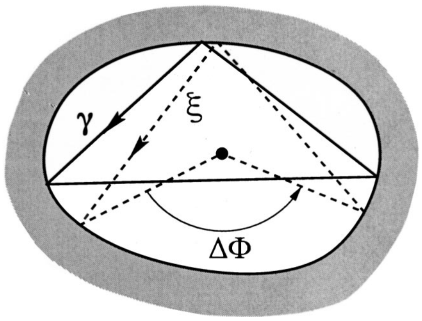

FIG. 3. Example of a periodic orbit, labeled by γ, and a diffractive orbit with one scattering event, labeled by ξ.

Eq. (19) can be abbreviated by $\hat{Q}u(\mathbf{r})$, where $\hat{Q}$ is the integral operator acting on u. Equation (19) is a Fredholm equation of the second kind, and it has nontrivial solutions only if the determinant $\Delta(E) := \det[\mathbf{1} - \hat{Q}(E)]$ vanishes. This condition determines the quantum energies of the problem. For a summary of the properties of the Fredholm determinant $\Delta(E)$ for two-dimensional billiards without fields with corresponding references, see Ref. [16].

From the condition of the vanishing of the Fredholm determinant, one can obtain an expression for the density of states in terms of the integral operator $\hat{Q}$. It is given by

$$d(k) = d_{\mathrm{sm}}(k) + \frac{1}{\pi}\frac{d}{dk}\,\mathrm{Im}\sum_{n=1}^{\infty}\frac{1}{n}\mathrm{Tr}\,\hat{Q}^n(k), \tag{20}$$

where

$$\mathrm{Tr}\,\hat{Q}^n(k) = (-2)^n \int_{\partial\mathcal{D}} ds_1 \cdots ds_n \partial_{\hat{n}_1} G_\alpha(\mathbf{r}_2,\mathbf{r}_1,E) \times \partial_{\hat{n}_2} G_\alpha(\mathbf{r}_3,\mathbf{r}_2,E)\cdots\partial_{\hat{n}_n} G_\alpha(\mathbf{r}_1,\mathbf{r}_n,E). \tag{21}$$

The sum in Eq. (20) is not convergent for real k, and for the derivation we assume that k has a sufficiently large imaginary part and that $\mathrm{Re}k > 0$. The density of states in Eq. (20) has a smooth part and a sum over oscillatory integrals. A semiclassical evaluation of the oscillatory integrals yields the leading semiclassical contributions to the density of states from periodic orbits and diffractive orbits. These contributions can be separated by writing G_α as sum of its geometrical and diffractive part. Then Eq. (21) consists of 2^n terms. The periodic orbit contributions are contained in the term that contains only geometrical Green functions. By evaluating this term in the stationary phase approximation, one obtains the usual Gutzwiller expression [17] for isolated periodic orbits in billiard systems, modified by an additional phase $2\pi m\alpha$, where m is the winding number of the orbit around the flux line. The terms with l diffractive Green functions, on the other hand, contain the contributions of diffractive orbits that are scattered l times on the flux line. An example of a periodic orbit and a diffractive orbit with one scattering event is shown in Fig. 3.

In this paper we consider only diffractive orbits that are scattered once on a flux line. We thus have to evaluate an integral with a product of $n-1$ geometrical Green functions and one diffractive Green function. This integral can be considerably simplified by applying a composition law for the geometrical part of the Green functions,

$$G_g^{(n)}(\mathbf{r},\mathbf{r}',E) \approx (-2)^n \int_{\partial\mathcal{D}} ds_1 \cdots ds_n \times G_g(\mathbf{r}_1,\mathbf{r}',E) \times \partial_{\hat{n}_1} G_g(\mathbf{r}_2,\mathbf{r}_1,E)\cdots\partial_{\hat{n}_n} G_g(\mathbf{r},\mathbf{r}_n,E), \tag{22}$$

where the approximate sign denotes that the integrals are evaluated in stationary phase approximation. The composition law was proved for ordinary billiard systems in Ref. [12] and it is a semiclassical version of the multiple reflection expansion of the Green function of Balian and Bloch. Since the presence of a flux line adds only a phase to the Green function which does not effect the stationary points in leading order, the composition law holds also in the present case and the phase is simply additive. The semiclassical expression for $G_g^{(n)}$ is then (see Ref. [12])

$$G_g^{(n)}(\mathbf{r}_2,\mathbf{r}_1,E) = \sum_{\gamma_n} \frac{1}{\sqrt{8\pi k|\tilde{M}_{12}|}} \exp\left\{ik\tilde{L} - i\frac{\pi}{2}\tilde{\nu} - i\frac{3\pi}{4} + i\alpha\phi_{21}\right\}. \tag{23}$$

Here the sum runs over all trajectories, labeled by γ_n, which run from $\mathbf{r}_1$ to $\mathbf{r}_2$ and are reflected n times on the boundary in between. ϕ_{21} is the total winding angle of a trajectory around the flux line. It can be written as $\phi_{21} = 2\pi m + \Delta\phi$, where m is an integer and $|\Delta\phi| \leq \pi$. Furthermore, $\tilde{M}_{12}$ is the 12-element of the stability matrix, $\tilde{L}$ is the length of the trajectory, and $\tilde{\nu}$ is the number of conjugate points from $\mathbf{r}_1$ to $\mathbf{r}_2$. The stability matrix $\tilde{M}$ is evaluated at unit energy and is energy independent. We use a tilde here in order to distinguish the quantities from the corresponding ones for the diffractive orbit. All quantities depend on the particular trajectory, but in order to avoid complicated notation an additional index γ_n is dropped. With Eq. (22) one obtains the following expression for the partial contribution to the level density from diffractive orbits with one scattering event and n reflections on the boundary:

$$d_{\mathrm{part}} = \frac{4}{\pi}\,\mathrm{Im}\,\frac{d}{dk}\int_{\partial\mathcal{D}} ds_1 ds_2 \partial_{\hat{n}_1} G_d(\mathbf{r}_2,\mathbf{r}_1,E) \times \partial_{\hat{n}_2} G_g^{(n-2)}(\mathbf{r}_1,\mathbf{r}_2,E). \tag{24}$$

We now insert Eqs. (23) and (15) with Eq. (11) for the semiclassical and diffractive Green functions, respectively. The normal derivative gives in both cases in leading order a factor $ik\cos\beta$, where β is the angle between the normal and the outgoing trajectory. We obtain

$$d_{\text{part}} = \text{Im} \sum_{\gamma_{n-2}} \frac{d}{dk} \frac{k \cos\beta_1 \cos\beta_2 \sin(\alpha\pi)}{2\pi^3 \sqrt{|\tilde{M}_{12}|(r_1+r_2)}} \times \exp\left\{ -i\frac{\pi}{2}\tilde{\nu} + i\alpha\phi_{21} - i\frac{\Delta\phi}{2} \right\} I, \tag{25}$$

where

$$I = \int_{\partial\mathcal{D}} ds_1 ds_2 \int_{-i\infty}^{i\infty} dz \frac{\exp\left\{ ik(\tilde{L}+r_1+r_2) - i\dfrac{2kr_1r_2}{r_1+r_2} z^2 \right\}}{z + \cos\dfrac{\Delta\phi}{2}}. \tag{26}$$

The main part in the derivation consists in the evaluation of the diffraction integral I. If all three integrals are evaluated by a stationary phase approximation, one obtains the contribution of diffractive orbits in the GTD approximation. This expression diverges when $|\Delta\phi| = \pi$. In order to obtain a semiclassical approximation that is uniformly valid for all angles, one has to take the dependence of the denominator on the integration variables into account. One can do this by expanding the exponent, in Eq. (26) up to second order in s_1, s_2, and z, and the denominator up to first order in these variables. In this way, in the denominator one obtains

$$\cos\frac{\Delta\phi}{2} \approx \cos\frac{\Delta\phi_0}{2} + \frac{1}{2}\left(\frac{s_1\cos\beta_1}{r_1} - \frac{s_2\cos\beta_2}{r_2} \right) \sin\frac{\Delta\phi_0}{2}. \tag{27}$$

This method corresponds to a particular choice of a uniform approximation. It yields an approximation that is correct at the ''optical boundary'' $|\Delta\phi| = \pi$ and in the GTD limit, and it interpolates between them. There are other possibilities to obtain a uniform approximation, for example by mapping the exponent onto a quadratic function in the three variables and then choosing an appropriate approximation for the amplitude function. This reflects the fact that uniform approximations are in general not unique. For example, a different interpolating approximation can be obtained by dropping the sine term in Eq. (27) which corresponds to replacing it by its value at the optical boundary.

The evaluation of the integral I is rather lengthy. It consists in carrying out the expansions and performing linear transformations of the variables such that, finally, the denominator depends only on one of the variables and the integral can be expressed in terms of the modified Fresnel function. A comparison with Ref. [12] shows, however, that the same diffraction integral occurs for the diffraction on billiard corners. For that reason, the calculations do not have to be done again, and the result can be inferred from this paper. One has $(c>0)$

$$\int_{-\infty}^{\infty} ds_1 \int_{-\infty}^{\infty} ds_2 \int_{-i\infty}^{i\infty} dz \frac{\exp\{ik(\tilde{L}+r_1+r_2-cz^2)\}}{a+z+b\left(\dfrac{s_1\cos\beta_1}{2r_1} - \dfrac{s_2\cos\beta_2}{2r_2} \right)}$$
$$= -\frac{4\pi^2 \text{sgn}(a)\tau}{k|b|\cos\beta_1\cos\beta_2} \sqrt{\frac{2r_1r_2|\tilde{M}_{12}|}{c|\text{Tr}\, M-2|}} \times K\left(i^\kappa \left|\frac{a}{b}\right| \sqrt{\frac{2k|M_{12}|}{|\text{Tr}\, M-2|}} \right) e^{ikL - i\pi(\nu+\kappa-\tilde{\nu})/2} + B, \tag{28}$$

where B denotes a boundary contribution whose origin is the discontinuity of the diffractive part of the Green function. It is canceled by a corresponding boundary contribution from the geometrical part of the Green function. In Eq. (28), L and M denote the length and stability matrix of the orbit, respectively, and ν is the number of conjugate points along the orbit. κ is given by

$$\kappa = \begin{cases} 0 & \text{if } \dfrac{M_{12}}{\text{Tr}\, M-2} > 0 \\ 1 & \text{if } \dfrac{M_{12}}{\text{Tr}\, M-2} < 0, \end{cases} \tag{29}$$

and $\tau = 1-2\kappa$.

With Eq. (28), and noting that the derivative in leading order gives a factor (iL), one obtains the final result for the contribution of a diffractive orbit ξ:

$$d_\xi(k) = -\text{Re}\left[\frac{2\tau L \sin(\alpha\pi) e^{ikL - i\pi\mu/2 + i\phi_{21}\alpha - i\Delta\phi/2}}{\pi \left| \sin\left(\dfrac{\Delta\phi}{2}\right) \right| \sqrt{|\text{Tr}\, M-2|}} \times K\left(i^\kappa \left| \cot\frac{\Delta\phi}{2} \right| \sqrt{\frac{2k|M_{12}|}{|\text{Tr}\, M-2|}} \right) \right], \tag{30}$$

where $\mu = \nu + \kappa$ agrees with the usual definition of the Maslov index for periodic orbits.

Formula (30) is the main result of this paper. It describes the contribution of a diffractive orbit to the density of states, and is valid for all scattering angles $\Delta\phi$ and for $0<\alpha<1$. It is assumed that the orbit is isolated and generic, in particular that $\text{Tr}\, M \neq 2$ and that $M_{12} \neq 0$. If these conditions are not satisfied then the formula has to be modified. This is analogous to typical semiclassical approximations in terms of classical trajectories. For example, periodic orbit contributions to the density of states have to be modified if the orbits occur in families or undergo bifurcation (case $\text{Tr}\, M = 2$), and contributions to the Green function have to be modified if the final point of a trajectory is conjugate to the initial point (case $M_{12} = 0$). An example for a system with families of diffractive orbits is treated in Sec. IV. Finally we note that a slightly simpler approximation than Eq. (30) can be obtained by dropping the sine term in the denominator in Eq. (30) and replacing the cotangent by a cosine, corresponding to the discussion after Eq. (27).

The use of the full Fresnel function in Eq. (30) is necessary in an angular region around the forward direction with width of order $k^{-1/2}$. For angles outside this range the Fresnel function can be replaced by its leading asymptotic form, which results in

$$d_\xi(k) \approx \text{Re}\left(\frac{L \sin(\alpha\pi)}{\pi \cos(\Delta\phi/2)} \frac{1}{\sqrt{2\pi k|M_{12}|}} \exp\left\{ ikL - i\frac{\pi}{2}\nu + i\alpha\phi_{21} - \frac{i}{2}\Delta\phi - i\frac{3\pi}{4} \right\} \right). \tag{31}$$

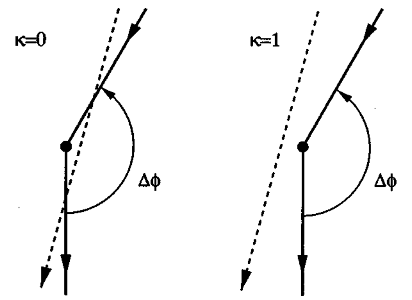

FIG. 4. Parts of a diffractive orbit and a nearby periodic orbit for $\kappa=0$ and $\kappa=1$.

This agrees with the GTD approximation for the diffractive orbit [18]:

$$d_\xi(k)=\mathrm{Re}\left(\frac{L}{\pi}G_g^\xi(\mathbf{r}_2,\mathbf{r}_1)\mathcal{D}(\phi_1,\phi_2)\right). \tag{32}$$

It is a contribution that is of order $1/\sqrt{k}$ smaller than the contribution of a isolated periodic orbit. In Eq. (32), G_g^ξ denotes the contribution from the trajectory ξ to the geometrical part of the Green function, where $\mathbf{r}_1=\mathbf{r}_2$ is the position of the flux line.

In the opposite limiting case at $|\Delta\phi|=\pi$ the uniform approximation is of the same order as that of a periodic orbit and it is discontinuous. As $|\phi|$ goes through π, the contribution makes a step of size

$$d_\xi(k)|_{\Delta\phi=\pi-0}-d_\xi(k)|_{\Delta\phi=-\pi+0}=-\frac{2\tau L\sin(\alpha\pi)}{\pi\sqrt{|\mathrm{Tr}\,M-2|}}\times\sin\left(kL-\frac{\pi}{2}\mu+(2m+1)\pi\alpha\right). \tag{33}$$

In order to understand this discontinuity we consider an angle $\Delta\phi=\pi-\varepsilon$ which is infinitesimally different from π. By examining the linearized motion around the diffractive orbit one finds that there is, in general, a periodic orbit in an infinitesimal neighborhood of the diffractive orbit. This orbit is obtained from the conditions that $dq=dq'$ and $dp=dp'-\varepsilon$ (at energy $E=1$), where the primed and unprimed quantities are infinitesimal perpendicular deviations from the starting point and end point of the diffractive orbit, respectively. From these conditions one finds that the position of the periodic orbit is given by $dq=-\varepsilon M_{12}/(\mathrm{Tr}\,M-2)$. Depending on the sign of the left-hand side, i.e., on the value of κ, there can be two possible cases that are shown in Fig. 4 for positive $\Delta\phi$ near π.

If one moves the flux line in a way that $\Delta\phi$ goes through π, then the flux line crosses this periodic orbit at the same instant. For the periodic orbit the semiclassical contribution is also discontinuous, since the winding number of the periodic orbit changes. For a primitive orbit the winding number changes by $+1$ if $\kappa=0$ and by -1 if $\kappa=1$. By writing the product of sines in Eq. (33) as a sum of two cosines, one can show that the two discontinuities cancel exactly and the sum of both contributions is continuous. This shows that the uniform approximation for diffractive contributions is necessary in order to make semiclassical approximations continuous if the position of a flux line is changed.

IV. DIFFRACTIVE ORBITS IN THE CIRCULAR BILLIARD

A simple example in which diffractive orbits are not isolated is a circular billiard with a flux line in its center. This system is integrable since the energy and the angular momentum around the center are conserved. All diffractive orbits run from the flux line to the boundary, and are reflected back directly onto the flux line. They appear in one- or more-parameter families, and their lengths are multiples of $2R$, where R is the radius of the circle. Contributions of these diffractive orbits to the density of states were observed in Ref. [19].

We are interested in the leading order semiclassical contributions of the diffractive orbits. For this purpose one cannot apply formula (30) since the orbits have a stability matrix with trace 2. Although one can in principle obtain the diffractive contributions from the boundary integral method, it is now much more convenient to start from the torus-quantization conditions for integrable systems [Einstein-Brillouin-Keller (EBK) conditions]. In this way one can obtain all leading order diffractive contributions to the density of states at once, even those for multiple diffraction.

The exact solutions of the Schrödinger equation are given by the solutions of the flux line in a plane (4) with a different normalization constant and the additional condition that the wave functions have to vanish at $r=R$. From this condition follows that the energies are determined by the zeros of the Bessel functions $E_{m,n}=\hbar^2k_{m,n}^2/(2M)$, where $k_{m,n}=j_{|m-\alpha|,n+1}/R$, and $j_{\nu,n}$ is the nth zero of the Bessel function with index ν.

The EBK quantization conditions yield semiclassical approximations to these energy levels. They have the forms

$$\frac{1}{2\pi}\oint d\phi p_\phi=\hbar m,\quad m\in\mathbb{Z},$$

$$\frac{1}{2\pi}\oint dr p_r=\hbar\left(n+\frac{3}{4}\right),\quad n=0,1,2,\ldots. \tag{34}$$

Due to the conservation of the angular momentum, the first condition gives $p_\phi=\hbar m$ and the second condition is evaluated with the energy conservation law $E=(p_r^2+(p_\phi-\hbar\alpha)^2/r^2)/(2M)$, and yields

$$\sqrt{k_{m,n}^2R^2-(m-\alpha)^2}-|m-\alpha|\arccos\frac{|m-\alpha|}{k_{m,n}R}=\pi\left(n+\frac{3}{4}\right), \tag{35}$$

which determines $k_{m,n}$ as a function of the two quantum numbers m and n.

From Eq. (35) the periodic orbit contributions to the density of states are obtained by applying the Poisson summation formula [20]

$$
\begin{aligned}
d(k)=&\sum_{M,N=-\infty}^{\infty}\int_{-\infty}^{\infty}dm\int_{-3/4}^{\infty}dn e^{2\pi i(Mm+Nn)}\delta(k-k_{m,n})\\
=&\sum_{M,N=-\infty}^{\infty}\int_{\alpha-kR}^{\alpha+kR}dm\frac{1}{\pi k}\sqrt{k^2R^2-(m-\alpha)^2}\\
&\times\exp\{2\pi i(Mm+Nn(m,k))\}\\
=&\sum_{M,N=-\infty}^{\infty}\int_{0}^{kR}dm\frac{1}{\pi k}\sqrt{k^2R^2-m^2}\exp\bigg\{2\pi iM(m+\alpha)\\
&+2iN\bigg[\sqrt{k^2R^2-m^2}-m\arccos\frac{m}{kR}\bigg]-\frac{3\pi}{2}iN\bigg\}\\
&+[\alpha\to-\alpha]. \qquad (36)
\end{aligned}
$$

We now consider the main semiclassical contributions to the integrals in Eq. (36). Altogether these are four contribution. One is the only nonoscillatory term $M=N=0$, which yields the leading area term for the mean density of states:

$$
d_A(k)=\frac{2}{\pi k}\int_0^{kR}dm\sqrt{k^2R^2-m^2}=\frac{1}{2}kR^2. \qquad (37)
$$

This agrees with the leading term in Weyl's law $Ak/(2\pi)$, with area $A=\pi R^2$.

The second main contribution arises from the stationary points of the integrals. A stationary phase approximation gives the contributions of the periodic orbits that have also been obtained in Ref. [19],

$$
\begin{aligned}
d_{po}(k)=&\sum_{N=2}^{\infty}\sum_{M+1}^{[N/2]}g_{M,N}\sqrt{\frac{4k}{\pi N}R^3\sin^3\frac{\pi M}{N}}\\
&\times\cos\bigg(2NkR\sin\frac{\pi M}{N}-\frac{3\pi}{2}N+\frac{\pi}{4}\bigg)\cos(2\pi M\alpha), \qquad (38)
\end{aligned}
$$

where $g_{M,N}=1$ if $M=N/2$ and $g_{M,N}=2$ if $M\neq N/2$. This factor arises from the fact that the stationary points for $M=N/2$ lie on the end point $m=0$ of the integrals in Eq. (36) and give only half the contribution.

The remaining two contributions follow from the boundaries of the oscillatory integrals. They can be obtained by an integration by part, which yields

$$
b.c.\ \text{of}\ \bigg\{\int_{-\infty}^{z}dxg(x)e^{if(x)}\bigg\}=-i\frac{g(z)}{f'(z)}e^{if(z)} \qquad (39)
$$

for an upper end of an integration range. If z is on the lower end of an integration range the end point contribution is given by minus the right hand side of Eq. (39).

With Eq. (39), for the contribution from $m=kr$ one obtains

$$
\begin{aligned}
d_L(k)=&\sum_{N,M=-\infty}^{\infty}{}'\frac{1}{\pi k}\\
&\times\frac{\sqrt{k^2R^2-m^2}\exp\Big\{2\pi iM(m+\alpha)-\frac{3\pi}{2}iN\Big\}}{2\pi iM-2iN\arccos\frac{m}{kR}}\Bigg|_{m\to kR}\\
&+[\alpha\to-\alpha]\\
=&\frac{2R}{\pi}\sum_{N=1}^{\infty}\frac{\sin\Big(\frac{3\pi}{2}N\Big)}{N}=-\frac{R}{2}, \qquad (40)
\end{aligned}
$$

where the prime denotes that the term $(N,M)=(0,0)$ is excluded from the sum since it corresponds to a nonoscillatory integral. The result in Eq. (40) can be identified with the perimeter term in the asymptotic expansion of the mean density of states.

From the other end points of the integrals at $m=0$, one obtains

$$
\begin{aligned}
d_d(k)=&\frac{iR}{2\pi^2}\sum_{\substack{M,N=-\infty\\ M\neq N/2}}^{\infty}\frac{1}{M-\frac{N}{2}}\exp\bigg\{2\pi iM\alpha+2iNkR\\
&-\frac{3\pi}{2}iN\bigg\}+[\alpha\to-\alpha]=d_d^e(k)+d_d^o(k). \qquad (41)
\end{aligned}
$$

Here the terms $M=N/2$ have to be excluded from the sum since they have already been taken into account by the stationary phase evaluation. For convenience the sum is split into two parts, corresponding to a summation over even and odd values of N, respectively.

For the first part N is replaced by $2N$, the summation index M is shifted by N, and terms for positive and negative values of M are combined:

$$
\begin{aligned}
d_d^e(k)=&-\frac{R}{\pi^2}\sum_{N=-\infty}^{\infty}\sum_{M=1}^{\infty}\frac{\sin[2\pi\alpha M]}{M}\exp\bigg\{i2N\bigg(\pi\alpha+2kR\\
&-\frac{3\pi}{2}\bigg)\bigg\}+[\alpha\to-\alpha]\\
=&\frac{2R}{\pi}(1-2\alpha)\sum_{N=1}^{\infty}\sin\bigg(2N\bigg(2kR-\frac{3\pi}{2}\bigg)\bigg)\\
&\times\sin(\pi\alpha 2N); \qquad (42)
\end{aligned}
$$

and for the second part N is replaced by $2N+1$, the summation index M is shifted by N, and terms for $M\geq 1$ and $M<1$ are combined:

$$
\begin{aligned}
d_d^o(k)=&-\frac{2R}{\pi^2}\sum_{N=-\infty}^{\infty}\sum_{M=1}^{\infty}\frac{\sin[\pi\alpha(2M-1)]}{2M-1}\exp\bigg\{i(2N+1)\\
&\times\bigg(\pi\alpha+2kR-\frac{3\pi}{2}\bigg)\bigg\}+[\alpha\to-\alpha]\\
=&\frac{2R}{\pi}\sum_{N=0}^{\infty}\sin\bigg((2N+1)\bigg(2kR-\frac{3\pi}{2}\bigg)\bigg)\\
&\times\sin(\pi\alpha(2N+1)). \qquad (43)
\end{aligned}
$$

The formulas for evaluating the summations in Eqs. (40), (42), and (43) can be found in Ref. [21] and are valid for $0<\alpha<1$.

Collecting all results, the complete trace formula is given by

$$d(k)\approx\bar{d}(k)+\sum_{N=2}^{\infty}\sum_{M=1}^{[N/2]}g_{M,N}\sqrt{\frac{4k}{\pi N}R^3\sin^3\frac{\pi M}{N}}\times\cos\left(2NkR\sin\frac{\pi M}{N}-\frac{3\pi}{2}N+\frac{\pi}{4}\right)\cos(2\pi M\alpha)+\sum_{N=1}^{\infty}\frac{2R}{\pi}\sin\left(2NkR-\frac{3\pi}{2}N\right)\sin(\pi N\alpha)-2\alpha\sum_{N=1}^{\infty}\frac{2R}{\pi}\sin(4NkR-3\pi N)\sin(2\pi N\alpha). \quad (44)$$

It consists of the mean level density, the contributions of periodic orbits, and the contributions of diffractive orbits which are smaller by an order $k^{-1/2}$ than those of the periodic orbits. The formula is similar to the corresponding one for a harmonic oscillator with a flux line [22].

The diffractive orbit term in Eq. (44) can be given a more direct interpretation since it can be transformed into a sum of δ functions by using the Poisson summation formula. One obtains

$$d_d(k)=-\frac{R}{2\pi}\sum_{n=-\infty}^{\infty}\left[\delta\left(\frac{kR}{\pi}-\frac{3}{4}+\frac{\alpha}{2}+n\right)-\delta\left(\frac{kR}{\pi}-\frac{3}{4}-\frac{\alpha}{2}+n\right)\right]+\frac{\alpha R}{\pi}\sum_{n=-\infty}^{\infty}\times\left[\delta\left(\frac{2kR}{\pi}-\frac{3}{2}+\alpha+n\right)-\delta\left(\frac{2kR}{\pi}-\frac{3}{2}-\alpha+n\right)\right]. \quad (45)$$

The argument of one of the δ functions can be identified with the semiclassical quantization condition for eigenvalues with vanishing angular momentum ($m=0$): $kR\approx\pi\alpha/2+3\pi/4+n\pi$. Since the full trace formula produces delta peaks at the eigenvalues given by the EBK conditions (35), the diffractive orbits have the following role: they contribute to peaks at eigenvalues with vanishing angular momentum, and they cancel wrong peaks that are produced by the periodic orbit sum.

The fact that the periodic orbits produce wrong peaks can be understood by noting that the periodic orbit contributions (38) are invariant under $\alpha\to-\alpha$. Due to this symmetry the periodic orbits give also rise to wrong peaks at $kR\approx-\pi\alpha/2+3\pi/4+n\pi$. The first two terms in Eq. (45) provide a correction to this failure in the approximation for states with zero angular momentum. The other two terms in Eq. (45) are necessary in order that the approximation is invariant under $\alpha\to1-\alpha$, since the spectrum is invariant under this replacement.

A test of the trace formula (44) is presented in Fig. 5, which shows a comparison between quantum mechanical and semiclassical results for the Fourier transform (with a Gaussian cutoff) of the oscillatory part of the density of states. The value of α is chosen to be $\alpha=0.25$, since for this value the periodic orbit contributions start at $L=8R$. The difference between the two curves cannot be seen on this scale.

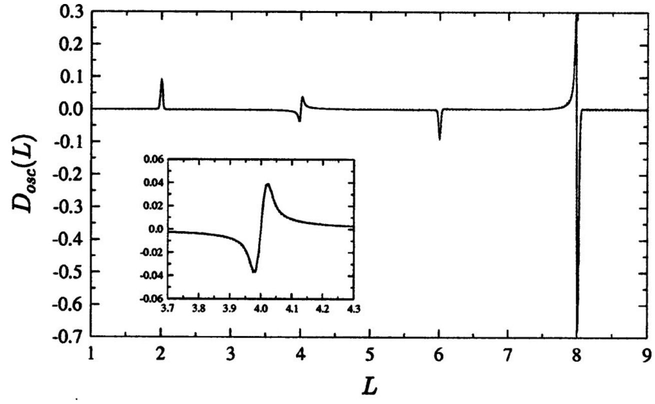

FIG. 5. Fourier transform of the oscillatory part of the density of states for the circular billiard with $\alpha=0.25$ and $R=1$ (full line) in comparison with the semiclassical approximation (dotted line). Dimensionless units are used in which $\hbar=2M=1$. Inset: Magnification of one peak.

V. CONCLUSIONS

One general property of uniform approximations for isolated diffractive orbits is that they make semiclassical approximations continuous as a system parameter is changed. They cancel discontinuities in semiclassical contributions of periodic orbits. In billiards with concave boundaries or with corners, those discontinuities are connected with the appearance or disappearance of periodic orbits. In the present case the discontinuity is due to a phase change in periodic orbit contributions. In addition, the diffraction on a flux line is very similar to the diffraction on corners. The final formula is expressed in terms of the same interpolating function, but it is also simpler since it consists only of one term instead of four. This suggests, for example, that a semiclassical study of two-dimensional systems which are nonintegrable but in which the classical motion is still restricted to a two-dimensional surface in phase space, might be performed more easily on billiards with a flux line instead of pseudointegrable polygonal billiards.

In this paper we considered only diffractive orbits that are scattered once on a flux line. The same method can be used to obtain semiclassical contributions of diffractive orbits with multiple scattering, but the formulas become increasingly more complex and have to be expressed in terms of multiple Fresnel integrals. The treatment of an integrable billiard with a flux line like the circular billiard is much simpler. There all leading order diffractive contributions including those from multiple diffraction can be obtained in one step from the EBK conditions. Moreover, they can be summed up and shown to contribute only to states with zero angular momentum.

One remaining question is whether in semiclassical arguments concerning spectral statistics in chaotic systems it is sufficient to consider only periodic orbits. One argument for this is that the semiclassical contributions of most diffractive orbits (GTD region) are by an order $1/\sqrt{k}$ smaller than those of periodic orbits, where k is the wave number. For scattering angles near the forward direction they contribute more strongly, up to the order of a periodic orbit, but the corresponding angular regime of this transitional region decreases proportional to $1/\sqrt{k}$. So one might argue that diffractive orbits become less and less important in the semiclassical regime.

Let us discuss this point in more detail. By applying the trace formula in order to resolve adjacent energy levels with wave numbers of order k, one has to take into account all orbits up to the Heisenberg length $L_H \propto k$. In a chaotic system the number of diffractive orbits increases exponentially with the orbit length. If we assume that the scattering angle is uniformly distributed, then the relative number of diffractive orbits in the transitional region decreases like $1/\sqrt{k}$. However, the total number of diffractive orbits in the transitional region is still increasing exponentially due to the exponential increase of all diffractive orbits. A similar argument can be applied to orbits with multiple scattering. It is not obvious that these orbits can be neglected. Moreover one can show that even in the GTD approximation diffractive orbits have a non-vanishing influence on spectral statistics in the semiclassical limit [23].

ACKNOWLEDGMENTS

Financial support by the Deutsche Forschungsgemeinschaft in the form of a ''Habilitandenstipendium'' (SI 380/2-1) is gratefully acknowledged.

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