# Periodic Orbit Theory of Diffraction

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(Received 21 January 1994)

An extension of the Gutzwiller trace formula is given that includes diffraction effects due to hard wall scatterers or other singularities. The new trace formula involves periodic orbits which have arcs on the surface of singularity and which correspond to creeping waves. A new family of resonances in the two-disk scattering system can be well described which is completely missing if only the traditional periodic orbits are used.

PACS numbers: 05.45.+b, 03.20.+i, 03.65.Sq

The Gutzwiller trace formula [1] is an increasingly popular tool for analyzing semiclassical behavior. Recently, it has been demonstrated that using proper mathematical apparatus, like Gutzwiller–Voros [2] zeta functions, cycle expansions [3], or quantum Fredholm determinants [4], the trace formula can successfully predict individual resonances of open scattering systems [5]; it is possible to compute systematic $\hbar$ corrections [6] and to extend the formula for systems with regular domains [7]. The physical content of the trace formula is the geometrical optical approximation of quantum mechanics via canonical invariants of closed classical orbits. This approximation is very accurate when periodic orbits sufficiently cove the phase space of the chaotic system. This is not the case when the number of obstacles is small or their distance is large compared to their typical size. In such cases it is very important to take into account the next-to-geometrical effects.

In this Letter we study how the *geometric theory of diffraction* (GTD) for hard core potentials can be incorporated in the periodic orbit theory. Such a problem occurs where the wavelength of a quantum mechanical (or optical) wave is very large compared with the spatial variation of a repulsive potential, e.g., at the boundaries of microwave guides, optical fibers, superconducting squids, or circuits in the ballistic evolution of electrons, i.e., in most of the devices used for so-called macroscopic quantum mechanical (or optical) experiments. First we summarize from the classical papers of Keller [8] how the Green's function in the shadowed regions of configuration space can be computed by the concept of GTD. Then we incorporate the periodic rays with diffracted ray arcs to the trace formula. It is possible to derive the diffraction part of the Green's function directly from the semiclassical approximation of the Feynman path integral in the neighborhood of a hard curved wall [9]. We have chosen Keller's approach here, since it is more suitable for computing the trace of the Green's function, without further approximations.

It has been known for quite a long time that the scattering amplitude in the shadowed region behind an obstacle can be well reproduced by allowing diffracted rays in addition to geometrical ones [8]. The diffracted rays connecting two points in the configuration space in the presence of sharp objects can be derived from an extension of Fermat's variational principle of classical mechanics [8]. The usual Fermat principle states that the classical trajectories connecting two positions $q_{\mathcal{A}}$ and $q_{\mathcal{B}}$ in configuration space are those smooth curves which make the action stationary. If the configuration space is bounded by hard walls, a generalized variational principle, introduced by Keller [8], has to be applied. This principle requires new classes of curves. We have to consider for each triplet of integers $r, s, t \geq 0$ the class of curves $\mathcal{D}_{rst}$ with $r$ smooth arcs on the surface, $s$ points on the edges, and $t$ points on the vertices of the boundary or the discontinuity. The curves of the GTD are those which make the action stationary within one of the classes $\mathcal{D}_{rst}$. The class $\mathcal{D}_{000}$ corresponds to the usual geometrical orbits. In this Letter, we concentrate on two-dimensional problems, where the simplest nontrivial curves are of class $\mathcal{D}_{100}$ and $\mathcal{D}_{001}$ [Figs. 1(a) and 1(b), respectively], whereas edge diffraction $\mathcal{D}_{010}$ is not possible. Once we know the generalized ray we can compute semiclassically the Green's function $G(q_{\mathcal{A}}, q_{\mathcal{B}}, E)$, tracing the ray along it [8]. In Fig. 1(a) ($\mathcal{D}_{100}$) the trajectory—obtained from the generalized variational principle—is tangent to the surface of the hard wall obstacle at points $\mathcal{A}'$ and $\mathcal{B}'$. The Green's function $G(q_{\mathcal{A}}, q_{\mathcal{A}'}, E)$ can be computed semiclassically by the energy domain Van Vleck propagator (for a single classical trajectory)

$$G(q, q', E) = \frac{2\pi}{(2\pi i\hbar)^{3/2}} D_V^{1/2}(q, q', E) e^{\frac{i}{\hbar} S(q,q',E) - \frac{i}{2}\nu\pi}, \tag{1}$$

where $D_V(q, q', E) = |\det(-\partial^2 S/\partial q_i \partial q_j')|/|\dot{q}||\dot{q}'|$ is the Van Vleck determinant and $\nu$ is the Maslov index (see Ref. [10] for definitions).

When the geometrical ray hits the surface of the obstacle, it creates a source for the diffracted (creeping) wave. The strength of the source is proportional to the Green's function at the incidence of the ray

$$Q_{\rm diff} = D G_{\rm inci}. \tag{2}$$

The diffraction constant $D$ depends on the local geometry and the nature of the diffraction. It has been determined in Ref. [8] from the asymptotic semiclassical expansion of

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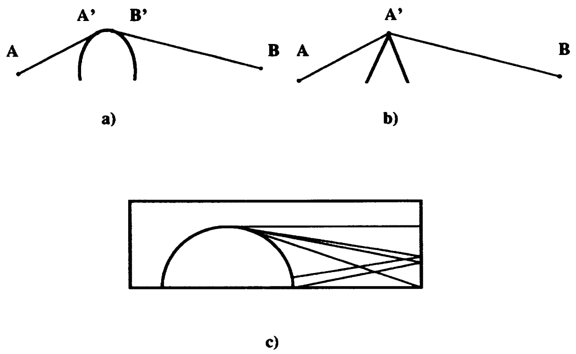


FIG. 1. The simplest classes $\mathcal{D}_{100}$ (a) and $\mathcal{D}_{001}$ (b) of curves in two dimensions. In the window (c): the first four basic orbits in the fundamental domain of the two-disk system.

the exact solution in some simple geometry [8] (see also [11]). Its form is

$$D_l = 2^{1/3}3^{-2/3}\pi e^{5i\pi/12}(k\rho)^{1/6}/\mathrm{Ai}'(x_l). \qquad (3)$$

Here $\mathrm{Ai}'(x)$ is the derivative of the Airy integral $\mathrm{Ai}(x) = \int_0^\infty dt\cos(xt - t^3)$, $k = \sqrt{2mE/\hbar}$ is the wave number, $\rho$ is the radius of the obstacle at the source of the creeping ray, and $x_l$ are the zeros of the Airy integral, which can be approximated as $x_l = 6^{1/3}[3\pi(l - 1/4)]^{2/3}/2$ in the semiclassical limit. The index $l \geq 1$ refers to the possibility of initiating creeping rays with different modes, each with its own profile. In practice only the low modes contribute to the Green's function. The source then initiates a ray creeping along the surface. During the creeping of the ray the amplitude decreases, which can be understood as a process analogous to the radiation processes of electrodynamics. The radiated intensity is proportional to the intensity of the ray:

$$\frac{d}{ds}A_l(s,E)^2 = -2\alpha_l(s,E)A_l(s,E)^2, \qquad (4)$$

where $s$ is the length measured along the surface and $A_l(s,E)$ is the complex amplitude of the Green's function along the surface. The coefficient $\alpha_l(s,E)$ depends on the local curvature of the surface, $1/\rho(s)$, and it has the structure $\alpha_l(s,E) = x_l e^{-i\pi/6}[k/6\rho(s)^2]^{1/3}$ (see Ref. [12]), where the index $l$ refers again to the different modes of the creeping wave. The Green's function for the creeping ray of mode $l$ is then given by

$$G_l^D(q_{\mathcal{A}'}, q_{\mathcal{B}'}, E) = e^{-\int_0^L ds\,\alpha_l(s,E)} e^{\frac{i}{\hbar}S(q_{\mathcal{A}'},q_{\mathcal{B}'},E)}, \qquad (5)$$

where $L$ is the length of the arc of the creeping ray, and $S(q_{\mathcal{A}'}, q_{\mathcal{B}'}, E)$ is the action along it. The creeping ray at the point $\mathcal{B}'$ initiates a pure geometrical ray. The source of this ray is located in $\mathcal{B}'$, and its strength is again given by Eqs. (2) and (3) due to the invariance of the Green's function against the interchange of the variables $q_{\mathcal{A}'}$ and $q_{\mathcal{B}'}$. The total Green's function is then the product of the Green's functions and diffraction coefficients along the ray:

$$G(q_{\mathcal{A}}, q_{\mathcal{B}}, E) = G(q_{\mathcal{A}}, q_{\mathcal{A}'}, E)\sum_{l=1}^{\infty} D_{l,\mathcal{A}'}G_l^D(q_{\mathcal{A}'}, q_{\mathcal{B}'}, E) \times D_{l,\mathcal{B}'}G(q_{\mathcal{B}'}, q_{\mathcal{B}}, E). \qquad (6)$$

In a general situation, when the ray consists of several pure geometric and creeping arcs, the Green's function can also be written as a product of partial Green's functions and diffraction constants.

To incorporate diffraction effects into the trace formula, one should compute the trace of the Green's function derived above. As in the case of the Gutzwiller trace formula—derived from a pure geometrical approximation of the Green's function—the trace receives the leading contributions from tubes encircling the closed curves, which now can have diffractional arcs too. We can handle separately the pure geometric cycles and the cycles with *at least one diffractional arc* along one of the obstacles:

$$\mathrm{Tr}\, G(E) \approx \mathrm{Tr}\, G_G(E) + \mathrm{Tr}\, G_D(E), \qquad (7)$$

where $\mathrm{Tr}\, G_G(E)$ is the ordinary Gutzwiller trace formula, while $\mathrm{Tr}\, G_D(E)$ is the new trace formula corresponding to the nontrivial cycles of the GTD. $\mathrm{Tr}\, G_{Dz}(E)$ can be computed by using appropriate Watson [11,13] contour integrals. For technical details we invite the reader to see Refs. [14] and [15]. Here we communicate the general result, and the detailed calculation will be published elsewhere [16]. If we denote by $q_i, i = 1,\ldots,n$ (with $q_{n+i} \equiv q_i$), the points along the closed cycle, where the ray changes from diffraction to pure geometric evolution or vice versa [see $\mathcal{A}'$ and $\mathcal{B}'$ in Fig. 1(a)], the trace for cycles with *at least one diffractional arc* can be expressed as the product

$$\mathrm{Tr}\, G_D(E) = \sum_{\text{cycles}} \frac{T(E)}{i\hbar}\prod_{i=1}^{n} D(q_i)G(q_i, q_{i+1}, E), \qquad (8)$$

where $T(E)$ is the time period of the cycle (without repeats) and $D(q_i)$ is the diffraction constant (3) with the radius of curvature $\rho$ given locally at the point $q_i$. The creeping mode index $l$ and the corresponding summations [see, e.g., (6)] are suppressed here for keeping the notation simple. $G(q_i, q_{i+1}, E)$ is alternately the Van Vleck propagator, if $q_i$ and $q_{i+1}$ are connected by pure geometric arcs, or is given by (5) in case $q_i$ and $q_{i+1}$ are the boundary points of a creeping arc. Note this formula applys only for cycles with at least one creeping section. Such cycles have the special property that their pertinent energy domain Green's functions are multiplicative [see, e.g., (6) with the summations over the creeping mode numbers of course included consistently]. This does not hold for pure geometrical cycles.

The eigenenergies can be recovered from the Gutzwiller–Voros spectral determinant [2] $\Delta(E)$, which is related to the trace formula as

$$\mathrm{Tr}\, G(E) = \frac{d}{dE} \ln \Delta(E) . \tag{9}$$

The full semiclassical determinant can be written as the *formal* product of two spectral determinants, one corresponding to pure geometrical and one to new cycles $\Delta(E) = \Delta_G(E)\Delta_D(E)$ due to the additivity of the traces. The product is only formal, since the eigenenergies are not given by the zeros of $\Delta_G(E)$ or $\Delta_D(E)$ individually, but have to be calculated from a curvature expansion of the *combined* determinant $\Delta(E)$ itself.

The diffraction part of the spectral determinant is

$$\Delta_D(E) = \exp\left( - \sum_{p,r=1}^{\infty} \frac{1}{r} \prod_{i=1}^{n_p} [D(q_i^p)G(q_i^p, q_{i+1}^p, E)]^r \right), \tag{10}$$

where the summation goes over closed primitive (nonrepeating) cycles $p$ and the repetition number $r$. The product of Green's functions should be evaluated for $q_i^p$ belonging to the primitive cycle $p$. After summation over $r$, the spectral determinant can be written as

$$\Delta_D(E) = \prod_p (1 - t_p) \tag{11}$$

with

$$t_p = \prod_{i=1}^{n_p} D(q_i^p)G(q_i^p, q_{i+1}^p, E), \tag{12}$$

where $q_i^p$ belongs to the primitive cycle $p$. As mentioned before, the mode numbers $l$ of the diffraction constants and the corresponding summations have been suppressed for notational simplicity; they can be easily restored as, e.g., in the final expression (19).

We can conclude that the diffractional part $\Delta_D(E)$ of the spectral determinant shares some nice features of the periodic orbit expansion of the dynamical zeta functions [3], and it can be expanded as

$$\Delta_D(E) = 1 - \sum_p t_p + \sum_{p,p'} t_p t_{p'} - \cdots . \tag{13}$$

The weight (12) has the following property which helps in radically reducing the number of relevant contributions in the expansion. If two different cycles $p$ and $p'$ have at least one common piece in their diffraction arcs, then the two cycles can be composed to one longer cycle $p + p'$, and the weight corresponding to this longer cycle is the product of the weights of the short cycles

$$t_{p+p'} = t_p t_{p'} . \tag{14}$$

As a consequence, the product of primitive cycles, which have at least one common piece in their diffraction arcs, can be reduced in such a way that the composite cycles are exactly cancelled in the curvature expansion

$$\prod_p (1 - t_p) = 1 - \sum_b t_b , \tag{15}$$

where $t_b$ are *basic* primitive orbits which cannot be composed from shorter primitive orbits.

To demonstrate the importance of the diffraction effects to the spectra, we have calculated the $A_1$ resonances of the scattering system of two equally sized hard circular disks with disk separation $R = 6a$, where $a$ is the radius of one disk. In this system there is only one geometrical periodic cycle along the line connecting the centers of the disks. Its stability $\Lambda_p = 9.898\,9794$ and action $S_p = kL_p = k4a$ yield the geometrical part of the spectral determinant [15,17]

$$\Delta_G(k) = \prod_{j=0}^{\infty} \left( 1 + \frac{e^{ikL_p}}{\Lambda_p^{(1+4j)/2}} \right), \tag{16}$$

where $k = \sqrt{2mE}/\hbar$ and $2m = \hbar = 1$, and leads to the following predictions for the semiclassical $A_1$ resonances

$$k_{n,j}^{\mathrm{res}} = [\pi(2n - 1) - i \tfrac{1+4j}{2} \ln \Lambda_p]/L_p \tag{17}$$

with $n = 1, 2, 3, \ldots$. Note in the above expressions $(1 + 4j)/2$ replaces the usual weight $(1 + 2j)/2$, since the geometrical orbit in the two-disk problem lies on the boundary of the fundamental domain [17].

Figure 1(c) shows the first four new basic cycles in the fundamental domain [17]. We computed the geometrical data of the first ten orbits and used them to construct the creeping and geometrical Green's functions. The semiclassical Green's function in free space is asymptotically $(kR \gg 1)$

$$G_0(q, q', E) = -\frac{i}{4} \left( \frac{2}{\pi k R} \right)^{1/2} e^{ikR - i\frac{\pi}{4}} , \tag{18}$$

where $R = |q - q'|$. If the ray connecting $q$ and $q'$ is reflected once or more from the curved hard walls before hitting tangentially one of the surfaces, we can keep track of the change in the amplitude by the help of the Sinai–Bunimovich curvatures.

By computing the curvatures $\kappa_i$ right after the reflections, and knowing the distances $l_i$ between the $i$th and the $(i + 1)$th points of reflections, the factor $R$ in the Green's function (18) has to be changed to the effective radius $R^{\mathrm{eff}} = R_0 \prod_{i=1}^{m} (1 + l_i \kappa_i)$ where $R_0$ is the distance between $q$ and the first point of reflection along the ray starting from $q$, and $m$ is the number of reflections from a disk. The effective radius $R_b^{\mathrm{eff}}$, the length of the geometrical arc $L_b^G$, and the length of the diffraction part $L_b^D$ of the first ten orbits with creeping sections are listed in Table I. To each

TABLE I. Table of the first ten basic cycles $t_b$ which include creeping sections in the fundamental region of two-disk problem (with disk separation $R = 6a$). The cycles are labelled by their number $m_b$ of geometrical reflections from one of the disks. The length of the geometrica ırc $L_b^G$, the effective radius $R_b^{\rm eff}$, and the length of the diffraction section $L_b^D$ are listed in units of the disk radius $a$.

| $m_b$ | $L_b^G/a$ | $R_b^{\rm eff}/a$ | $L_b^D/a$ |
|---|---|---|---|
| 0 | 5.65685 | 5.65685 | 3.82126 |
| 0 | 6.00000 | 6.00000 | 3.14159 |
| 1 | 9.83215 | 58.16784 | 3.47648 |
| 1 | 9.79795 | 58.78775 | 3.54430 |
| 2 | 13.81654 | 578.14066 | 3.50740 |
| 2 | 13.81309 | 579.74342 | 3.51425 |
| 3 | 17.81499 | 5729.64981 | 3.51048 |
| 3 | 17.81464 | 5732.23550 | 3.51118 |
| 4 | 21.81483 | 56728.70010 | 3.51079 |
| 4 | 21.81479 | 56732.26871 | 3.51086 |

cycle in the list, there is a whole sequence of cycles which wind around the disk $m_w$ times. For these orbits one has to add $2\pi a m_w$ to the diffraction length $L_b^D$. The diffraction part of the spectral determinant is finally given by

$$\Delta_D(k) = 1 - \sum_{b,l}(-1)^{m_b} C_l \frac{a^{1/3} e^{i\pi/12} e^{ik(L_b^G + L_b^D) - \alpha_l L_b^D}}{k^{1/6}\sqrt{R_b^{\rm eff}}} \times \frac{1}{1 - e^{2\pi(ik-\alpha_l)a}}, \tag{19}$$

where $C_l = \pi^{3/2} 3^{-4/3} 2^{-5/6}/\mathrm{Ai}'(x_l)^2$, and the summation for the windings $m_w$ gives the factor $1/(1 - e^{2\pi(ik-\alpha_l)^a})$. We computed the spectra by truncating the product

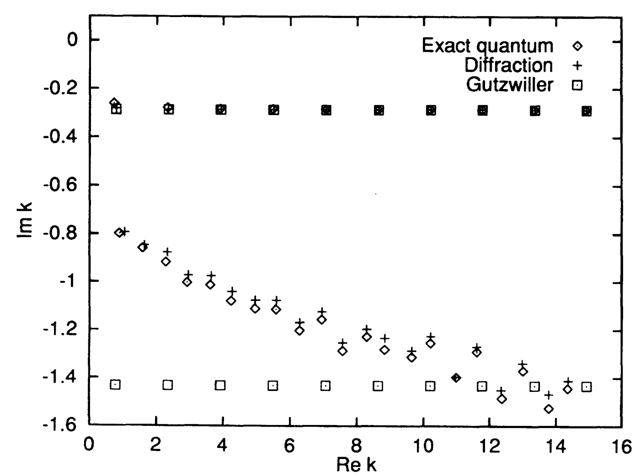


FIG. 2. Resonances for the $A1$ subspace of the two-disk system (with disk separation $R = 6a$) in the complex $k$ plane in units of the disk radius $a$. The diamonds label the exact quantum mechanical resonances, which are the poles of the scattering matrix. The crosses are their semiclassical approximations, including the diffraction terms derived in this paper. The boxes refer to the ordinary Gutzwiller semiclassical approximation [Eq. (17), $j = 0, 1$], where the diffraction effects are not included.

$\Delta_G(k)\Delta_D(k)$ at maximal cycle length 5 and using only the $l = 1$ term in the now restored summation over the creeping mode number. The exact quantum mechanical resonances were computed following Ref. [14].

The leading semiclassical resonances are given equally well with and without creeping modifications. In Fig. 2 we can see that the new formula describes the resonances of the two-disk system with a few-percent error, while the computation based on the geometrical cycle alone, Eq. (16), gives completely false results for the next-to-leading resonances [see Eq. (17)].

The authors are very grateful to P. Cvitanović for encouraging the project. A. W. thanks NORDITA and NBI for hospitality. G. V. and P. E. R. thank SNF for support and G. V. acknowledges the support of the Széchenyi Foundation, Phare Accord H 9112-0378 German-Hungarian Cooperation 62, and OTKA F4286.

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