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Exact trace formulas for a class of one-dimensional ray-splitting systems

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Using quantum graph theory we establish that the ray-splitting trace formula proposed by Couchman *et al.* [Phys. Rev. A **46**, 6193 (1992)] is exact for a class of one-dimensional ray-splitting systems. Important applications in combinatorics are suggested.

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I. INTRODUCTION

Gutzwiller's trace formula, established in the late 1960s and early 1970s, states that it is possible to obtain the level density of a bounded Hamiltonian dynamical system with semiclassical accuracy, based entirely on the information provided by its classical periodic orbits [1,2]. According to Gutzwiller the density of energy states can be written as a sum over prime periodic orbits and their repetitions,

$$\begin{aligned} \rho(E) &= \sum_n \delta(E - E_n) \\ &= \bar{\rho}(E) + \frac{1}{\pi\hbar} \operatorname{Re} \sum_p T_p(E) \\ &\quad \times \sum_{\nu=1}^{\infty} A_{p\nu}(E) e^{i\nu[S_p(E)/\hbar + \varphi_p(E)],} \end{aligned} \quad (1.1)$$

where $\bar{\rho}(E)$ is the average density of states, S_p is the classical action of the prime periodic orbit p ,

$$T_p = \frac{\partial S_p(E)}{\partial E} \quad (1.2)$$

is its period, and $\varphi_p(E)$ is its Maslov phase. Gutzwiller derived the preexponential factors $A_{p\nu}$ in semiclassical approximation, expressing them in terms of the stability properties of the corresponding periodic orbits.

The orbits used to construct the sum (1.1) are obtained at a given value of the energy E . On the other hand it is known that, as the energy of a generic, nonhyperbolic system changes, the structure of the phase space changes and with it the set of periodic orbits. This phenomenon is called "phase-space metamorphosis" [3]. Phase-space metamorphosis, in general, is accompanied by the creation and destruction of periodic orbits giving rise to the interesting phenomenon of ghost orbits [4]. Therefore, in general, the sum in Eq. (1.1) will change as a function of E in the sense that it may acquire or lose certain terms. However, apart from hyperbolic systems [5], there exists an interesting class of systems, that are free of such metamorphoses of the phase space. These are the scaling systems, for which the action functional $S_p(E)$ for any periodic orbit p decouples into the product of an energy-dependent part $f(E)$ and the "reduced action" S_p^0 , which depends only on the geometry of the periodic orbit,

$$S_p(E) = f(E)S_p^0. \quad (1.3)$$

Examples of such systems are various billiard systems, and also (with suitable definitions of scaling parameters) the hydrogen atom in strong electric and/or magnetic fields [2,6,7]. For such systems neither the geometry of the phase space nor the geometry of the set of periodic orbits changes with energy. Therefore the structure of the sum (1.1) can be defined once and is valid for all values of E . In such cases it is interesting to investigate the relationship between the fixed set of periodic orbits (the periodic orbit spectrum) and the quantum energy spectrum.

Direct derivation of Gutzwiller's trace formula, as presented originally by Gutzwiller, is based on the saddle point approximation. This implies that this formula is meant to work only semiclassically, i.e., to predict only the highly excited energy levels with semiclassical accuracy. Indeed, for generic billiard domains, Gutzwiller's formula is not exact [1]. However, in certain special cases Eq. (1.1) is known to predict the entire energy spectrum exactly. An example is the harmonic oscillator. Moreover, exact "Gutzwiller-like" trace formulas do exist. A theorem by Anderson and Melrose [8] states that for any billiard there exists a set of preexponential factors A_α that makes the relationship (1.1) exact. Other exact Gutzwiller-like trace formulas are obtained in the context of quantum graph theory [9–11]. We show that ray-splitting systems [12] provide further examples of exact Gutzwiller-like trace formulas. A specific example, a scaling one-dimensional step billiard, closely related to quantum graphs, is presented in the following section together with its generalized ray-splitting Gutzwiller formula. In Sec. III we present a proof for the exactness of the ray-splitting Gutzwiller formula. In Sec. IV we define the ray-splitting Z function and relate it to cycle expansion techniques. In Sec. V we make use of the exactness of the ray-splitting Gutzwiller formula to prove a nontrivial combinatorial identity. In Sec. VI we discuss our results and conclude the paper.

II. MODEL

In this section we study the spectrum and the generalized ray-splitting Gutzwiller formula for the one-dimensional scaling step billiard [12–16] (Fig. 1)

$$V(x) = \begin{cases} 0, & \text{for } 0 < x \leq b \\ V_0 = \lambda E & \text{for } b < x < 1, \end{cases} \quad (2.1)$$

This, in turn, suggests that there exists an exact formula of the type (1.1). That this is indeed the case is proved in Sec. III below.

A natural generalization of Gutzwiller's trace formula, which includes the contributions from the non-Newtonian ray-splitting orbits, was obtained previously in [12]. Speaking in terms of the step potential (2.1), instead of just a single orbit bouncing between $x=0$ and $x=1$, a generic orbit may now be reflected off or transmitted through the ray-splitting boundary at $x=b$ any number of times in arbitrary sequence. As a result, the set of *primitive non-Newtonian orbits* becomes infinite. In a one-dimensional system the numbers of these reflections and transmissions are the only characteristics of the orbits, and therefore any orbit can be characterized uniquely and completely by a binary sequence of symbols \mathcal{L} and \mathcal{R} that keep track of each reflection off the left (\mathcal{L}) or the right (\mathcal{R}) wall of the potential well. The corresponding generalized Gutzwiller sum includes all primitive Newtonian and non-Newtonian periodic orbits and their repetitions,

$$\rho(E) = \bar{\rho}(E) + \frac{1}{\pi} \operatorname{Re} \sum_p T_p \sum_{\nu=1}^{\infty} [(-1)^{\chi(p)} t^{2\tau(p)} r^{\sigma(p)}]^\nu e^{i\nu S_p}, \quad (2.9)$$

where $\bar{\rho} = [b + \beta(1-b)] / (2\pi k)$ is the average level density, r , defined by Eq. (2.6), is the quantum reflection coefficient, $t = \sqrt{1-r^2}$ is the transmission coefficient, $\sigma(p)$ and $2\tau(p)$ are the number of reflections and transmissions of the primitive orbit p at the potential step, and $\chi(p)$ counts the total number of times the orbit reflects off the walls and off the potential step to the right of the ray-splitting boundary. Note that $(-1)^{\chi(p)} = e^{i\varphi_p}$ and explicitly defines the Maslov phase in Eq. (1.1).

If we denote the actions of the shortest orbits (\mathcal{R} and \mathcal{L}) by $S_{\mathcal{R}}$ and $S_{\mathcal{L}}$, respectively, the action S_p of any orbit can be expressed as a sum,

$$S_p = n_{\mathcal{L}} S_{\mathcal{L}} + n_{\mathcal{R}} S_{\mathcal{R}}, \quad (2.10)$$

for certain integers $n_{\mathcal{L}}$ and $n_{\mathcal{R}}$ (generally different from σ and τ). The level density (2.9) contains only even powers of the transmission coefficient t , because every periodic orbit transmits an even number of times through the ray-splitting boundary.

III. EXACTNESS OF THE RAY-SPLITTING TRACE FORMULA

Using quantum graph theory [9–11], it is possible to show that the expression (2.9) is exact. We prove this below after presenting some basic ideas of quantum graph theory.

From the perspective of quantum graph theory, the quantization of a particle in the potential (2.1) is treated as a scattering problem on the graph

$$\bullet_1 \text{---} \bullet_2 \text{---} \bullet_3 \quad (3.1)$$

with three vertices and two bonds described by the connectivity matrix [9–11]

$$C = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}. \quad (3.2)$$

On every bond connecting vertices i and j , one defines a free particle wave function ψ_{ij} , which satisfies the following vertex conditions:

$$\psi_{ij}(\xi=0) = \varphi_i, \quad \psi_{ij}(\xi=L_{ij}) = \varphi_j, \quad (3.3)$$

where ξ is the coordinate along a particular bond of length L_{ij} , so that the wave functions on different bonds match on every vertex. The general solution satisfying the vertex conditions is

$$\begin{aligned} \psi_{ij}(\xi) &= \frac{\varphi_i C_{ij}}{\sin[k\beta_{ij}L_{ij}]} \sin[k\beta_{ij}(L_{ij}-\xi)] \\ &+ \frac{\varphi_j C_{ij}}{\sin[k\beta_{ij}L_{ij}]} \sin[k\beta_{ij}\xi]. \end{aligned} \quad (3.4)$$

The presence of the coefficients β_{ij} allows us to generalize the formalism developed in [9–11]. For the derivatives we have the continuity conditions

$$\sum_{j<i} C_{ij} \psi'_{ji}(\xi=L_{ij}) = \sum_{j>i} C_{ij} \psi'_{ij}(\xi=0). \quad (3.5)$$

For the case of the potential (2.1),

$$\psi_{12}(\xi) = \frac{\varphi_2}{\sin(kb)} \sin(k\xi), \quad (3.6)$$

$$\psi_{23}(\xi) = \frac{\varphi_2}{\sin[k\beta(1-b)]} \sin[k\beta(1-b-\xi)]. \quad (3.7)$$

The matching and continuity conditions at vertex 2 result in

$$\beta \tan(kb) + \tan[k\beta(1-b)] = 0 \quad (3.8)$$

or

$$\sin[k(l_1+l_2)] - r \sin[k(l_1-l_2)] = 0, \quad (3.9)$$

which is the same as Eq. (2.4). The lengths l_1 and l_2 , defined in Eq. (2.5) turn out to be the weighted bond lengths.

The same quantization condition can be obtained from considering the scattering process at every vertex of the graph (3.1). The vertex scattering matrix is given by

$$\sigma_{jii'}^{(i)} = g_{jj'}^{(i)} C_{ji} C_{ij'}, \quad (3.10)$$

where the index i refers to the vertex under consideration, $g_{jj'}^{(i)}$ are coefficients that depend on the physics of the scattering at the vertex i , and C_{ij} are the matrix elements of the connectivity matrix determining the geometry of the graph. At the ‘‘dead end’’ vertices 1 and 3 of the graph (3.1) we have $\sigma_{j11j'}^{(1)} = \sigma_{j33j'}^{(3)} = -1$. For the central vertex it is easy to show that

$$\sigma_{j22j'}^{(2)} = \begin{pmatrix} r & t \\ t & -r \end{pmatrix}. \quad (3.11)$$

The graph scattering matrix, describing the graph as a whole, is given by

$$S = \begin{pmatrix} 0 & -D \\ D\sigma^{(2)} & 0 \end{pmatrix}, \quad (3.12)$$

where the matrix

$$D = \begin{pmatrix} e^{il_1k} & 0 \\ 0 & e^{il_2k} \end{pmatrix} \quad (3.13)$$

accounts for the phases accumulated along the bonds. The quantization condition [9–11]

$$\det(1 - S) = 0, \quad (3.14)$$

results in

$$e^{2i(l_1k+l_2k)} - r(e^{2il_1k} - e^{2il_2k}) = 1. \quad (3.15)$$

This is the same as Eq. (3.9).

With the help of

$$\ln \det(1 - S) = - \sum_{n=1}^{\infty} \frac{1}{n} \text{Tr}(S^n), \quad (3.16)$$

the quantization condition (3.14) can be written alternatively as a sum over the periodic orbits of the graph. Indeed, since the scattering matrix is defined geometrically using the graph connectivity matrix, its indices correspond to the vertices i and j connected by a bond if the matrix element $C_{ij} \neq 0$. The trace of the n th power of this matrix is defined on the set of all the possible cyclical n -bond sequences. Using Eqs. (3.10) and (3.12) we obtain $\text{Tr}(S^{2n+1}) = 0$ and

$$\text{Tr}(S^{2n}) = 2 \sum_{n_{\mathcal{L}} + n_{\mathcal{R}} = n} (-1)^{\chi} r^{\sigma} t^{2\tau} e^{2ikL_n}, \quad (3.17)$$

where $n_{\mathcal{L}}$ and $n_{\mathcal{R}}$ give the number of times the left (\mathcal{L}) and the right (\mathcal{R}) bonds of Eq. (3.1) occur in the sequence, $L_n = n_{\mathcal{L}}l_1 + n_{\mathcal{R}}l_2$, σ is the number of reflections from the middle vertex, and 2τ is the number of transmissions through it. Since the reflection coefficient coming from the scattering matrix (3.11) can be positive or negative, the factor $(-1)^{\chi}$ is needed to keep track of how many times it appears with a minus sign. It also keeps track of how many times a given orbit scatters off the walls.

There are two possibilities for L_n . Either it corresponds to a prime periodic orbit, or it corresponds to a bond sequence that retraces itself ν times. In this case L_n is ν times the length of a single (primitive) traversal L_p , and the preexponential factor is the ν th power of the factor corresponding to the shortest closed bond sequence. Alternatively, these closed bond sequences can be viewed as periodic orbits traced by a particle moving on the graph.

On the other hand, from the analytical properties of $\det[1 - S(E)]$ [11], it is easy to relate it to the spectral counting function $N(E)$,

$$N(E) = \bar{N}_W(E) - \frac{1}{2} + \frac{1}{\pi} \text{Im} \sum_{n=1}^{\infty} \frac{1}{n} \text{Tr}(S^n), \quad (3.18)$$

where $\bar{N}_W(E)$ is the average spectral staircase function (the Weyl term). Putting all these ingredients together, one arrives at the trace formula (2.9).

The exactness of Eq. (2.9) can be understood on the basis of the dramatic increase of the number of primitive non-Newtonian orbits included in it. As the orbit length L_p in Eq. (2.9) increases, non-Newtonian orbits proliferate exponentially, providing additional information about the structure of the potential $V(x)$.

It is interesting to compare Eq. (2.9) with the results produced by Gutzwiller's trace formula without ray splitting. For the step potential (2.1) there exists only one Newtonian periodic orbit with classical action S_N which bounces between the left and the right walls of the well (Fig. 1). Therefore Eq. (2.9) predicts

$$\rho(E) = \bar{\rho}(E) + \frac{T_N}{\pi} \sum_{\nu=1}^{\infty} \cos(\nu S_N) = T_N \sum_{m=-\infty}^{\infty} \delta(S_N - 2\pi m), \quad (3.19)$$

where

$$S_N = 2kb + 2k\beta(1-b) = S_N^0 k, \quad (3.20)$$

$T_N = \partial S_N / \partial E$, and $\bar{\rho} = T_N / 2\pi$. Since only a single periodic orbit contributes, Eq. (3.19) predicts a periodic spectrum for a particle in the step potential (2.1). Moreover, the Fourier image

$$F(s) = \int \rho(E) e^{-isk} dE = [S_N^0]^2 \sum_{m=-\infty}^{\infty} \delta[mS_N^0 - s] \quad (3.21)$$

of the density of states produces δ peaks at integer multiples of the reduced action S_N^0 of the (only) Newtonian orbit of the system. Figure 3 shows that the exact spectrum of the problem is not periodic, which illustrates that the trace formula (1.1) [(2.9), respectively] without non-Newtonian orbits predicts a wrong energy level distribution.

A straightforward generalization of the ideas and procedures discussed above provides a proof of the exactness of Eq. (2.9) for the whole class of N -step scaled potentials

$$V(x) = V_i = \lambda_i E, \quad b_{i-1} < x < b_i, \quad i = 1, \dots, N, \quad (3.22)$$

where $b_0 = 0$, $b_N = 1$, and λ_i is the scaling coefficient for the i th interval $[b_{i-1}, b_i]$.

IV. RAY-SPLITTING Z FUNCTION

Despite its exponentially decreasing terms, Eq. (2.9) converges only conditionally due to the exponential proliferation

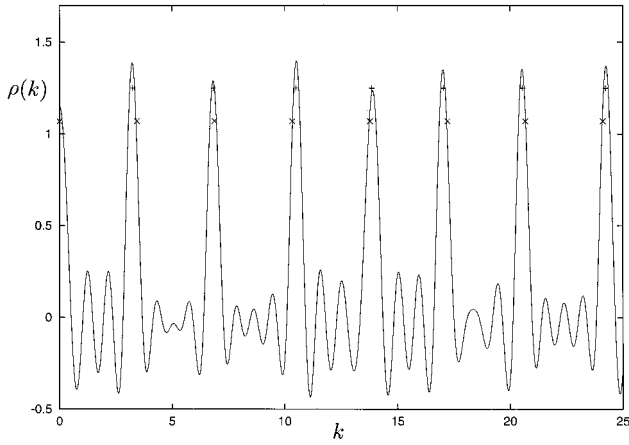


FIG. 3. Contribution of the 43 shortest Newtonian and non-Newtonian periodic orbits (up to binary code length 7) to the density of states of the step potential shown in Fig. 1. The exact energy eigenvalues (+) are close to the locations of the peaks. For comparison the energy levels predicted by the Newtonian orbits alone are also shown (\times).

of the non-Newtonian orbits. Therefore, one should specify a physically meaningful way of partial summation for this series. In practice, one could certainly consider the shortest periodic orbits in order to get an approximation for Eq. (2.9). Figure 3 presents the contribution of the 43 shortest periodic orbits. This corresponds to including all periodic orbits up to binary code length 7 (e.g., $\mathcal{LRRL\mathcal{L}\mathcal{L}\mathcal{L}\mathcal{L}$). Figure 3 shows that the peaks give a very accurate representation of the actual positions of the roots.

Since Eq. (2.9) is a geometric series with respect to the repetition index ν , this part of the summation can be performed immediately, yielding

$$\rho(E) = \bar{\rho}(E) + \frac{1}{\pi} \operatorname{Re} \sum_p T_p \frac{(-1)^{\chi(p)} t^{2\tau(p)} r^{\sigma(p)} e^{iS_p(E)}}{1 - (-1)^{\chi(p)} t^{2\tau(p)} r^{\sigma(p)} e^{iS_p(E)}}. \quad (4.1)$$

Using the relation (1.2), the density of states can be written as

$$\rho(E) = \bar{\rho}(E) - \frac{1}{\pi} \operatorname{Im} \frac{\partial}{\partial E} \ln Z(E), \quad (4.2)$$

where

$$Z(E) = \prod_p [1 - (-1)^{\chi(p)} t^{2\tau(p)} r^{\sigma(p)} e^{iS_p(k)}] \quad (4.3)$$

is an analog of the Fredholm determinant associated with the ray-splitting system (2.1) and the sum (2.9), considered as a function of the coefficients r and t . One can consider a cycle expansion [18] of the product (4.3) in powers of r or t . A natural choice for the expansion variable would be the smaller one of r, t . Physically, this asymmetry determines whether reflection or transmission is the dominant process.

V. COMBINATORICS

In quantum graph theory the representation of the quantum level density in the form of a Gutzwiller-like trace formula is exact [9–11]. In special cases both the level density and the trace formula can be evaluated analytically and give rise to combinatorial identities. This idea was successfully implemented by Schanz and Smilansky, who obtained a host of new and nontrivial combinatorial identities [19]. Additional identities are generated whenever Eq. (3.9) can be solved analytically. We illustrate the method by choosing β such that $l_1 = b$ and $l_2 = \beta(1 - b) = b$ in Eq. (3.9). In this case (3.9) becomes $\sin(2kb) = 0$, solved by $k_n = n\pi/(2b)$. The corresponding periodic level density can be obtained directly using the conventional Poisson formula,

$$\rho(E) = \sum_{n=1}^{\infty} \delta\left(E - \frac{\pi^2 n^2}{4b^2}\right) = \frac{b}{\pi k} \sum_{m=-\infty}^{\infty} e^{im4bk}. \quad (5.1)$$

It is interesting that the arguments of the exponents in Eq. (5.1) coincide with the actions of the repetitions of the Newtonian orbit, $S_N = 4bk$. This coincidence is due to the special choice of parameters $l_1 = l_2 = b$ assumed in this case.

Alternatively, the level density (5.1) can be expressed via Eq. (2.9). Equating the prefactors of terms with the same action results in the sum rule

$$1 = \frac{1}{T_N} \sum_{p\nu} T_p [(-1)^{\chi(p)} t^{2\tau(p)} r^{\sigma(p)}]^\nu. \quad (5.2)$$

Here $T_N = 2b/k$ and the sum on the right-hand side is over all periodic orbits, Newtonian and non-Newtonian, that add up to the same multiple of the Newtonian action S_N .

The sum rule (5.2) can be recast into a combinatorial theorem on the set W_Λ of cyclically nonequivalent binary codes of even length $\Lambda = 2M$ over the symbols \mathcal{L} and \mathcal{R} in the following way. (i) For every word $w \in W_\Lambda$ compute the primitive time T_w defined as $T_w = M/\nu_w$, where ν_w is the number of repetitions of the shortest subcode in w . (ii) Scan each word $w \in W_\Lambda$ and assign

$$w \rightarrow (-1)^{\alpha_w} (r^2)^{\beta_w} (t^2)^{\gamma_w} \quad (5.3)$$

according to the substitutions

$$\mathcal{LR} \rightarrow t, \quad \mathcal{RL} \rightarrow t, \quad \mathcal{LL} \rightarrow r, \quad \mathcal{RR} \rightarrow -r. \quad (5.4)$$

Then, with $r^2 + t^2 = 1$, we have

$$\sum_{w \in W_\Lambda} T_w (-1)^{\alpha_w} (r^2)^{\beta_w} (t^2)^{\gamma_w} = 1, \quad (5.5)$$

which is equivalent to the sum rule (5.2). Stated differently, Eq. (5.5) is the same as

$$\sum_{w \in W_\Lambda, \beta_w = \beta} (-1)^{\alpha_w} T_w = \binom{M}{\beta}. \quad (5.6)$$

VI. DISCUSSION AND CONCLUSIONS

Since Atle Selberg discovered his famous trace formula [20], more exact trace formulas have been found. There are many cases in which the geometrical information contained in the set of closed geodesics (periodic orbits) can be used to reconstruct the spectrum exactly. Gutzwiller provided a physical theory that parallels these results. His formula points the way to establish *approximate* relationships, which involve physical rather than geometrical concepts. In particular, Gutzwiller uses the semiclassical saddle point approximation, valid under certain physical conditions, in order to derive the pre exponential factors in Eq. (1.1) in a form, that is valid for a wide class of dynamical systems.

However, Gutzwiller's theory does not imply that these sums are necessarily approximate. There exist different approaches to establish exact relationships between the spectra of operators and the spectra of periodic orbits. The above method, based on the intuitively clear idea of ray splitting, provides an example that is physical, lies outside the scope of Gutzwiller's approach, and is exact.

This result immediately suggests many important applications. First, from the mathematical point of view, one can derive statements about the behavior of the zeros of a wide class of almost periodic functions. Second, the exactness of Eq. (2.9) provides a convenient way to prove many combinatorial identities, expressible in terms of periodic orbits in Eq. (2.1). Lastly, it provides a nontrivial way to obtain Feynman's path integrals in a well-defined limit. It is a natural idea to approximate arbitrary one-dimensional potentials by a steplike profile such as (3.22), for which (2.9) is exact. Taking the limit in which the size of the steps tends to zero, one can approximate the shape of any smooth potential with any accuracy. As the number of steps increases, the sum over the non-Newtonian orbits leads to Feynman's path integral.

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