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LETTER TO THE EDITOR

Ray splitting with ghost orbits: explicit, analytical and exact solution for spectra of scaling step potentials with tunnelling

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Online at stacks.iop.org/JPhysA/38/L563**Abstract**

In the familiar concept of ray splitting, a ray incident on an interface splits into reflected and transmitted rays. Tunnelling adds something new to ray splitting: an incident Newtonian ray splits into a reflected Newtonian ray and a transmitted ray with complex classical action—a *ghost orbit*. Using novel periodic-orbit expansion techniques, we are able to compute explicitly and analytically energy eigenvalues of an energy-scaling one-dimensional step potential. Inclusion of all periodic orbits in our series expansions, in particular a class of orbits called *pure ghosts* with imaginary classical action, makes our formulae *exact*. We suggest an experiment that may be used to verify the importance of pure ghosts.

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Ray splitting, a term coined by Couchman *et al* [1] in their investigation of acoustic and quantal systems having sharp interfaces, is a venerable concept dating at least as far back as the work of Snell [2] on the reflection and transmission of light rays at an air–water interface. In the quantum mechanical context, ray splitting has important consequences such as addition of a universal ray-splitting correction term to the density of states [3] and production of non-Newtonian periodic orbits. Both the importance of non-Newtonian orbits and the universal ray-splitting correction have been confirmed in recent microwave experiments with dielectric inserts [4, 5].

To illustrate the concept of non-Newtonian classical orbits, consider a classical particle with energy $E > V_0$ in the one-dimensional potential $V(x)$ shown in figure 1. According to Newtonian mechanics, the particle executes a periodic motion between the walls \mathcal{L} and \mathcal{R} of the potential $V(x)$ represented by the periodic orbit P_1 in figure 1. However, for the exact quantal description of the particle, the orbits P_2 and P_3 are equally important. It was shown

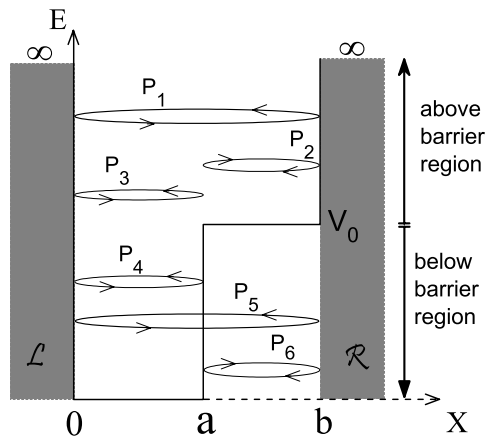


Figure 1. Step potential $V(x)$ illustrating various types of classical periodic orbits contributing to the quantal dynamics of a particle in $V(x)$. P_1 : Newtonian orbit bouncing between the potential walls \mathcal{L} and \mathcal{R} ; P_2, P_3 : non-Newtonian above-barrier reflection orbits; P_4 : Newtonian orbit for $E < V_0$, bouncing between potential wall \mathcal{L} and the potential step at $x = a$; P_5 : complex action ghost orbit for $E < V_0$ bouncing between potential walls \mathcal{L} and \mathcal{R} ; P_6 : ‘pure ghost’ with purely imaginary action bouncing entirely below the potential barrier V_0 .

both experimentally [4] and theoretically [6, 7] that P_2 and P_3 are ‘real’ in the sense that they, too, produce clear peaks in the Fourier transform of the level density. Because P_2 and P_3 do not exist in Newtonian mechanics, they are called *non-Newtonian orbits* [4]. Though non-Newtonian, P_2 and P_3 are, nevertheless, proper classical orbits in the following sense. The reflection amplitude r for a quantum particle of energy E incident on a potential step of height V_0 is

$$r = \frac{\sqrt{E} - \sqrt{E - V_0}}{\sqrt{E} + \sqrt{E - V_0}}. \quad (1)$$

Because \hbar does not appear in (1), r is a classical quantity: even in the classical limit of $\hbar \rightarrow 0$, and even though $E > V_0$, the reflection amplitude stays finite. Therefore, in order to be exact, a periodic-orbit expansion technique must include the classical, but non-Newtonian, orbits P_2 and P_3 . It was shown recently [8, 9] that exact, explicit quantization formulae for the above-barrier ($E > V_0$) energy spectrum of the potential shown in figure 1 are obtained by including P_2 and P_3 as well as all periodic orbits and their repetitions that can be constructed by combining P_2 and P_3 .

Direct, exact periodic-orbit expansions of individual energy levels [8, 9] is a new direction in quantum mechanics. This letter presents the first exact, explicit periodic-orbit expansions of energy levels in the tunnelling regime $E < V_0$. In this regime, Newtonian mechanics allows for the existence of a single classical orbit, called P_4 in figure 1. On it a particle bounces between the potential wall \mathcal{L} and the potential step at $x = a$. We find that to obtain exact energy formulae it is necessary to include in the periodic-orbit expansions the so-called *ghost orbits* [10], which are (partially) under-barrier orbits having complex classical action. Ghost orbits have already been seen in atomic physics experiments [11, 12]. Examples of ghost orbits in figure 1 are P_5 and P_6 .

Ghost orbits lead to a new type of ray splitting whereby a Newtonian ray incident on the barrier splits into a reflected Newtonian ray with real action and a transmitted ghost ray with imaginary action.

Combining a Newtonian section ($0 < x < a$) with real classical action and a non-Newtonian section ($a < x < b$) with imaginary action, the total action of P_5 is complex, so in analogy to nomenclature used in the contemporary literature [10], it is a ghost orbit. We will show that even the orbit P_6 , bouncing *entirely under* the barrier, is important for a proper quantal description of a particle in $V(x)$. Moreover, this orbit must be included to obtain *exact* quantal formulae for the energy spectrum of a particle in $V(x)$. Finally, we propose an experimental scheme for measuring properties of P_6 such as its imaginary action.

Our derivation of an explicit, exact expression for the spectrum of a quantal particle in the potential of figure 1 focuses on the *scaling* case [8, 9] characterized by $V_0 = vE$, where v is a real number. Since this letter focuses on the tunnelling regime, we choose $v > 1$, which corresponds to $E < V_0$. The spectral equation of a quantal particle in this $V(x)$ is

$$\eta \sin(ka) \cosh(\eta kd) + \cos(ka) \sinh(\eta kd) = 0, \tag{2}$$

where $d = b - a$ and $\eta = \sqrt{v - 1}$. We denote the positive solutions of (2) by k_n , $n = 1, 2, 3, \dots$; they define the energy spectrum according to $E_n = \hbar^2 k_n^2 / 2M$, where M is the mass of the particle.

We define the staircase of the solutions k_n of (2) by [13] $\mathcal{N}(\chi) = \sum_{n=1}^{\infty} \theta(\chi - \chi_n)$, where $\chi = ka$, $\chi_n = k_n a$, and $\theta(\chi) = 0$, for $\chi < 0$, $\theta(\chi) = 1/2$ for $\chi = 0$ and $\theta(\chi) = 1$, for $\chi > 0$. Based on the scattering quantization approach pioneered in [14, 15], we compute $\mathcal{N}(\chi)$ explicitly according to

$$\mathcal{N}(\chi) = -\frac{1}{2} + \frac{\chi}{\pi} + \frac{\phi(\chi)}{\pi} + \frac{1}{2\pi} \text{Im Tr} \sum_{m=1}^{\infty} \frac{1}{m} S^{2m}(\chi). \tag{3}$$

The 2×2 scattering matrix in (3) is given by

$$S(\chi) = \begin{pmatrix} 0 & R(\chi) e^{i\chi} \\ -e^{i\chi} & 0 \end{pmatrix}, \tag{4}$$

where $R(\chi) = r[1 - r^* \exp(-2\gamma\chi)] / [1 - r \exp(-2\gamma\chi)]$ and $\gamma = \eta d/a$; r is the reflection amplitude for $b \rightarrow \infty$ that is given, according to (1), by $r = [1 - i\eta] / [1 + i\eta]$. The function $\phi(\chi)$ in (3) is

$$\phi(\chi) = \arctan \left[\frac{1}{\eta} \tanh(\gamma\chi) \right]. \tag{5}$$

Noting that the solution χ_n , and only χ_n , is contained in the interval $[\xi_n^{(-)} = (n - \frac{1}{2})\pi, \xi_n^{(+)} = (n + \frac{1}{2})\pi]$, we have

$$\int_{\xi_n^{(-)}}^{\xi_n^{(+)}} \mathcal{N}(\chi) d\chi = (n - 1)[\chi_n - \xi_n^{(-)}] + n[\xi_n^{(+)} - \chi_n], \tag{6}$$

which can be solved for χ_n , with the result

$$\chi_n = n\pi - \frac{\phi_n}{\pi} - \frac{1}{\pi} \text{Im} \sum_{m=1}^{\infty} \frac{(-1)^m}{m} \int_{\xi_n^{(-)}}^{\xi_n^{(+)}} R^m(\xi) e^{2mi\xi} d\xi, \tag{7}$$

where

$$\phi_n = \int_{\xi_n^{(-)}}^{\xi_n^{(+)}} \phi(\chi) d\chi = \pi \arctan \left(\frac{1}{\eta} \right) + \text{Im} \sum_{m=1}^{\infty} \frac{r^m}{m^2 \gamma} e^{-2nm\gamma\pi} \sinh(m\gamma\pi). \tag{8}$$

To check our algebra, we compared $\chi_n^{(\text{ana})}$ computed with equation (7) with $\chi_n^{(\text{num})}$ computed by direct numerical solution of equation (2) for $n = 1, \dots, 100$ and many different choices

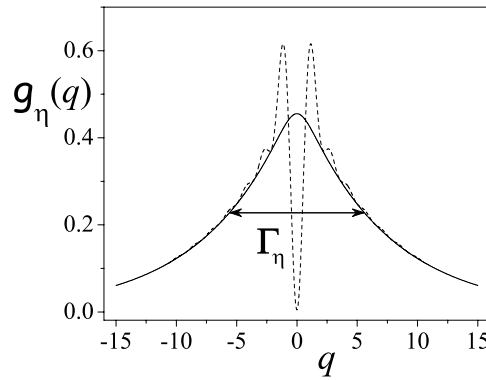


Figure 2. Full line: scaling function $g_\eta(q)$ used for extracting the reduced action of pure ghosts from numerical or experimental spectral data. Dashed line: regularized Fourier transform $f^{(N)}(\sigma = q\gamma)$ for $N = 30$.

of v and the ratio a/b . We found that in all cases, $|\chi_n^{(\text{ana})} - \chi_n^{(\text{num})}|$ can be made as small as desired. Thus, our algebra is correct. It is important to emphasize here that equation (7) does not define a procedure for obtaining improved computational speed; it was never meant to be. Equation (7) is an *intellectual* advance: for the first time, bound-state energy levels are analytically calculated exactly and explicitly for a scaling system in the tunnelling regime.

The explicit formula (7) allows for an interpretation in terms of periodic orbits, for which figure 1 will be useful. Expanding R into a power series in r yields an expression that starts with unity. Thus, we see that the leading term of the sum in (7) corresponds to the summation of all possible Newtonian orbits of the type P_4 . The remaining terms correspond to all possible ghost orbits of the type P_5 . Even the pure ghosts of the type P_6 contribute decisively to the explicit formula (7). We see this by inspecting equation (5), which can be expanded into a power series over all pure ghosts whose actions are multiples of $2i\gamma\chi$.

So far we computed energy levels χ_n in terms of periodic orbits. But the reverse procedure works too. Given the spectrum $\{\chi_n\}_{n=1}^\infty$, the Fourier transform $\mathcal{F}(\sigma) = \sum_{n=1}^\infty \cos(\sigma\chi_n)$ reveals its periodic-orbit contents. $\mathcal{F}(\sigma)$ consists of a picket fence of two-periodic peaks on a smooth background. Peaks at $\sigma = \pm 2, \pm 4, \dots$ are signatures of the Newtonian orbit P_4 and its repetitions, and of ghost orbits of type P_5 and their repetitions. The smooth background in \mathcal{F} is due to the imaginary parts of the complex actions of the ghost orbits of types P_5 and P_6 . Of particular importance is a peak at $\sigma = 0$, which corresponds to the pure ghost P_6 and its repetitions. The smooth part of the peak at $\sigma = 0$ is given by the regularized Fourier transform $f(\sigma) = \mathcal{F}(\sigma) - \delta(\sigma) + 1/2$, valid in the vicinity of $\sigma = 0$. It is given explicitly by $\pi f(\sigma) = \int_0^\infty \phi'(\chi) \cos(\sigma\chi) d\chi$. Equation (5) implies that $f(\sigma)$ scales in σ/γ , i.e. $f(\sigma) = g_\eta(\sigma/\gamma)$. The scaling function g_η is shown as the full line in figure 2 for $v = 1.02$. Its full width at half maximum is denoted by Γ_η . We discuss now how the scaling property can be turned into a method for the experimental extraction of ghost-orbit information.

We propose to study experimentally the properties of non-Newtonian ghost orbits with a quasi-one-dimensional (q1D) dielectric-loaded microwave cavity shown schematically in figure 3. The dielectric-filled region I ($0 < x < a$) is assumed to have relative electric permittivity $\kappa_e = \epsilon/\epsilon_0 > 1$ and relative magnetic permeability $\kappa_m = 1$; vacuum ($c^2\mu_0\epsilon_0 = \kappa_e = \kappa_m = 1$) or air ($\kappa_e \simeq \kappa_m \simeq 1$) fills region II ($a < x < b$). The setup shown in figure 3 allows experimental implementation of the Schrödinger equation for a quantal particle in the potential $V(x)$ of figure 1. Both the cavity height H and cavity width W are

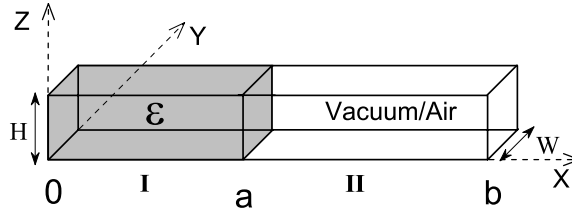


Figure 3. Sketch of the proposed quasi-one-dimensional microwave setup for extracting ghost-orbit information from experimental resonance spectra. Coupling the width W of the cavity to the microwave frequency ω allows scaled spectra to be taken in the tunnelling regime.

assumed to be small compared to the cavity length b , such that

$$H \ll \frac{c\pi}{\omega\sqrt{\kappa_e}} < W < \frac{2\pi c}{\omega\sqrt{\kappa_e}} \quad (9)$$

for all operating frequencies ω of interest. In this case, the oscillating modes of the cavity are transverse magnetic modes of the type TM_{n10} , $n = 1, 2, \dots$, where n is the mode index in the x -direction, the index ‘1’ indicates that only the first mode is excited in the y -direction and the index ‘0’ means that the electric field $E_z^{(n)}(x, y)$ of the TM_{n10} cavity mode is independent of z . Thus, $E_z^{(n)}(x, y) = \psi_n(x) \sin(\pi y/W)$. Since $E_z^{(n)}(x, y)$ satisfies $[\Delta + \kappa_e \omega^2/c^2]E_z = 0$ [16], we have

$$\psi_n''(x) - \left(\frac{\pi}{W}\right)^2 \psi_n(x) + \frac{\kappa_e \omega^2}{c^2} \psi_n(x) = 0. \quad (10)$$

If we now assume that the width W of the cavity is coupled to the cavity frequency via $W = s/\omega$, where s is a constant, (10) turns into an energy-scaling problem of the scaling Schrödinger type considered above. Thus, the potential shown in figure 1 is experimentally realizable and is, therefore, more than an academic problem. Indeed, defining $E = \omega^2[\kappa_e - (\pi c/s)^2]/c^2$, we obtain $-\psi_n''(x) = E_n \psi_n(x)$ in region I and $-\psi_n''(x) + v E_n \psi_n(x) = E_n \psi_n(x)$ in region II, where $v = (\kappa_e - 1)/[\kappa_e - (\pi c/s)^2]$. Proper adjustment of s allows realization of the cases $v < 1$ (above-barrier case), $v = 1$ (degenerate case) and $v > 1$ (below-barrier, tunnelling case). In the tunnelling case, e.g., together with (9), we have $\pi c/\sqrt{\kappa_e} < s < \min(\pi c, 2\pi c/\sqrt{\kappa_e})$. At a frequency of 1 GHz and $\kappa_e \approx 2$, this implies $10 \text{ cm} < W < 15 \text{ cm}$, a convenient dimension for experimental work.

The q1D cavity setup shown in figure 3 can be used (i) to verify the importance of ghost orbits and (ii) to extract experimentally the reduced action $\hat{S}_6 = S_6/(2i\chi) = \gamma$ of the pure ghost P_6 from a measured sequence $\chi_1, \chi_2, \dots, \chi_N$ of scaled resonance frequencies. From N measured frequencies, we may construct the finite- N approximation of the regularized Fourier transform $f(\sigma)$ according to $f^{(N)}(\sigma) = \sum_{n=1}^N [\cos(\sigma \chi_n) - \cos(\sigma n\pi)] u(\chi_n)$, where $u(\chi)$ is a weight function which suppresses the Gibbs phenomenon [4, 5]. Fitting $g_\eta(\sigma/\gamma)$ to $f^{(N)}(\sigma)$, the experimental value for the reduced action of the pure ghost P_6 is given by

$$\gamma^{(\text{exp})} = \Gamma_N / \Gamma_\eta. \quad (11)$$

Surprisingly few states are needed for extracting Γ_N . The dashed line in figure 2 plots $f^{(N)}$ using χ_n values obtained numerically for $v = 1.02$ with $a/b = 3/4$, $u(\chi) = \cos^2[(\pi/2)\chi/\chi_N]$ and $N = 30$. Figure 2 shows that there is no problem to extract Γ_N from this plot. The dip at $\sigma = 0$ becomes narrower for larger N . As shown in figure 2, it does not limit our ability to extract Γ_N .

The setup we propose resembles the quasi-two-dimensional (q2D) cavity setups pioneered by Stöckmann and Stein [17] and now routinely used for the microwave investigations of 2D quantum chaos; see e.g. [4, 5, 18–20]. However, ours differs in one crucial respect: the width W must be variable because q1D microwave spectra are not naturally scaling for a cavity with fixed dimensions, whereas the spectra of q2D cavities are scaling [3]. Though a cavity with variable side length has been used to measure parametric correlations of energy levels in a Sinai ray-splitting billiard [21], the variable dimension we propose introduces the complication of keeping the width of a dielectric insert equal to the cavity width W . A liquid dielectric could solve this problem and afford an additional advantage: use of mixtures of liquids would allow κ_c to be adjusted continuously.

Although one dimensional, our system is not trivial. According to figure 1, contributing periodic orbits can be enumerated with the help of a binary ‘ \mathcal{L} , \mathcal{R} ’ code [22]. The number of binary code words of length B is 2^B . Thus, the number of periodic orbits contributing to (7) grows exponentially. New in our system is that the ‘lion’s share’ of the exponentially proliferating orbits are orbits with complex action (ghost orbits). We note that although an infinite number of exponentially proliferating periodic orbits have to be summed, the sum nevertheless converges to the correct results for the energy levels χ_n [23].

There are essentially two ways to treat tunnelling semiclassically: the method of complex time and the method of complex phase space. The former leads to the theory of instantons [24], which, at this point, is not developed far enough to yield explicit, exact spectral formulae in the tunnelling regime. We opted for the latter method, which leads to classical paths with complex actions, i.e. ghost orbits. But in contrast to semiclassical methods, we emphasize that our method is *exact*. It provides us with exact periodic-orbit expansions of individual energy eigenvalues in the tunnelling regime.

In summary, we report several innovations: (i) a new type of ray splitting involving ghost rays; (ii) direct, exact periodic-orbit expansions of energy levels in the tunnelling regime; (iii) a proposed new dielectric-loaded cavity setup for taking scaled energy spectra; and (iv) a scheme for an experimental test of the manifestations of ‘pure ghosts’.

Although this letter focuses on the case of a single, scaling step potential, we have recently constructed explicit, analytical solutions for scaling δ -function potentials and piecewise constant scaling potentials consisting of several steps [23]. Moreover, although we have not actually written them out explicitly, we are able to prove that exact periodic-orbit expansions exist for a class of piecewise constant scaling potentials with an arbitrary number of steps as long as their spectral equations satisfy a certain ‘regularity condition’ [8, 9, 23]. A technique called the ‘ m -scheme’ in [9] may be used to overcome this restriction and serve as a basis for providing a proof for the existence of exact periodic-orbit expansions for the spectra of all piecewise constant scaling potentials.

Let us mention in closing that the spectral equation (2) is a transcendental equation that can be written as an exponential sum [25] with complex arguments. Thus, the formulae for explicit solutions in the tunnelling regime presented in this letter, together with earlier results in the above-barrier regime [8, 9], coupled with our recent advances [23], are the beginning of a systematic theory for the explicit, analytical calculation of the zeros of exponential sums.

Acknowledgments

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