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Theory of resonant scattering in two dimensions

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Abstract
We present an analytical approach to elastic scattering processes in two dimensions which is based on a formalism of resonant states for potentials having cylindrical symmetry. We obtain an expression for the elastic cross section in terms of the resonant states of the problem. Using the unitarity condition on the S-matrix we also derive an exact relationship between the elastic cross section and the local density of states. We exemplify our findings by considering a δ-potential.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

The first ideas for a theory of resonant states originated at the end of the twenties of the last century with the work of Gamow on nuclear radioactive decay [1]. He considered a situation where a particle, initially confined inside a three-dimensional region by a potential barrier, goes out of it by tunnelling. In order to describe the above process, Gamow restricted the discussion to spherically symmetric systems and looked for stationary solutions to the Schrödinger equation which at large distances consist of purely outgoing waves. He realized that the absence of incoming waves in the solution is fulfilled if the energy eigenvalues are complex. These ideas led to one of the first successful theories applying tunnelling phenomena to real systems. In 1939, Siegert also considered purely outgoing boundary conditions to derive a dispersion formula for elastic scattering by a potential of finite range [2]. The same definition of resonant states was also used by Humblet and Rosenfeld to formulate a theory of nuclear reactions [3]. Subsequent developments involved the analytical properties of the outgoing Green's function to the problem [4, 5]. These led to expansions of this function and to a consistent normalization condition for resonant states [5]. The extension of this formalism to

one dimension, for potentials that vanish beyond a distance, modifies the expression for the normalization condition [6, 7].

The design and construction of quantum corrals following the seminal work by Eigler *et al* [8, 9], by positioning atoms on top of a metal surface using the scanning tunnelling microscope, has opened the way to investigate electronic properties in two-dimensional quantum nanostructures. Measurements of the differential conductance $\mathrm{d}I/\mathrm{d}V$, which is proportional to the local density of states, in these systems exhibit well-defined resonance peaks as a function of the applied voltage, thus providing evidence of quantized resonance electron confinement in these structures [10]. Recently, work on resonant expansions of the local density of states in two dimensions has been applied to the description of coherent and incoherent processes in quantum corrals [11]. Other approaches have considered numerical calculations based on multiple s-wave scattering theory, as discussed in [10, 12].

Inspired by the above considerations, in this work we develop an analytical theory of resonant states in two dimensions for potentials having cylindrical symmetry and apply it to derive an expansion for the outgoing Green's function to the problem and the corresponding resonant expansions for the S-matrix and the elastic cross section. We also relate the elastic cross section to the local density of states using the unitarity condition obeyed by the scattering function. This in principle would permit us to relate a measurement of the elastic cross section with measurements of the differential conductance. It is worth mentioning that although previous work has addressed the derivation of the cross section in terms of the scattering matrix [13, 14], to our knowledge, a treatment involving resonant expansions is lacking in the literature that might be useful for the experimental analysis of resonant electronic properties in artificial quantum structures. We complete our analysis by presenting in an appendix a detailed derivation of the normalization condition for resonant states that follows from the residue at a complex pole of the Green's function, which is strictly different from that in three and one dimensions [5, 7].

The paper is organized as follows. Section 2 provides a relationship between the S-matrix and the outgoing Green's function of the problem that leads to an analytical expression for the elastic cross section and to a relationship between this quantity and the local density of states. Section 3 discusses resonant expansions of the quantities presented in the previous section. In section 4 the delta-potential is considered to exemplify our findings and compare them with exact analytical calculations. Finally, section 5 yields the concluding remarks and appendix A provides a detailed derivation of the normalization condition for resonant states in two dimensions.

2. Scattering in 2D

Let the Hamiltonian of a particle in two dimensions be denoted by $H = H_0 + V_0(r)$, where H_0 refers to free propagation and $V_0(r)$ represents a cylindrical symmetric potential of finite range, i.e. $V_0(r) = 0$ for $r > R$, that allows for tunnelling between the internal and external regions of the system. The rotational symmetry of the potential allows us to separate the wavefunction of the problem into polar coordinates, i.e. $\Psi(\mathbf{r}) = (1/\sqrt{2\pi})\,\psi_\ell(k, r)\exp(\mathrm{i}\ell\phi)$, where $\ell = 0, \pm 1, \pm 2, \ldots$ denotes the angular momentum quantum number. It then follows that $\psi_\ell(k, r)$ obeys the two-dimensional radial Schrödinger's equation,

$$\frac{\mathrm{d}^2}{\mathrm{d}r^2}\psi_\ell(k, r) + \frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r}\psi_\ell(k, r) + [k^2 - \mathcal{V}_0(r)]\psi_\ell(k, r) = 0, \tag{1}$$

where $\mathcal{V}_0(r) = 2mV_0(r)/\hbar^2 + \ell^2/r^2$, m being the mass of the particle. It is convenient to write the solution to the Schrödinger equation along the region $r \geqslant R$ as

$$\psi_\ell(k, r) = \tfrac{1}{2}\left[H_\ell^-(kr) + S_\ell(k)H_\ell^+(kr)\right], \tag{2}$$

where S_ℓ denotes the ℓ-wave component of the S-matrix of the problem and $H_\ell^-(kr)$ and $H_\ell^+(kr)$ denote, respectively, the ingoing and outgoing Hankel functions of integer order [16].

2.1. Relationship between S_ℓ and the outgoing Green's function

The outgoing Green's function $G_\ell^+(r, r'; k)$ of the problem satisfies the equation

$$\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + [k^2 - \mathcal{V}_0(r)]\right)G_\ell^+(r, r'; k) = \eta\frac{\delta(r - r')}{r}, \tag{3}$$

where

$$\eta = \frac{2m}{\hbar^2}. \tag{4}$$

The boundary condition satisfied by the outgoing Green's function at $r = R$ reads

$$\frac{\partial}{\partial r}G_\ell^+(r, r'; k)\bigg|_{r=R} = g_\ell(k)G_\ell^+(R, r'; k), \tag{5}$$

where $g_\ell(k)$ is defined as

$$g_\ell(k) = \frac{1}{H_\ell^+(kR)}\left[\frac{\mathrm{d}}{\mathrm{d}r}H_\ell^+(kr)\right]_{r=R}. \tag{6}$$

Let us now apply Green's theorem to equations (A.1) and (1), that is multiply equation (A.1) by $\psi_\ell(k, r)$ and equation (1) by $G_\ell^+(r, r'; E)$, subtract one equation from the other and integrate the resulting expression along the internal region of the potential interaction, namely

$$R\left[\psi_\ell(k, r)\frac{\partial}{\partial r}G_\ell^+(r, r'; k) - G_\ell^+(r, r'; k)\frac{\mathrm{d}}{\mathrm{d}r}\psi_\ell(k, r)\right]_{r=R} = \eta\psi_\ell(k, r'); \qquad r' \leqslant R. \tag{7}$$

Using equation (A.2) we may write equation (7) as

$$\eta\psi_\ell(k, r') = RG_\ell^+(R, r'; k)\left[\frac{H_\ell^{+'}(kR)}{H_\ell^+(kR)}\psi_\ell(k, R) - \psi_\ell'(k, R)\right]; \qquad r' \leqslant R \tag{8}$$

where the prime denotes the derivative with respect to r evaluated at $r = R$. Along the external region of the interaction, $\psi_\ell(k, r)$ is given by the linear combination of incoming and outgoing solutions given by equation (2), which may be used into the right-hand side of equation (8) to obtain

$$\psi_\ell(k, r') = \mathrm{i}D_\ell(kR)G_\ell^+(R, r'; k)H_\ell^-(kR), \qquad r' \leqslant R \tag{9}$$

where we have used that the Wronskian $W\big(H_\ell^-(kr), H_\ell^+(kr)\big)\big|_{r=R} \equiv \big[H_\ell^-(kR)H_\ell^{+'}(kR)) - H_\ell^+(kR)H_\ell^{-'}(kR)\big] = 4\mathrm{i}/\pi R$ and we define $D_\ell(kR) = 2\big/\big[\pi\eta H_\ell^-(kR)H_\ell^+(kR)\big]$. In order to get an expression for $S_\ell(k)$, in terms of the outgoing Green's function, we evaluate equation (9) at $r' = R$ and make use of equation (2) to obtain after a simple algebraic manipulation,

$$S_\ell(k) = \left[2\,\mathrm{i}D_\ell(kR)\;G_\ell^+(R, R; k) - 1\right]\frac{H_\ell^-(kR)}{H_\ell^+(kR)}. \tag{10}$$

Note that for $kR \gg 1$, we may use the asymptotic expressions of the Hankel functions of integer order [16], to have $D_\ell(kR) = kR/\eta$ and $H_\ell^-(kR)\big/H_\ell^+(kR) = \exp[-\mathrm{i}(2kR - \pi\ell - \pi/2)]$, which simplifies the expressions given by (9) and (10).

2.2. Elastic cross section

The total elastic cross section of the problem may be written as

$$\sigma(E) = \sum_{\ell} \sigma_\ell(E), \tag{11}$$

where $\sigma_\ell(E)$ is given by

$$\sigma_\ell(E) = \frac{1}{k}|S_\ell(E) - 1|^2. \tag{12}$$

Substitution of equation (10) into equation (12) yields

$$\sigma_\ell(E) = \frac{4}{k}\left| f_\ell + \mathrm{i}D_\ell(kR)G_\ell^+(R, R; k)\frac{H_\ell^-(kR)}{H_\ell^+(kR)}\right|^2, \tag{13}$$

where

$$f_\ell = -\frac{J_\ell(kR)}{H_\ell^+(kR)}, \tag{14}$$

with $J_\ell(kR)$ being the ordinary Bessel function of integer order.

On the other hand, it is well known that for elastic processes the difference between the asymptotic incoming and outgoing waves is given by a change in the phase. Hence, S_ℓ reads

$$S_\ell = \mathrm{e}^{2\mathrm{i}\delta_\ell}, \tag{15}$$

and consequently the corresponding expression for the elastic cross section may also be written as

$$\sigma_\ell(E) = \frac{4}{k}\sin^2\delta_\ell. \tag{16}$$

2.3. Relationship between the cross section and the local density of states

The unitarity condition for the scattering function, $S_\ell(k)S_\ell^*(k) = 1$, implies using equation (10),

$$D_\ell(kR)\left|G_\ell^+(R, R; k)\right|^2 = -\mathrm{Im}\left[G_\ell^+(R, R; k)\right]. \tag{17}$$

The left-hand side of equation (17) is proportional to the local density of states at $r = R$, namely

$$\rho_\ell(k, R) = -\frac{1}{2\pi^2}\mathrm{Im}\left[G_\ell^+(R, R; k)\right]. \tag{18}$$

It then follows using equations (13), (17) and (18) that the elastic cross section may be written as the sum of the hard-disc scattering cross section σ^{HD}, a term proportional to the local density of states ρ_ℓ, calculated at the boundary radius $r = R$, plus an interference contribution, namely

$$\sigma_\ell(E) = \sigma_\ell^{\mathrm{HD}}(E) + \frac{8\pi^2}{k}D_\ell(kR)\rho_\ell(E, R) - \frac{8}{k}D_\ell(kR)\mathrm{Im}\left[G_\ell^+(R, R; E)f_\ell^*(k)\frac{H_\ell^-(kR)}{H_\ell^+(kR)}\right], \tag{19}$$

where the hard-disc cross section reads

$$\sigma_\ell^{\mathrm{HD}} = \frac{4}{k}|f_\ell(k)|^2 = \frac{4}{k}\left|\frac{J_\ell(kR)}{H_\ell^+(kR)}\right|^2. \tag{20}$$

3. Resonant expansions

3.1. Definition of a resonant state

Resonant states are defined as solutions to equation (1) such that beyond the range of the potential these consist of purely of outgoing waves. It follows from time-reversal considerations that the above condition implies that the values of k cannot be real. Indeed the condition is satisfied for an infinite set of complex values $\{k_{\ell n}\}$ distributed symmetrically with respect to the imaginary axis on the lower half of the complex k-plane. This allows us to define the resonant functions $\{u_{\ell n}(r)\}$ as solutions to the Schrödinger equation,

$$\frac{\mathrm{d}^2}{\mathrm{d}r^2}u_{\ell n}(r) + \frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r}u_{\ell n}(r) + \left[k_{\ell n}^2 - \mathcal{V}_0(r)\right]u_{\ell n}(r) = 0, \tag{21}$$

satisfying the purely outgoing solution,

$$u_{\ell n}(r) = \mathcal{A}_\ell(k_{\ell n})H_\ell^+(k_{\ell n}r), \qquad r \geqslant R. \tag{22}$$

Hence, joining at $r = R$ the internal and external solutions yields the boundary condition

$$\left.\frac{\mathrm{d}}{\mathrm{d}r}u_{\ell n}(r)\right|_{r=R_-} = g(k_{\ell n})u_{\ell n}(R_-), \tag{23}$$

where R_- indicates that the functions $u_{\ell n}(r)$ correspond to the solutions along the internal region and

$$g(k_{\ell n}) = \frac{1}{H_\ell^+(k_{\ell n}R)}\left[\frac{\mathrm{d}}{\mathrm{d}r}H_\ell^+(k_{\ell n}\,r)\right]_{r=R}. \tag{24}$$

Since $k_{\ell n}$ is complex, i.e. $k_{\ell n} = \alpha_{\ell n} - \mathrm{i}\beta_{\ell n}$, with $\alpha_{\ell n}, \beta_{\ell n} > 0$, the corresponding complex energy reads

$$E_{\ell n} = k_{\ell n}^2\big/\eta = \mathcal{E}_{\ell n} - \mathrm{i}\Gamma_{\ell n}/2, \tag{25}$$

where η is defined by (4).

The probability density of a resonant state increases exponentially with distance but decays exponentially as a function of time,

$$|u_{\ell n}(r,t)|^2 \sim \frac{2}{\pi\left(\alpha_{\ell n}^2 + \beta_{\ell n}^2\right)r}\,\mathrm{e}^{2\beta_{\ell n}r}\,\mathrm{e}^{-\Gamma_{\ell n}t/\hbar}. \tag{26}$$

The above behaviour implies that the usual rules of normalization and eigenfunction expansions do not apply for resonant states. An alternative way to define resonant states, that leads to a consistent normalization condition, follows from the residues at the complex poles of the outgoing Green's function $G_\ell^+(r, r'; k)$ of the problem, and a derivation of eigenfunction expansions involving these states is discussed in the following subsections.

3.2. Expansion of the outgoing Green's function

For a finite range interaction, the outgoing Green's function $G_\ell^+(r, r'; k)$, as a function of k, can be extended analytically to the whole complex k-plane. Complex poles are seated on the lower half of the k-plane. To each complex pole k_n there corresponds, from time-reversal invariance, a complex pole k_{-n} situated symmetrically with respect to the imaginary axis, i.e. $k_{-n} = -k_n^*$. In what follows we shall consider a description in the complex energy E-plane. Since the relationship between the energy and the wavenumber is quadratic, a single-valued outgoing Green's function on the energy plane requires two Riemann sheets. We choose as the 'physical sheet' the one displayed in figure 1, namely, formed by a cut along the negative imaginary axis and complex poles seated on the fourth quadrant.

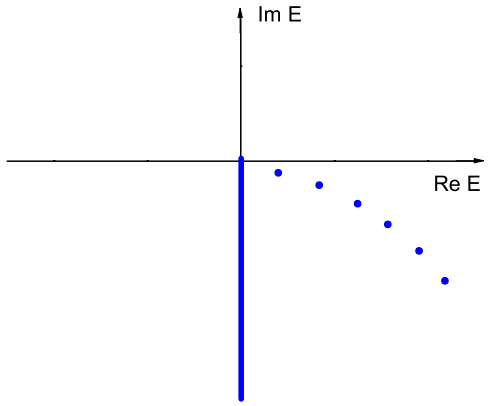

Figure 1. Location of poles and the energy cut in the complex energy plane.

In this section we consider an expansion of the outgoing Green's function $G_\ell^+(r, r'; E)$ in terms of its complex energy poles and residues, the later, as shown in the appendix, being proportional to the resonant states of the problem. In order to obtain the expansion of $G_\ell^+(r, r'; E)$ we take a large but finite closed contour C on the E'-plane that includes a finite number of contours C_i, around each complex pole, a contour C_E around a real energy value E and a closed contour C_s that excludes the cut L and embraces all those contours, i.e. $C = \sum_i C_i + C_E + C_s$. We then consider the Cauchy integral,

$$\mathcal{J} = \frac{1}{2\pi \mathrm{i}} \oint_C \frac{G_\ell^+(r, r'; E')\,\mathrm{d}E'}{E' - E} = 0. \tag{27}$$

Evaluating the contributions of each contour by Cauchy integral theorem and using the residues given by equation (A.12), we obtain

$$G_\ell^+(r, r'; E) = \sum_{n=1}^{N} \frac{u_{\ell n}(r) u_{\ell n}(r')}{E - \mathcal{E}_{\ell n} - \mathrm{i}\Gamma_{\ell n}/2} + Z_\ell(E), \tag{28}$$

where $Z_\ell(E)$ accounts for the contribution of contour C_s, which we assume to be a background term that varies slowly with energy in the region of interest.

A useful expression relating the width $\Gamma_{\ell n}$ to the corresponding resonant function $u_{\ell n}(r)$ follows by considering the Green's theorem between equation (21) and its complex conjugate, integrating from $r = 0$ to $r = R$, to obtain

$$\left\{ r \left[u_{\ell n}^*(r) \frac{\mathrm{d}}{\mathrm{d}r} u_{\ell n}(r) - u_{\ell n}(r) \frac{\mathrm{d}}{\mathrm{d}r} u_{\ell n}^*(r) \right] \right\}_0^R + \left(k_{\ell n}^2 - k_{\ell n}^{*2}\right) \int_0^R |u_{\ell n}(r)|^2\, r\, \mathrm{d}r = 0. \tag{29}$$

Using now the boundary condition given by equation (23) and its complex conjugate into equation (29) and recalling that $k_{\ell n}^2 - k_{\ell n}^{*2} = -\mathrm{i}\eta\Gamma_{\ell n}$, allows us to express the decay width $\Gamma_{\ell n}$ in terms of the corresponding resonant state as

$$\Gamma_{\ell n} = \frac{2}{\eta} \operatorname{Im}\left[g(k_{\ell n})\right] \frac{R\,|u_{\ell n}(R)|^2}{I_{\ell n}}, \tag{30}$$

where

$$I_{\ell n} = \int_0^R |u_{\ell n}(r)|^2\, r\, \mathrm{d}r. \tag{31}$$

3.3. Resonant expansion of the scattering function

Let us now substitute the outgoing Green's function given by equation (28), evaluated at $r = r' = R$, into equation (10). This leads to the expansion of the scattering function

$$S_\ell(E) = \left(2\mathrm{i}D_\ell(kR)\sum_n^N \frac{u_{\ell n}^2(R)}{E - \mathcal{E}_{\ell n+}\mathrm{i}\Gamma_{\ell n}/2} - 1\right)\frac{H_\ell^-(kR)}{H_\ell^+(kR)}, \tag{32}$$

where we have dropped the non-resonant background term $Z_\ell(E)$. Let us now express $u_{\ell n}(R) = |u_{\ell n}(R)|\exp(\mathrm{i}\phi_{\ell n})$ and make use of equation (30) to write equation (32) as

$$S_\ell(E) = \left(\mathrm{i}\frac{\eta}{R}D_\ell(kR)\sum_n^N C_{\ell n}\frac{\Gamma_{\ell n}\,\mathrm{e}^{2\mathrm{i}\phi_{\ell n}}}{E - \mathcal{E}_{\ell n} + \mathrm{i}\Gamma_{\ell n}/2} - 1\right)\frac{H_\ell^-(kR)}{H_\ell^+(kR)}, \tag{33}$$

where

$$C_{\ell n} = \frac{I_{\ell n}}{\mathrm{Im}[g(k_{\ell n})]}, \tag{34}$$

with $g(k_{\ell n})$ given by equation (24).

Substitution of equation (33) into equation (12) gives the expression for the elastic scattering cross section,

$$\sigma_\ell(E) = \frac{4}{k}\left|f_\ell + \mathrm{i}\frac{\eta}{R}D_\ell(kR)\sum_n^N C_{\ell n}\frac{(\Gamma_{\ell n}/2)\,\mathrm{e}^{2\mathrm{i}\phi_{\ell n}}}{E - \mathcal{E}_{\ell n} + \mathrm{i}\Gamma_{\ell n}/2}\frac{H_\ell^-(kR)}{H_\ell^+(kR)}\right|^2, \tag{35}$$

where f_ℓ stands for the hard-disc scattering function given by equation (14).

For an isolated sharp resonance, i.e. ($\mathcal{E}_{\ell n\pm 1} - \mathcal{E}_{\ell n} \gg \Gamma_{\ell n}$ and $\mathcal{E}_{\ell n} \gg \Gamma_{\ell n}$). Then $\alpha_{\ell n} \gg \beta_{\ell n}$ and $\beta_{\ell n} \ll 1$ and also $\mathrm{Im}\,u_{\ell n}(R) \approx 0$. Hence, the resonance phase $\phi_{\ell n} \approx \mathrm{Im}\,u_{\ell n}(R)/\mathrm{Re}\,u_{\ell n}(R) \approx 0$. As a consequence, the expression for the cross section in two dimensions becomes

$$\sigma_\ell^{B-W}(E) = \left(\frac{4\eta^2}{kR^2}\right)|D_\ell(kR)C_{\ell n}|^2\frac{\Gamma_{\ell n}^2/4}{(E - \mathcal{E}_{\ell n})^2 + \Gamma_{\ell n}^2/4}, \tag{36}$$

which except for a prefactor characteristic of two dimensions corresponds to the well-known *Breit–Wigner formula* [15].

3.4. Resonant expansion of the local density of states at $r = R$

Substitution of equation (28), with $r = r' = R$, into equation (18) yields the expression for the local density of states

$$\rho_\ell(E, R) = \frac{1}{2\pi^2}\sum_n |u_{\ell n}(R)|^2\frac{(\Gamma_{\ell n}/2)\cos 2\phi_{\ell n} - (E - \mathcal{E}_{\ell n})\sin 2\phi_{\ell n}}{(E - \mathcal{E}_{\ell n})^2 + (\Gamma_{\ell n})^2/4}, \tag{37}$$

where we have used $u_{\ell n}(R) = |u_{\ell n}(R)|\exp(\mathrm{i}\phi_{\ell n})$ and we have dropped the background contribution $\mathrm{Im}\,Z_\ell(E)$. Using equation (30) one may write equation (37) as

$$\rho_\ell(E, R) = \frac{1}{2\pi^2}\frac{\eta}{R}\sum_n C_{\ell n}\frac{\Gamma_{\ell n}}{2}\frac{(\Gamma_{\ell n}/2)\cos 2\phi_{\ell n} - (E - \mathcal{E}_{\ell n})\sin 2\phi_{\ell n}}{(E - \mathcal{E}_{\ell n})^2 + (\Gamma_{\ell n})^2/4}. \tag{38}$$

A sharp isolated resonance implies that $\phi_{\ell n} \approx 0$, since $\mathrm{Re}\,u_{\ell n} \gg \mathrm{Im}\,u_{\ell n}$. In such a case, for energies E_{res} around a resonance energy $\mathcal{E}_{\ell n}$, we obtain, using equation (35), that the elastic cross section is proportional to the local density of states, namely

$$\sigma_\ell(E_{\mathrm{res}}) \approx \frac{8\pi^2\eta}{kR}D_\ell^2(kR)C_{\ell n}\rho_\ell(E_{\mathrm{res}}, R). \tag{39}$$

In particular for quantum corrals, where $kR \gg 1$, the above equation becomes

$$\sigma_\ell(E_{\rm res}) \approx \frac{8\pi^2 R}{\eta}\rho_\ell(E_{\rm res}, R), \tag{40}$$

where we have used that $D_\ell \approx kR/\eta$ and $C_{\ell n} \approx 1/\alpha_n$.

4. Example

In this section we discuss both the elastic scattering cross section and the local density of states, for a system described by a delta potential of intensity λ at a radius R, namely

$$V(r) = \lambda\delta(r - R). \tag{41}$$

For the sake of simplicity we shall restrict the discussion to the case $\ell = 0$ and hence we drop that index in the following expressions.

4.1. Exact solution

Along the internal region of the potential the solution to the problem reads

$$\psi(k, r) = C J_0(kr); \qquad r \leqslant R, \tag{42}$$

where $J_0(kr)$ stands for the ordinary Bessel function of integer order [16] and along the external region, $r \geqslant R$, we may write, using equation (2),

$$\psi(k, r) = \tfrac{1}{2}[H_0^-(kr) + S(k)H_0^+(kr)]; \qquad r \geqslant R. \tag{43}$$

It then follows immediately by the continuity of the above solutions at $r = R$, that,

$$S(k) = -\frac{-2\mathrm{i} - \pi R\eta\lambda J_0(kR)H_0^-(kR)}{2\mathrm{i} - \pi R\eta\lambda J_0(kR)H_0^+(kR)}. \tag{44}$$

Substitution of equation (44) into equation (12) yields an exact analytical expression for the elastic cross section. On the other hand, using equations (10) and (44), allows us to write the exact analytical expression for $G^+(R, R; k)$ as

$$G^+(R, R; k) = \pi\eta\frac{J_0(kR)H_0^+(kR)}{2i - \pi R\eta\lambda J_0(kR)H_0^+(kR)}, \tag{45}$$

which permits us to evaluate the local density of states using equation (18).

4.2. Resonant states and complex poles

Along the internal region for the δ-potential, the resonant solution to equation (21) reads

$$u_n(r) = \mathcal{C}_n J_0(k_n r); \qquad r \leqslant R, \tag{46}$$

and, following equation (22), along the external region, the solution is given by

$$u_n(r) = \mathcal{A}_n H_0^+(k_n r); \qquad r \geqslant R. \tag{47}$$

From the continuity of the solutions at $r = R$ and the corresponding discontinuity of the first derivatives, due to the δ-potential, we obtain the eigenvalue equation for the complex poles k_n,

$$2\mathrm{i} - \lambda\pi R J_0(k_n R)H_0^+(k_n R) = 0. \tag{48}$$

Since in our case, $k_n R \gg 1$, equation (48) may be written as the approximate expression,

$$F(k_n) \equiv 2\mathrm{i}k_n - \lambda[\mathrm{e}^{\mathrm{i}(2k_n R - \pi/2)} + 1] = 0. \tag{49}$$

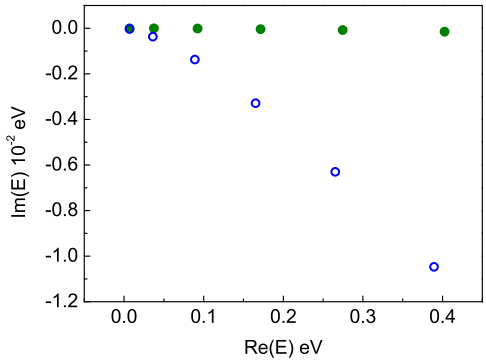

Figure 2. Plot of the first six resonance poles on the complex energy plane, for a δ-potential of radius $R = 9.0$ nm and intensity $\lambda = 3.48$ nm^{-1}.

The above equation allows us to obtain simple approximate analytical solutions for the complex poles k_n [11],

$$k_n \approx a_n^0 \left[1 - \frac{1}{\lambda R}\right] - \mathrm{i}\frac{1}{R\lambda^2}\left(a_n^0\right)^2, \tag{50}$$

where $a_n^0 = (2n+1)\pi/4R$, with $n = 1, 3, 5, \ldots$.

The above solutions may be used as an input into the well-known Newton–Raphson iterative method to obtain the poles with any degree of accuracy. However, using equation (50) into equation (25) allows us to write the real and imaginary parts of the complex energy poles E_n, respectively, as

$$\mathcal{E}_n \approx \frac{\hbar^2}{2m}\left[\frac{(2n+1)\pi}{4R}\left(1 - \frac{1}{\lambda R}\right)\right]^2 \tag{51}$$

and

$$\Gamma_n \approx \frac{\hbar^2}{2m}\left[(2n+1)\pi\right]^3\left(\frac{1}{2R^4\lambda^2}\right). \tag{52}$$

It turns out that equations (51) and (52) provide a very good approximation to the exact complex energy values. Figure 2 exhibits a plot of a few resonance poles for the parameters of the δ-potential: $\lambda = 3.48$ nm^{-1} and $R = 9.0$ nm. Here we consider as the effective mass for the electron $m^* = 0.38\, m_e$, with m_e being the electron mass, which is typical of quantum corrals formed by Fe adatoms on a surface of Cu(1,1,1) [8–10].

4.3. Comparison of exact and resonant expansion solutions

For an infinite value of the intensity, i.e. $\lambda \to \infty$, one obtains the hard-disc situation, where the cross section σ^{HD} is given by equation (20). The physically interesting case arises for finite values of λ, since then, particles may tunnel into the internal region of the corral at resonance energies as described by equation (35). The resonance energies $\mathcal{E}_n$ and decay widths Γ_n are a function of the potential parameters, namely the radius R and the intensity λ.

Having obtained the poles allows us to determine the normalized resonance functions $u_n(r)$, using equation (A.13), and the coefficients $C_{\ell n}$, given by equation (34), that together with the resonance energies $\mathcal{E}_n$ and the decay widths Γ_n are the necessary input to evaluate the resonance contribution to the cross section given by equation (35). Figure 3 exhibits the

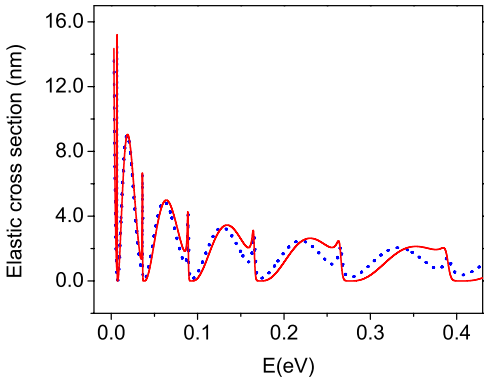

Figure 3. Comparison of the exact (solid line) and resonant expansion (dotted line) expressions for the elastic cross section as a function of the energy E with $\lambda = 5.0\ \mathrm{nm}^{-1}$ and $R = 9.0$ nm.

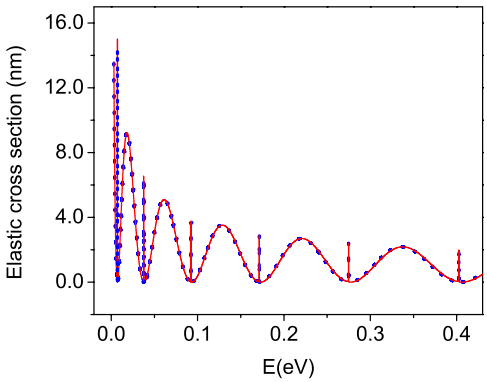

Figure 4. Comparison of the exact (solid line) and resonant expansion (dotted line) expressions for the elastic cross section as a function of the energy E with $\lambda = 50.0\ \mathrm{nm}^{-1}$ and $R = 9.0$ nm.

cross section versus energy for an energy range involving the first six resonance poles for $\lambda = 5.0\ \mathrm{nm}^{-1}$ and $R = 9.0$ nm. By comparing with the exact solution, obtained using by equations (12) and (44), we appreciate that the first three resonances are fairly well described by the resonance expansion given by equation (35) (dotted line). We observe that as the energy increases the agreement gets worse, indicating that the background contribution ceases to be negligible. Figure 4 presents the case for a larger value of λ, namely $\lambda = 50.0\ \mathrm{nm}^{-1}$. Here one observes an excellent agreement between the exact (solid line) and resonance solution (dotted line) along the exhibited range of energies. This follows because in this case the resonances are sharper and more isolated than in the previous example and hence the background contribution remains negligible.

Figures 5 and 6 exhibit two examples comparing the local density of states $\rho(E, R)$ for the exact calculation (solid line), that follows from equations (18) and (45), and the corresponding resonance expansion, given by equation (38). Here the values for the intensities of the δ-potential are, respectively, $\lambda = 50.0\ \mathrm{nm}^{-1}$ and $\lambda = 150.0\ \mathrm{nm}^{-1}$. Again, as the intensity λ increases, we observe that the agreement between the exact and the resonance expansion becomes better.

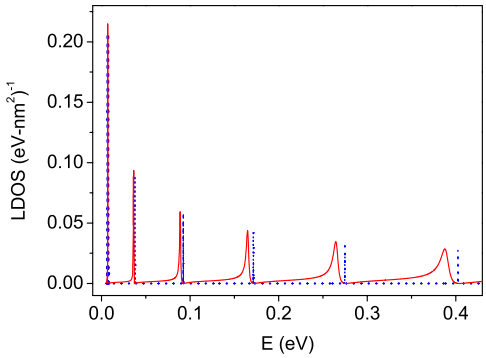

Figure 5. Comparison of the exact (solid line) and resonant expansion (dotted line) expressions for the local density of states as a function of the energy E with $\lambda = 50.0\ \mathrm{nm}^{-1}$ and $R = 9.0$ nm.

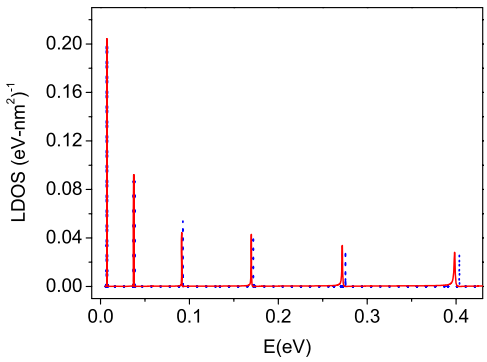

Figure 6. Comparison of the exact (solid line) and resonant expansion (dotted line) expressions for the local density of states as a function of the energy E with $\lambda = 150.0\ \mathrm{nm}^{-1}$ and $R = 9.0$ nm.

5. Concluding remarks

We have obtained that the resonant expansion for the outgoing Green's function to the problem (28) may lead to analytical expressions for both the S-matrix and the elastic cross section for potentials with cylindrical symmetry in two dimensions, as given respectively, by equations (33) and (35). Using the unitarity condition obeyed by the S-matrix in terms of the Green's function, given by equation (17), we have derived a relationship between the cross section and the local density of states for elastic processes (19). We have also obtained that near an isolated sharp resonance these two quantities are proportional to each other, as shown by equation (40). This might be useful for the experimental verification of these quantities.

An interesting extension, that will be considered elsewhere, follows by using Laplace transform techniques to obtain the retarded time-dependent Green's function of a two-dimensional system to study the time evolution of decay of an initially prepared state within the system, in a fashion similar as in three dimensions [17].

Acknowledgments

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Appendix. Determination of the residue at a pole of the outgoing Green's function in two dimensions

In what follows it is shown that the residue of $G_\ell^+(r, r'; k)$ near one of the complex energy poles is proportional to the functions $u_{\ell n}(r)$ and $u_{\ell n}(r')$. In doing so we extend to two dimensions the derivation given in three dimensions by García Calderón and Peierls [5]. This leads to a normalization condition that differs from that in three [5], and in one [7], dimensions. Hence, for the sake of completeness, we provide a detailed derivation of the residue at the complex pole in two dimensions.

The outgoing Green's function, of a given partial wave ℓ, for the Hamiltonian H defined in section 2 satisfies the equation

$$\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + [k^2 - \mathcal{V}_0(r)]\right) G_\ell^+(r, r'; k) = \eta \frac{\delta(r - r')}{r}, \tag{A.1}$$

where η is given by equation (4), m is the mass of the particle and E denotes the energy of the particle. The boundary condition of the outgoing Green's function at $r = R$ reads

$$\frac{\partial}{\partial r} G_\ell^+(r, r'; k)\bigg|_{r=R} = g(k_{\ell n}) G_\ell^+(R, r'; k). \tag{A.2}$$

Here $g(k_{\ell n})$ is defined by equation (24). It is convenient, for simplicity, to perform the analysis in the complex k^2-plane. Hence, near a complex pole one may write

$$G_\ell^+(r, r'; k) = \eta \frac{C_{\ell n}(r, r')}{k^2 - k_{\ell n}^2} + \chi_\ell(r, r'; k), \tag{A.3}$$

where the $C_{\ell n}(r, r')$ is the residue and $\chi_\ell(r, r'; k)$ is regular at the pole. Substitution of equation (A.3) into equation (A.1) gives

$$\frac{\eta}{k^2 - k_{\ell n}^2}\left[\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + [k^2 - \mathcal{V}_0(r)]\right] C_{\ell n}(r, r') + \left[\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + [k^2 - \mathcal{V}_0(r)]\right] \chi(r, r'; k) - \eta \frac{\delta(r - r')}{r} = 0. \tag{A.4}$$

Adding and subtracting $k_{\ell n}^2 C_{\ell n}(r, r') \big/ \left(k^2 - k_{\ell n}^2\right)$ to equation (A.4) and taking the limit $k^2 \to k_{\ell n}^2$ leads to the following expressions:

$$\left[\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \left[k_{\ell n}^2 - \mathcal{V}_0(r)\right]\right] C_{\ell n}(r, r') = 0 \tag{A.5}$$

and

$$\left[\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \left[k_{\ell n}^2 - \mathcal{V}_0(r)\right]\right] \chi_\ell(r, r'; k_n) + \eta\, C_{\ell n}(r, r') = \eta \frac{\delta(r - r')}{r}. \tag{A.6}$$

Now substitution of equation (A.3) into the boundary condition given by equation (A.2), followed by adding and subtracting $g(k_{\ell n}) C_{\ell n}(r, r') \big/ \left(k^2 - k_{\ell n}^2\right)$, and then taking the limit $k^2 \to k_{\ell n}^2$ yields

$$\frac{\partial}{\partial r} C_{\ell n}(r, r')\bigg|_{r=R} = g(k_{\ell n}) C_{\ell n}(R, r') \tag{A.7}$$

and

$$\frac{\partial}{\partial r} \chi_\ell(r, r'; k)\bigg|_{r=R} = g(k_{\ell n}) \chi_\ell(R, r'; k) + \frac{\dot{g}(k_{\ell n})}{2k_{\ell n}} \eta C_{\ell n}(R, r'). \tag{A.8}$$

Equation (A.5) for $C_{\ell n}(r, r')$ and the corresponding boundary condition given by equation (A.7) are identical to equation (21) for $u_{\ell n}(r)$ and its boundary condition, given by equation (23). Consequently, it follows that these functions are proportional, that is

$$C_{\ell n}(r, r') = u_{\ell n}(r) P(r'). \tag{A.9}$$

Multiplying equation (A.6) by $u_{\ell n}(r)$ and equation (21) by $\chi_\ell(r, r'; k)$, subtracting one from the other, and integrating from $r = 0$ to $r = R$, yields

$$\left[r \left(u_{\ell n}(r) \frac{\partial}{\partial r} \chi_\ell(r, r'; k_n) - \chi_\ell(r, r'; k_n) \frac{\mathrm{d}}{\mathrm{d}r} u_{\ell n}(r) \right) \right] \Bigg|_0^R + \eta \int_0^R u_{\ell n}(r) C_{\ell n}(r, r') r \, \mathrm{d}r = \eta u_{\ell n}(r'). \tag{A.10}$$

Using equations (23), (A.8) and (A.9) into equation (A.10) allows us to write the following expression for $P(r')$:

$$P(r') = \frac{u_{\ell n}(r')}{\int_0^R u_{\ell n}(r)^2 r \, \mathrm{d}r + \left[R \, u_{\ell n}^2(R) \big/ 2k_{\ell n} \right] \dot{g}(k_{\ell n})}. \tag{A.11}$$

Hence, the residue of the outgoing Green's function at the pole $k_{\ell n}^2$ may be written as

$$C_{\ell n}(r, r') = u_{\ell n}(r) u_{\ell n}(r'), \tag{A.12}$$

provided the resonant states are normalized according to the condition

$$\int_0^R u_{\ell n}^2(r) \, r \, \mathrm{d}r + R \frac{u_{\ell n}^2(R)}{2k_{\ell n}} \dot{g}(k_{\ell n}) = 1 \tag{A.13}$$

where

$$\dot{g}(k_{\ell n}) = \left[\frac{\mathrm{d}}{\mathrm{d}k} g(k) \right]_{k = k_{\ell n}}. \tag{A.14}$$

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