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Optical potentials using resonance states in supersymmetric quantum mechanics

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Optical potentials using resonance states in Supersymmetric Quantum Mechanics

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Abstract. Complex potentials are constructed as Darboux-deformations of short range, radial nonsingular potentials. They behave as optical devices which both refracts and absorbs light waves. The deformation preserves the initial spectrum of energies and it is implemented by means of a Gamow-Siegert function (resonance state). As straightforward example, the method is applied to the radial square well. Analytical derivations of the involved resonances show that they are 'quantized' while the corresponding wave-functions are shown to behave as bounded states under the broken of parity symmetry of the related one-dimensional problem.

1. Introduction

Solutions of the Schrödinger equation associated to complex eigenvalues $\epsilon = E_\alpha$ and satisfying purely outgoing conditions are known as Gamow-Siegert functions [1, 2]. These solutions represent a special case of scattering states for which the 'capture' of the incident wave produces delays in the scattered wave. The 'time of capture' can be connected with the lifetime of a decaying system (resonance state) which is composed by the scatterer and the incident wave. Then, it is usual to take $\text{Re}(\epsilon)$ as the binding energy of the composite while $\text{Im}(\epsilon)$ corresponds to the inverse of its lifetime. The Gamow-Siegert functions are not admissible as physical solutions into the mathematical structure of Quantum Mechanics since, in contrast with conventional scattering wave-functions, they are not finite at $r \to \infty$. Thus, such a kind of functions is acceptable in Quantum Mechanics only as a convenient model to solve scattering equations. However, because of the resonance states relevance, some approaches extend the formalism of quantum theory so that they can be defined in a precise form [3–9].

In this paper the Gamow-Siegert functions are analyzed not to precisely represent decaying systems but to be used as the cornerstone of complex Darboux-transformations in Supersymmetric Quantum Mechanics (Susy-QM). The 'unphysical' behaviour of these solutions plays a relevant role in the transformation: While the Gamow-Siegert function u diverges at $r \to \infty$, the limit of its logarithmic derivative $\beta = -u'/u$ at $r \to \infty$ is a complex constant. This last function is used to deform the initial potential into a complex function. It is worth noticing that complex eigenvalues ϵ have been used as factorization constants in Susy-QM (see for instance [10–18] and the discussion on 'atypical models' in [19]). However, as far as we know, until the recent results reported in [20–22] the connection between Susy-QM and resonance states has been missing. Our interest in the present work is two-fold. First, we want to show that appropriate approximations lead to analytical expressions for the real and imaginary parts

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of the resonance energies in the case of radial short range potentials. Second, we want to enlarge the number of applications of the Darboux transformations in constructing new exactly solvable models in Quantum Mechanics.

In Section 2 the main aspects of solving the Schrödinger equation for radial, nonsingular short range potentials are reviewed. The relevance of the scattering amplitude $S(k)$ in the analysis of both the bounded and scattering wave-functions is clearly stated. In Section 3 the analytical properties of $S(k)$ as a function of the complex kinetic parameter k are studied. It is shown that poles of the scattering amplitude which live in the lower k–plane are connected with the Gamow-Siegert functions while the poles on the positive imaginary axis lead to bounded physical energies. The general aspects of the complex Darboux-transformations are included in Section 4. All the previous developments are then applied to the square radial well and new analytical expressions for the involved resonance energies are reported in Section 5. We conclude the paper with some concluding remarks in Section 6.

2. Short range radial potentials revisited

2.1. General considerations

Let us consider the Hamiltonian of one particle in the external, spherically symmetric field $U(\vec{r}) = U(r)$. The Schrödinger equation reduces to the eigenvalue problem:

$$H\psi(\vec{r}) \equiv \left(-\frac{\hbar^2}{2m}\Delta + U(r)\right)\psi(\vec{r}) = \mathcal{E}\psi(\vec{r}). \tag{1}$$

We are interested in potentials which decrease more rapidly than $1/r$ at large r. Indeed, $U(r)$ is a short-range potential (i.e., there exists $a \in \mathrm{Dom}(U) := D_U$ such that $U(r) = 0$ at $r > a$) which is nonsingular (i.e., $U(r)$ satisfies $r^2U(r) \to 0$ at $r \to 0$). The wave function $\psi(\vec{r})$ must be single-valued and continuous everywhere in D_U. Since the operators H, L^2, L_3 and P commute with each other, in spherical coordinates the Schrödinger equation (1) has solutions of the form

$$\psi_{\ell m}(\vec{r}) = R_\ell(r)Y_{\ell m}(\theta, \varphi) \tag{2}$$

where θ and φ are respectively the polar and the azimuthal angles, $R_\ell(r)$ is a function depending on r and $Y_{\ell m}(\theta, \varphi)$ stands for the spherical harmonics. For simplicity in calculations we shall use the function $u_\ell(r) = rR_\ell(r)$. The introduction of (2) into equation (1) yields:

$$\left[-\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + v(r)\right]u_\ell(r) := \left[-\frac{d^2}{dr^2} + V_\ell(r)\right]u_\ell(r) = k^2u_\ell(r) \tag{3}$$

with $v = 2mU/\hbar^2$ and $k^2 = E \equiv 2m\mathcal{E}/\hbar^2$ the dimensionless expressions for the potential and the kinetic parameter respectively. As usual, the effective potential V_ℓ is defined as the potential v plus the centrifugal barrier $\ell(\ell+1)/r^2$. Physical solutions $\psi(\vec{r})$ of (1) should be constructed with functions u_ℓ fulfilling the following boundary conditions:

$$\begin{cases} u_\ell(r) = 0 & r \to 0 \\ \frac{u_\ell(r)}{r} < \infty & r \to \infty \end{cases} \tag{4}$$

Furthermore, the function u_ℓ and its derivative u'_ℓ have to be continuous for $r > 0$ since (3) includes second order derivatives. As we shall see, the study of the involved matching conditions is simplified by introducing a function β_ℓ as follows

$$\beta_\ell(r) := -\frac{u'_\ell(r)}{u_\ell(r)} = -\frac{d}{dr}\ln u_\ell(r). \tag{5}$$

In general we will assume that the energy spectrum is composed by negative (bounded) and positive (scattering) energies. For the sake of notation we shall use the symbol $\phi_\ell(r)$ for the solutions of (3) which satisfy the boundary conditions (4); the symbol $u_\ell(r)$ will stand for general mathematical solutions of equation (3).

2.2. Bases of solutions

For arbitrary ℓ and $r > a$, the appropriate basis of solutions can be written in the form

$$u_\ell^{(+)}(r) = ikr\, h_\ell^{(1)}(kr), \qquad u_\ell^{(-)}(r) = -ikr\, h_\ell^{(2)}(kr) \tag{6}$$

where $h_\nu^{(1)}$ and $h_\nu^{(2)}$ are the spherical Hänkel functions of order $\nu = \ell$ (see e.g. [23]). For large values of kr in the region $r > a$, the functions (6) behave as follows

$$u_\ell^{(\pm)}(r) \approx \exp\left[\pm i\left(kr - \frac{\ell\pi}{2}\right)\right]. \tag{7}$$

Thereby, $u_\ell^{(+)}$ represents a diverging wave and describes particles moving with speed $\vartheta = k$ in all directions from the origin. In turn, the function $u_\ell^{(-)}$ represents a converging wave and describes particles moving with speed ϑ towards the origin.

It is worth noticing that the Schrödinger equation (3) is invariant under the change $k \to -k$. Hence, if $u_\ell(r,k)$ is solution of (3) for $E = k^2$, then $u_\ell(r,-k)$ is also a solution for the same energy. However, these last functions must differ at most in a constant factor because the solutions of (3) have to be single-valued. In contrast, up to a global phase, they interchange their roles at $r \to \infty$, as indicated by the relationship

$$u_\ell^{(\pm)}(r,k) = e^{i\pi\ell}\, u_\ell^{(\mp)}(r,-k), \quad r \to \infty. \tag{8}$$

On the other hand, the basis of solutions at $r < a$ may be written

$$u_\ell^{(1)}(r) = \frac{2\ell+1}{\Lambda_\ell}\, kr\, j_\ell(kr), \qquad u_\ell^{(2)}(r) = -\Lambda_\ell\, kr\, n_\ell(kr), \qquad \Lambda_\ell := \frac{2^{-\ell}\sqrt{\pi}}{\Gamma(\ell+1/2)} \tag{9}$$

where j_ℓ and n_ℓ are respectively the spherical Bessel and Neumann functions of order ℓ. For very small values of r we have

$$u_\ell^{(1)}(r \to 0) \approx (kr)^{\ell+1}, \qquad u_\ell^{(2)}(r \to 0) \approx \frac{1}{(kr)^\ell}. \tag{10}$$

2.2.1. Bounded states. Imaginary values of the kinetic parameter $k = \pm i\sqrt{|E|} \equiv \pm i\kappa$ correspond to negative values of the energy $E = k^2 = -\kappa^2$. As usual, we shall consider k to be in the upper complex k–plane I_+. In this way $u_\ell^{(-)}(r,\kappa)$ does not satisfy the boundary condition at $r \to \infty$ and $u_\ell^{(2)}(r,\kappa)$ does not fulfill the boundary condition at $r = 0$. Hence, the physical solutions should be constructed with $u_\ell^{(1)}(r,\kappa)$ and $u_\ell^{(+)}(r,\kappa)$. We write:

$$\phi_\ell(r,\kappa) = \begin{cases} \zeta_\ell(\kappa)\, u_\ell^{(1)}(r,\kappa)\, g_\ell(r,\kappa) & r < R \\ \xi_\ell(\kappa)\, u_\ell^{(+)}(r,\kappa) & r \geq R \end{cases} \tag{11}$$

where the intermediary function $g_\ell(r,\kappa)$ is equal to 1 at $r = 0$ and depends on the potential. The coefficients $\zeta_\ell(\kappa)$ and $\xi_\ell(\kappa)$ are complex numbers while the matching condition $\beta_\ell(a,\kappa) = \kappa$

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corresponds to a transcendental equation which is fulfilled for a set of discrete values of the kinetic parameter κ_n, $n = 0, 1, 2, \ldots$ Under these conditions the functions $\phi_\ell(r, \kappa_n)$ are finite and the integral

$$\int_0^{+\infty} |\phi_\ell(r, \kappa_n)|^2 dr \tag{12}$$

converges. Thereby, $|\phi_\ell(r, \kappa_n)|^2$ can be identified as the involved Born's probability density.

2.2.2. Scattering states. Positive energies $E = k^2$ correspond to real values of k and both solutions (7) remain finite in $r \geq a$. As a consequence, both of them are physically acceptable in this region. To analyze these solutions first let us consider the case $\ell = 0$ and, for the sake of simplicity, let us drop this subindex from the functions $u_\ell(r)$. The general solution in the free of interaction zone ($r > a$) may be written as

$$u_{\text{out}}(r) = \gamma(k) \left[u^{(-)}(r) - S(k) u^{(+)}(r) \right]. \tag{13}$$

The constant $\gamma(k)$ is the amplitude of the converging wave and does not depend on the potential $v(r)$. The scattering amplitude $S(k)$, in contrast, strongly depends on the potential and encodes the information of the scattering phenomenon. The matching condition between $u_{\text{out}}(r)$ and the solution $u_{\text{in}}(r)$ in the interaction zone reads

$$\beta_{\text{out}}(a) = \beta_{\text{in}}(a) \tag{14}$$

and can be satisfied by appropriate values of γ and S. Indeed, equation (14) is equivalent to the following matrix array

$$\left. \begin{pmatrix} u_{\text{in}} & u^{(+)} \\ u'_{\text{in}} & u'^{(+)} \end{pmatrix} \right|_{r=a} \begin{pmatrix} \gamma^{-1} \\ S \end{pmatrix} = \left. \begin{pmatrix} u^{(-)} \\ u'^{(-)} \end{pmatrix} \right|_{r=a} \tag{15}$$

the solution of which is given by the system of equations

$$\gamma = \left. \frac{W\left(u_{\text{in}}, u^{(+)}\right)}{2ik} \right|_{r=a}, \qquad S = \left. \frac{W\left(u_{\text{in}}, u^{(-)}\right)}{W\left(u_{\text{in}}, u^{(+)}\right)} \right|_{r=a}, \tag{16}$$

where $W(\cdot, \cdot)$ stands for the Wronskian of the involved functions.

To get a better idea of the roles played by each one of the terms in equation (13) let us consider the free motion ($v(r) = 0$) in the whole of D_v. From equations (6) and (9) we realize that a regular solution at the origin may be written as follows

$$u_{\text{free}}(r) \equiv u^{(-)}(r) - u^{(+)}(r) = -2ikr\, j_0(kr) = -2i \sin(kr). \tag{17}$$

This term can be introduced into equation (13) to get

$$u_{\text{out}}(r) = \gamma(k) \left[u_{\text{free}}(r) - (S(k) - 1) u^{(+)}(r) \right]. \tag{18}$$

Thus, the total wave function after scattering u_{out} is given by the wavepacket one would have if there were no scattering γu_{free} plus a scattered term $-\gamma(S-1)u^{(+)}$. This last example shows the important role played by the scattering amplitude in the analysis of positive energies.

On the other hand, the potential we are dealing with is neither a sink nor a source of particles, then the condition $|S(k)| = 1$ (elastic scattering) is true and we have

$$S(k) = e^{2i\delta(k)}. \tag{19}$$

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The scattering phase $\delta(k)$ represents the difference in phase of the outgoing parts. The situation is clear if one introduces (17) and (19) into equation (18) to get

$$u_{\text{out}}(r \to \infty) = -2i\gamma(k)\, e^{i\delta(k)}\, \sin(kr + \delta). \tag{20}$$

As we have indicated, the scattering states include $k \in \mathbb{R}$ since $E > 0$. However, the function (13) is also valid if k is one of the imaginary values of the kinetic parameter leading to the bounded energies $E_n = -\kappa_n^2$. Indeed, this case provides further information about the scattering amplitude. For $k_n = i\kappa_n$, the function (13) at $r \to \infty$ reads

$$u_{\text{out}}(r \to \infty, \kappa_n) \sim -2i\gamma(i\kappa_n) \left[e^{\kappa_n r} - S(i\kappa_n) e^{-\kappa_n r} \right]. \tag{21}$$

The first term in square brackets never vanishes ($\kappa_n > 0$), then the coefficient S must be singular at the complex point $k_n = i\kappa_n$. In other words, the points k_n are nothing but poles of the scattering amplitude. Since these points are in the upper complex k–plane I_+, we realize that $S(k)$ is a regular function in I_+ except at k_n, $n = 0, 1, 2, \ldots$ We shall use these results in the next sections.

Finally, similar expressions can be found for arbitrary azimuthal quantum numbers ℓ. A straightforward calculation gives

$$u_\ell(r) = \gamma_\ell(k) \left(u_\ell^{(-)}(r) - S_\ell(k) u_\ell^{(+)}(r) \right), \qquad r > a \tag{22}$$

the asymptotic behaviour of which reads

$$u_\ell(r \to \infty) \approx -2i\gamma_\ell(k) e^{i\delta_\ell(k)} \sin\left(kr + \delta_\ell(k) - \frac{\ell\pi}{2} \right). \tag{23}$$

The above discussed properties of the scattering amplitude $S(k)$ are easily generalized to the case of arbitrary angular momentum $S_\ell(k)$.

3. Gamow-Siegert functions

3.1. Analytic continuation of the scattering amplitude $S_\ell(k)$

In the previous section we realized that S_ℓ is a regular function in I_+ except at the points $k = i\kappa$ leading to bound states of the energy. In order to get a well behaved scattering amplitude in the whole of the complex k–plane, this function must be extended to be analytic in I_-. With this aim, first let us construct an arbitrary linear combination of the functions (7), it reads

$$u_\ell(r) = \zeta_\ell(k)\, u_\ell^{(-)}(r) - \xi_\ell(k)\, u_\ell^{(+)}(r) \equiv \zeta_\ell(k) \left[u_\ell^{(-)}(r) - S_\ell(k) u_\ell^{(+)}(r) \right]. \tag{24}$$

This function is regular at the origin if $u_\ell(r = 0) = 0$, then we arrive at the following relationship

$$S_\ell(k) = \frac{\xi_\ell(k)}{\zeta_\ell(k)} = \left. \frac{u_\ell^{(-)}(r)}{u_\ell^{(+)}(r)} \right|_{r=0}. \tag{25}$$

Now, after a change of sign in k, the coefficients of the single-valued function (24) should satisfy

$$-e^{i\pi\ell} \xi_\ell(-k) = \alpha \zeta_\ell(k), \qquad e^{i\pi\ell} \zeta_\ell(-k) = -\alpha \xi_\ell(k) \tag{26}$$

where α is a proportionality factor and we have used equation (8). In this way, the expression (25) leads to

$$S_\ell(k)\, S_\ell(-k) = 1. \tag{27}$$

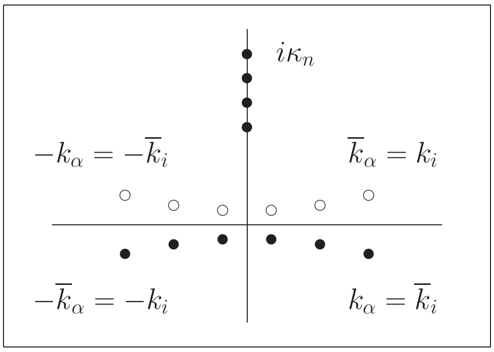

Figure 1. Schematic representation of the poles (disks) and the zeros (circles) of the scattering amplitude $S_\ell(k)$ in the complex k–plane. Bounded energies $E_n = -\kappa_n^2$ correspond to the poles located on the positive imaginary axis.

Let $k_i \in I_+$ be a zero of S_ℓ. From equation (27) we notice that the scattering amplitude is well behaved in I_- except at the point $-k_i$, for which $S_\ell(-k_i) \to \infty$. Thus, $-k_i \in I_-$ is a pole of S_ℓ.

On the other hand, if the kinetic parameter k is real, then the complex conjugate of any solution of equation (3) is also a solution for the same energy. However, the solution is unique so these last functions differ at most in a global phase. Thereby, in a similar form as in the previous case, we get

$$S_\ell(k)\,\overline{S}_\ell(k) = 1 \tag{28}$$

where the bar stands for complex conjugation. This last equation is a consequence of the elastic scattering we are dealing with since $|S_\ell(k)| = 1$. However, as k is real, also equation (28) has to be extended to the whole of the complex k–plane. The natural condition reads

$$S_\ell(k)\,\overline{S}_\ell(\overline{k}) = 1. \tag{29}$$

It is clear that $\overline{S}_\ell(\overline{k}_i)$ diverges because $k_i \in I_+$ is a zero of S_ℓ. In other words, $\overline{k}_i \in I_-$ is a pole of S_ℓ since $|S_\ell(\overline{k}_i)| \to \infty$. Moreover, as $-k_i$ is a pole of S_ℓ, from equation (29) we also notice that $\overline{S}_\ell(-\overline{k}_i) = 0$. Thus, $-\overline{k}_i$ is another zero of the scattering amplitude. In summary, if k_α (k_i) is a pole (zero) of S_ℓ, then $-\overline{k}_\alpha$ ($-\overline{k}_i$) is another pole (zero) while $\overline{k}_\alpha$ and $-k_\alpha$ ($\overline{k}_i$ and $-k_i$) are zeros (poles) of the scattering amplitude. In this way $S_\ell(k)$ is a meromorphic function of the complex kinetic parameter k, with poles restricted to the positive imaginary axis (bound states) and to the lower half-plane I_- (see Figure 1).

3.2. Resonance states

Let us express one of the poles of the scattering amplitude as $k_\alpha = \alpha_1 - i\alpha_2$, with α_1 an arbitrary real number and $\alpha_2 > 0$. The function (22), evaluated for k_α at $r \to \infty$ reads

$$u_\ell(r \to \infty, k_\alpha) \approx \gamma_\ell(k_\alpha) e^{-i(\alpha_1 r - \ell\pi/2)} \left[e^{-\alpha_2 r} - S_\ell(k_\alpha) e^{\alpha_2 r} \right]. \tag{30}$$

Observe that the first term in brackets vanishes for large values of $-\alpha_2 r$. Hence, there remains only the scattering, purely outgoing wave $e^{\alpha_2 r}$. As a consequence, the particle is maximally scattered by the potential field $v(r)$ and the wave function is not "well behaved" since it does not fulfill the boundary condition at $r \to \infty$. However, as we have seen, this last "unphysical behaviour" is not only natural but necessary to study the elastic scattering process of a particle by a short range, nonsingular radial field interaction. Wave functions behaving like (30) are known as Gamow-Siegert solutions of the Schrödinger equation (3). We write

$$u_\ell^{(GS)}(r) = \begin{cases} \theta_\ell\, g_\ell(r,k_\alpha)\, u_\ell^{(1)}(k_\alpha r) & r < R \\ \\ -\gamma_\ell(k_\alpha) S_\ell(k_\alpha) u_\ell^{(+)}(r,k_\alpha) & R \leq r \end{cases} \tag{31}$$

where θ_ℓ is a constant and the intermediary function $g_\ell(r,k_\alpha)$ is equal to 1 at $r=0$ and depends on the potential. Besides the matching condition (16), the Gamow-Siegert functions fulfill the purely outgoing boundary condition:

$$\lim_{r\to+\infty} \left\{ \beta_\ell^{(GS)}(r) + ik_\alpha \right\} = 0. \tag{32}$$

Our interest is now addressed to the Gamow-Siegert functions not precisely as describing a decaying system but as appropriate mathematical tools to study the construction of complex Darboux-deformed potentials.

4. Complex-Darboux deformations of radial potentials

4.1. General considerations

In order to throw further light on the function $\beta_\ell(r)$ we may note that (5) transforms the Schrödinger equation (3) into a Riccati one

$$-\beta_\ell'(r) + \beta_\ell^2(r) + \epsilon_\ell = V_\ell(r) \tag{33}$$

where the energy k^2 has been changed for the arbitrary number ϵ_ℓ. Remark that (33) is not invariant under a change in the sign of the function beta:

$$\beta_\ell'(r) + \beta_\ell^2(r) + \epsilon_\ell = V_\ell(r) + 2\beta_\ell'(r). \tag{34}$$

These last equations define a Darboux transformation $\widetilde{V}_\ell(r) \equiv \widetilde{V}_\ell(r,\epsilon_\ell)$ of the initial potential $V_\ell(r)$. If ϵ_ℓ is a nontrivial complex number, then the Darboux-deformation is necessarily a complex function

$$\widetilde{V}_\ell(r) = V_\ell(r) + 2\beta_\ell'(r) \equiv V_\ell(r) - 2\frac{d^2}{dr^2} \ln \varphi_\epsilon(r) \tag{35}$$

where the transformation function $u_\ell(r,\epsilon) \equiv \varphi_\epsilon(r)$ is the general solution of (3) for the complex eigenvalue ϵ_ℓ. The solutions $y_\ell(r) = y_\ell(r,\epsilon_\ell,\mathcal{E})$ of the non-Hermitian Schrödinger equation

$$-y_\ell''(r) + \widetilde{V}_\ell(r)\, y_\ell(r) = \mathcal{E} y_\ell(r) \tag{36}$$

are easily obtained

$$y_\ell(r) \propto \frac{\mathrm{W}(\varphi_\epsilon(r), u_\ell(r))}{\varphi_\epsilon(r)}, \tag{37}$$

where $u_\ell(r)$ is eigensolution of equation (3) with eigenvalue $\mathcal{E}$.

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4.2. New exactly solvable optical potentials

Let the transformation function $\varphi_\epsilon(r)$ be a Gamow-Siegert function (31). The *superpotential* $\beta_\ell^{(GS)}(r,k_\alpha)$ and the new potential $\widetilde{V}_\ell(r)$ behave at the edges of D_v as follows

$$\beta_\ell^{(GS)}(r,k_\alpha) = \begin{cases} -\frac{\ell+1}{r} & r\to 0 \\ -ik_\alpha & r\to+\infty \end{cases} \qquad \Rightarrow \qquad \widetilde{V}_\ell(r) = \begin{cases} V_{\ell+1}(r) & r\to 0 \\ V_\ell(r) & r\to+\infty \end{cases} \tag{38}$$

It is remarkable that even for an initial potential with $\ell = 0$ the corresponding Darboux-deformation contains a nontrivial centrifugal term in the interaction zone $r < a$. Notice also that the new potential is mainly a real function at the edges of D_v. Thus, the function $\mathrm{Im}(\widetilde{V}_\ell)$ is zero at the origin and vanishes at $r\to+\infty$. In general $\mathrm{Im}(\widetilde{V}_\ell)$ oscillates along the whole of $(0,+\infty)$ according with the level of excitation of the Gamow-Siegert solution $u_\ell^{(GS)}(r,k_\alpha)$: The higher the level of excitation the greater the number of oscillations. Such a behaviour implies a series of maxima and minima in $\mathrm{Im}(\widetilde{V}_\ell)$ which can be analyzed in terms of the optical bench [19].

As regards the physical solutions of the new potential it is immediate to verify that, in all cases (bounded and scattering states of the initial potential), the corresponding transformations fulfill the boundary condition at $r = 0$. The analysis of the behaviour at $r\to\infty$ is as follows.

4.2.1. Scattering states. Let $u_\ell(r)$ be a scattering state of the initial potential in $r > a$. At $r\to+\infty$, the corresponding Darboux-Deformation (37) behaves as follows

$$\lim_{r\to+\infty} y_\ell(r) = -i\gamma_\ell(k)\left[(k_\alpha+k)u^{(-)}(r) - (k_\alpha-k)S_\ell(k)u^{(+)}(r)\right]_{r\to+\infty} \tag{39}$$

where we have used equation (22). As we can see, the Darboux-deformations of u_ℓ behave as scattering states at $r > a$.

If the scattering state $u_\ell(r)$ is a Gamow-Siegert function and $k \neq k_\alpha, \overline{k}_\alpha, -k_\alpha, -\overline{k}_\alpha$, the Darboux-deformation preserves the purely outgoing condition (32). Special cases are:

(i) $k = k_\alpha \Rightarrow$ the Wronskian in (37) is zero and there is no transformation.

(ii) $k = \overline{k}_\alpha \Rightarrow S_\ell(\overline{k}_\alpha) = 0$, then $y_\ell(r)$ is an exponentially decreasing function.

(iii) $k = -k_\alpha \Rightarrow S_\ell(-k_\alpha) = 0$ and the coefficient of $u^{(-)}(r)$ vanishes, then $y_\ell(r) = 0$.

(iv) $k = -\overline{k}_\alpha \Rightarrow S_\ell(-\overline{k}_\alpha)\to\infty$, then $y_\ell(r)$ fulfills the purely outgoing condition (32).

4.2.2. Bounded states. If $I_+ \ni k = i\kappa = i\sqrt{|E|}$ the function $u_\ell(r,\sqrt{|E|})$ corresponds to one of the bounded states (11). Thereby, from equation (37) we get

$$\lim_{r\to+\infty} y_\ell(r,\sqrt{|E|}) \approx (ik_\alpha - \sqrt{|E|})\,\xi_\ell(\sqrt{|E|})\,e^{-i\frac{\ell\pi}{2}}\,e^{-\sqrt{|E|}\,r}. \tag{40}$$

Thus, the Darboux-deformations of bounded wave-functions vanishes at $r\to\infty$. However, although this new functions are square-integrable, they do not form an orthogonal set in the Hilbert space spanned by the initial square-integrable wave-functions [14] (see also [24] and the 'puzzles' with self orthogonal states [25]).

In the next section we are going to solve the Schrödinger equation for the radial square well. We shall get the solutions corresponding to complex energy eigenvalues and purely outgoing boundary conditions. Thus, we shall construct the involved Gamow-Siegert functions.

5. Gamow-Siegert states of the radial square well

Let us consider the potential

$$v(r) = \begin{cases} -v_0 & r < a \\ 0 & a \leq r \end{cases} \tag{41}$$

with a and v_0 positive real numbers. The regular solution of the Schrödinger equation (3) for this potential may be written

$$u_\ell(r) = \begin{cases} \theta qr\, j_\ell(qr) & r < a \\ -i\gamma_\ell(k)\, kr \left[h_\ell^{(2)}(kr) + S_\ell(k) h_\ell^{(1)}(kr)\right] & a \leq r \end{cases} \tag{42}$$

where the *interaction parameter* q is defined by $q^2 = v_0 + k^2$. For simplicity, we shall analyze the s-wave solutions ($\ell = 0$) for which the matching conditions (16) lead to

$$S(q) = -\left[\frac{ik\sin(qa) + q\cos(qa)}{ik\sin(qa) - q\cos(qa)}\right] e^{-2ika}, \qquad \gamma(k) = -\frac{\theta e^{ika}}{2ik}[ik\sin(qa) - q\cos(qa)]. \tag{43}$$

Let us take $\theta = 2ik$. The scattering amplitude $S(k)$ has zeros and poles which respectively correspond to the roots of the transcendental equations

$$\frac{iq}{k} = \tan(qa), \qquad -\frac{iq}{k} = \tan(qa). \tag{44}$$

Indeed, equations (44) correspond to the even and odd quantization conditions for negative energies if $k = i\kappa \in I_+$, just as it has been discussed in the previous sections. However, we are looking for points k_α in the complex k–plane such that $\mathrm{Re}(k_\alpha) \neq 0$ and $\mathrm{Im}(k_\alpha) \neq 0$. Thereby, if k_α is a pole of S, the converging wave in (42) vanishes. Then the Gamow-Siegert function reads

$$u_{\ell=0}^{(\mathrm{GS})}(r) = \begin{cases} 2ik_\alpha \sin[q(k_\alpha)r] & r < a \\ 2ik_\alpha \sin[q(k_\alpha)a]\, e^{ik_\alpha(r-a)} & a \leq r \end{cases} \tag{45}$$

In order to solve the second equation in (44) let us rewrite the scattering amplitude as

$$S(k) = -\left[\frac{e^{2iqa}(k+q) + (q-k)}{e^{2iqa}(k-q) - (q+k)}\right] e^{-2ika}. \tag{46}$$

In this way, the poles of S are also the solutions of the transcendental equation

$$e^{2iqa} = \frac{|k|^2 - |q|^2 + 2\mathrm{Re}(k\overline{q})}{|k-q|^2}. \tag{47}$$

If the interaction parameter q is real, then $\sin(2qa) = 0$ and we obtain the following quantization rule for the energy

$$q_n = \frac{\pi n}{2a} \quad \Rightarrow \quad E_n = \left(\frac{n\pi}{2a}\right)^2 - v_0, \quad n = 0, 1, \ldots \tag{48}$$

On the other hand, let k and q be the complex numbers $k = K_1 + iK_2$ and $q = Q_1 + iQ_2$. Then $q^2 = v_0 + \epsilon = (v_0 + \epsilon_1) + i\epsilon_2$, with $\epsilon = k^2$. Hence we have

$$Q_1^2 - Q_2^2 = v_0 + \epsilon_1, \qquad 2Q_1Q_2 = \epsilon_2 \tag{49}$$

and

$$K_1^2 - K_2^2 = \epsilon_1, \qquad 2K_1K_2 = \epsilon_2. \tag{50}$$

The imaginary part of equation (47) is $\sin(2Q_1a) = 0$ and we obtain the following quantization rule

$$Q_{1,n} = \frac{\pi n}{2a}, \quad n = 0, 1, \ldots \tag{51}$$

Therefore, if $|Q_2| << 1$, the first equation in (49) shows that equation (51) leads to $\epsilon_1 \approx E_n$. The second equation in (49), on the other hand, gives a value of ϵ_2 which is not necessarily equal to zero. In this way, we shall study the poles of S for which the complex points ϵ are such that $\mathrm{Re}(\epsilon) \approx E_n$ and $\mathrm{Im}(\epsilon) \approx -\frac{\Gamma}{2}$, with $0 < \Gamma << 1$. The main problem is then to approximate the adequate value of Γ as connected with the discreteness of Q_1 in (51). With this aim, for a given finite value of a we take $|Q_2|a << 1$. A straightforward calculation shows that the second equation in (44) uncouples into the system

$$Q_1 = \sqrt{v_0}\sin(Q_1a)\cosh(Q_2a), \qquad Q_2 = \sqrt{v_0}\cos(Q_1a)\sinh(Q_2a). \tag{52}$$

In turn, the second one of these last equations reduces to

$$\cos(Q_1a) \approx \frac{1}{a\sqrt{v_0}} = \frac{1}{\eta}. \tag{53}$$

Now, let $|\delta| << 1$ be a correction of Q_1 around the quantized values (51), that is $Q_1a \approx Q_{1,n}a + \delta$. Then, equation (53) leads to

$$\delta_n = -\frac{\sin(\pi n/2)}{\eta}, \quad n \text{ odd}. \tag{54}$$

Thus, only odd values of n are allowed into the approximation we are dealing with. Now, to ensure small values of Q_2 we propose $Q_2a = \sum_{m=1}^{+\infty} \lambda_m/\eta^m$. From (49) we have

$$\frac{\epsilon_1}{v_0} \approx -1 + \left(\frac{aQ_{1,n}}{\eta}\right)^2 - \frac{2aQ_{1,n}\sin(\pi n/2)}{\eta^3} + \frac{1-\lambda_1^2}{\eta^4} - \frac{2\lambda_1\lambda_2}{\eta^5} - \cdots \tag{55}$$

In order to cancel the term including η^{-4} we take $\lambda_1 = \pm 1$ (the appropriate sign will be fixed below). Higher exponents in the power of $1/\eta$ are dropped by taking $\lambda_{m>1} = 0$. In order to get $\epsilon_1 \to E_n$, after introducing (51) into (55), we realize that the condition $\eta >> 1$ allows us to drop the term including η^{-3}. Thus, at the first order in the approximation of Q_2a we get $\epsilon_1 \approx E_n$.

It is also necessary to have regard to the positiveness of energy ϵ_1, which is ensured whenever n exceeds a minimum value. Let us take $n := n_{\inf} + m$, $m \in \mathbb{Z}^+$, where $n_{\inf}$ is the ceiling function of $2\eta/\pi$, i.e. $n_{\inf} = \left\lceil \frac{2\eta}{\pi} \right\rceil = \left\lceil \frac{2a\sqrt{v_0}}{\pi} \right\rceil$. Since n is odd, the integer m is even (odd) if $n_{\inf}$ is odd (even). We finally arrive at

$$\mathrm{Re}(\epsilon) \approx \left(\left[\frac{(n_{\inf}+m)\pi}{2a\sqrt{v_0}} \right]^2 - 1 \right) v_0, \quad m = \begin{cases} 0, 2, 4, \ldots & n_{\inf} \text{ odd} \\ 1, 3, 5, \ldots & n_{\inf} \text{ even} \end{cases} \tag{56}$$

On the other hand, it is worth noticing that the introduction of $Q_2a = \pm 1/\eta$ and (54) into the second equation in (49) leads to the conclusion that $Q_2a = +1/\eta$ has to be dropped. The expression for the imaginary part of the complex energy ϵ is calculated as follows. First, let us rewrite equations (52) in the form

$$K_1 = \pm\sqrt{v_0}\sin(Q_1a)\sinh(Q_2a), \qquad K_2 = \pm\sqrt{v_0}\cos(Q_1a)\cosh(Q_2a). \tag{57}$$

Since $\epsilon_2 = -\Gamma/2$, from equations (50) we realize that the sign of K_1 must be the opposite one of K_2. The introduction of (53) into the second equation in (57) leads to

$$K_2 \approx \pm\frac{1}{a}\left(1 + \frac{1}{2\eta^2}\right) \tag{58}$$

where we have used $Q_2 a \approx -1/\eta$. If $\eta >> 1$ we get $aK_2 \approx \pm 1$. Then, this last result together with the real part of the factorization constant ϵ gives

$$K_1^2 = \epsilon_1 + K_2^2 \approx \epsilon_1 + \frac{1}{a^2}. \tag{59}$$

Thus, for $a^2\epsilon_1 > 1$ we obtain $K_1 \approx \pm\sqrt{\epsilon_1}$. Finally, the introduction of (58) and (59) into the second equation of (50) produces

$$\text{Im}(\epsilon) = -\frac{\Gamma}{2} \equiv -2|K_1|\,|K_2| \approx -\frac{2}{a}\sqrt{\text{Re}(\epsilon)}. \tag{60}$$

In Figure 2 we show the absolute value of the scattering amplitude close to one of its poles k_α and the corresponding zero $\bar{k}_\alpha$. Some of the first resonances are reported in Table 1 for different values of the potential strength v_0 and the cutoff a.

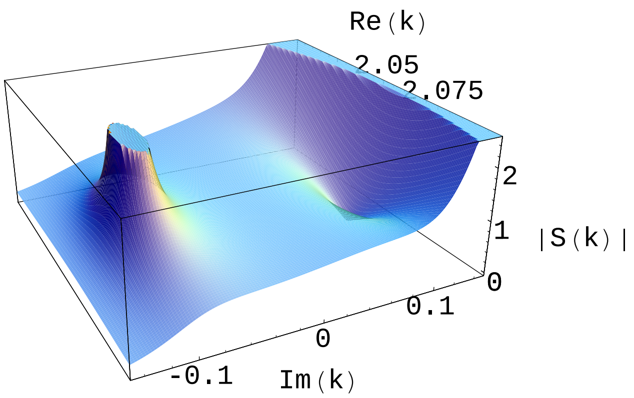

Figure 2. The absolute value of the scattering amplitude $S(k)$ close to the pole k_α (and the zero $\bar{k}_\alpha$) which corresponds to the first resonance $E_\alpha = k_\alpha^2$ of the square well reported in Table 1 for $n_{\text{inf}} = 64$. The limits of our approach give the number $k_\alpha = 2.063412 - i\,0.099882$.

5.1. Complex Darboux-deformations of the radial square well

Figure 3 shows the global behaviour of a typical Gamow-Siegert function associated with the radial square well. Notice the exponential growing of the amplitude for $r > a$. This kind of solutions are used in (35) to complex Darboux-deform the square well as it is shown in Figure 4.

The cardiod-like behaviour seems to be a profile of the complex potentials derived by means of Darboux-deformations (compare with [20] and [22]). In this case, the complex potential shows concentric cardiod curves for values of r inside the interaction zone, one of them is shown at the left of Figure 4. The real and imaginary parts of $\widetilde{V}_\ell(r)$ are then characterized by oscillations and changes of sign depending on the position in $r < a$. As a consequence, these complex potentials behave as an optical device which both refracts and absorbs light waves (see details in [22] and

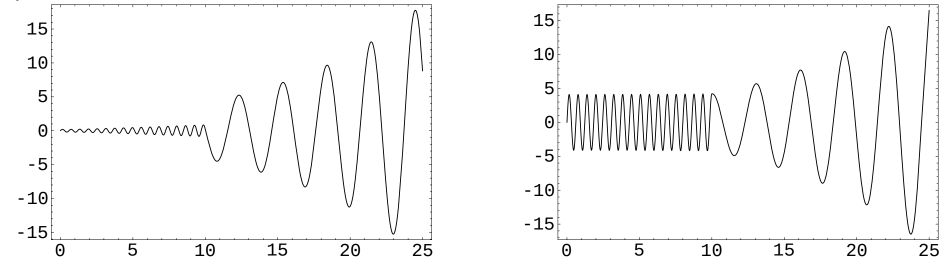

Figure 3. The real (left) and imaginary (right) parts of the Gamow-Siegert function (45) associated with the first resonance state reported in Table 1 for $n_{\text{inf}} = 64$.

discussions on the optical bench in [19]). The presence of this kind of oscillations is also noted at distances slightly greater than the cutoff $r = a$. Hence, the complex Darboux-deformations (35) are short range potentials which enlarge the initial 'interaction zone' as it is shown in the right part of Figure 4.

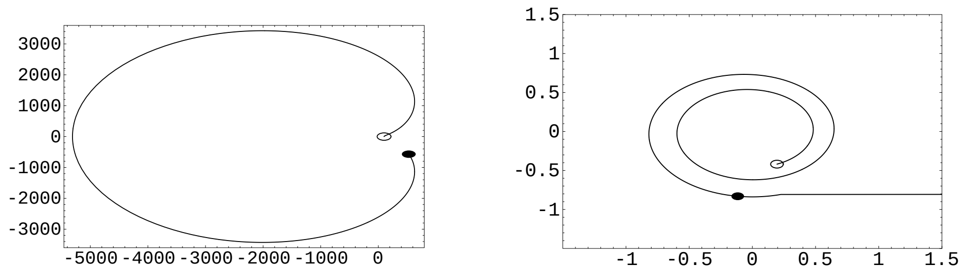

Figure 4. The Argand-Wessel diagram of the complex Darboux-deformed square well with $v_0 = 100$ and $a = 10$. Left: Detail of the cardiod-like behaviour of the new potential between $r = 9.8$ (disk) and $r = 10$ (circle). Right: The disk is evaluated at $r = 10.1$ and the circle at $r = 13$. As complementary information: $\widetilde{V}_0(r = 10) = 100.2255 - i\,0.8076$ and $\widetilde{V}_0(r = 10.1) = -0.1157 - i\,0.8306$.

Table 1. The first four resonance energies for the radial square well of intensity $v_0 = 100$ and cutoff $a = 10$ ($n_{\text{inf}} = 64$) and for the radial square well of intensity $v_0 = 1000$ and cutoff $a = 10$ ($n_{\text{inf}} = 202$). Notice that, in each case, the even values of m obtained for the related one-dimensional problem are missing (see e.g. Table A.1 of reference [22]).

	$n_{\text{inf}} = 64$	$n_{\text{inf}} = 202$
$m = 1$	$04.247696 - i\,0.412198$	$16.791319 - i\,0.819544$
$m = 3$	$10.761635 - i\,0.656098$	$36.925312 - i\,1.215324$
$m = 5$	$17.472966 - i\,0.836013$	$57.256697 - i\,1.513363$
$m = 7$	$24.381689 - i\,0.987556$	$77.785474 - i\,1.763921$

6. Concluding remarks

We have studied the elastic scattering process of a particle by short range, nonsingular radial field interactions. The poles of the involved scattering amplitude $S(k)$ play a relevant role in the construction of physical solutions connected with either bounded or scattering states of the energy. It has been shown that poles k_α in the lower half complex k–plane lead to the "unphysical" Gamow-Siegert functions which are necessary to depict the behaviour of the scattering phenomenon.

The Gamow-Siegert functions were used to transform the radial short range potentials into complex ones which preserve the initial energy spectrum. These new potentials are 'opaque' in the sense that they simultaneously emit and absorb flux, just as an optical device which both refracts and absorbs light waves. The transformation preserves the square-integrability of the solutions at the cost of producing non-orthogonal sets of wave-functions. It is also notable that scattering states are transformed into scattering states while deformed Gamow-Siegert functions can be either a new Gamow-Siegert function or an exponentially decreasing function depending on the involved kinetic parameter k and the pole k_α.

The method has been applied to the radial square well in the context of s-waves ($\ell = 0$). Analytical expressions were derived for the corresponding complex energies in the long lifetime limit (i.e., for small values of $|\text{Im}(E_\alpha)| = \Gamma/2$) and, as a consequence, such energies fulfill a 'quantization rule'. In contrast with the 'even' and 'odd' resonances of short range potentials defined in the whole of the straight-line (see e.g. [22]), the resonances of radial short range potentials are labelled by only odd (positive) integers. This result enforces the interpretation of Gamow-Siegert functions as representing quasi-bounded states: The bounded spectrum of a potential which is invariant under the action of the parity operator $v(x) = v(-x)$ includes odd and even functions. The symmetry is broken by adding an impenetrable wall at the negative part of the straight line and only the odd solutions are preserved. As we have shown, the same is true for resonance states.

Finally, the results reported in this paper are complementary to our previous work [22]. It is remarkable that explicit derivations of Gamow-Siegert functions are barely reported in the literature, not even for simple models like those studied here (however see [5, 20, 21, 26–29]). We hope our approach has shed some light onto the solving of the Schrödinger equation for complex energies and functions fulfilling the purely outgoing boundary condition.

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