Resonances in Cut-Off Potentials Determined by the Exterior Complex-Scaling Method

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Abstract. The resonances of one-dimensional short-range potentials defined by a cutoff are analyzed in terms of a modification of the well known complex-scaling method. Such a modification consists in transforming the eigenfunctions only in the zone where the potential is identically zero. As usual, the complex-scaled Hamiltonian is non-Hermitian and the functions that represent resonances become square-integrable. The method is illustrated by calculating the resonances of a concrete cut-off potential.

1. Introduction

Resonances in quantum mechanics are special cases of scattering states for which the 'capture' of the incident wave (projectile) by the scatterer produces delays in the scattered wave. They are represented by solutions of the Schrödinger equation associated to complex energy eigenvalues $\epsilon = E - i\Gamma/2$ and satisfying purely outgoing conditions. Here E is interpreted as the binding energy of a decaying system which is composed by the scatterer and the projectile, and $\tau = \hbar/\Gamma$ as the corresponding life-time. In contrast with the conventional scattering wave-functions, such a kind of solutions to the Schrödinger equation are not finite at large distances. Therefore, some approaches have been introduced to extend the formalism of quantum theory so that the resonance states can be defined in precise form (for detailed information see e.g. [1]). Of special interest, the complex-scaling method is useful to transform the resonance eigenfunctions into square-integrable functions [1–4]. The latter at the price of transforming the initial Hamiltonian into a non-Hermitian operator.

In the present paper we analyze the resonances associated with cut-off potentials which are defined as $V(x) = v(x)\,\Theta\,(\xi - |x|)$, with Θ the step function, and v a real-valued smooth function. The interval $[-\xi, \xi] \in \mathbb{R}$ defines an *interaction zone* where the potential is not identically zero, so that our model represents a short-range interaction centered at the origin of coordinates and delimited by the *cutoff* $\xi \geq 0$. As these potentials are not analytic in general, the conventional complex-scaling method is not necessarily applicable. Therefore, we shall follow the *exterior complex scaling method* [5] to transform the cut-off potentials outside the interaction zone only. With this aim we revisit the main points of the conventional complex-scaling method in Sec. 2. The modifications of the method addressed to study the cut-off potentials are indicated in Sec. 3 and some examples are given. In Sec. 4 we give some final remarks.

2. Complex Scaling

Let $k = k_r + ik_i = |k|e^{-i\beta}$ be the wave number defining an scattering wave with $k_r, k_i, \beta \in \mathbb{R}$. If $0 < \beta < \pi/2$ (equivalently, $k_r > 0$ and $k_i < 0$), then k is in the fourth quadrant of the complex k-plane and defines a resonance with 'complex energy' $\epsilon = k^2$. Therefore, the corresponding eigenfunctions are such that $u_\epsilon(x) \sim e^{\pm i|k|x \cos \beta} e^{\pm |k|x \sin \beta}$ as $x \to \pm\infty$. Using the operator

$$S_0 = e^{i\theta x \, d/dx}, \qquad \theta \in \mathbb{R}, \tag{1}$$

and the Baker-Campbell-Hausdorff formula [6] $e^A B e^{-A} = \{e^A, B\} = \sum_{n=0}^{\infty} \frac{1}{n!} \{A^n, B\}$, one can show that the initial Hamiltonian H is transformed into the non-Hermitian operator

$$S_0 H S_0^{-1} \equiv H_\theta^0 = -e^{-2i\theta} \frac{d^2}{dx^2} + V(xe^{i\theta}), \tag{2}$$

and that the new eigenfunction is such that $\widetilde{u}_\epsilon(x \to \pm\infty) = e^{\pm i|k|x \cos(\theta-\beta)} e^{\mp |k|x \sin(\theta-\beta)}$. Therefore, $\widetilde{u}_\epsilon$ is square-integrable whenever $0 < \theta - \beta < \frac{\pi}{2}$ [1]. In particular, for $\beta = 0$ we realize that the scattering states are transformed as $e^{\pm i|k|x} \to e^{\pm i|k|x \cos\theta} e^{\mp |k|x \sin\theta}$. That is, plane waves are transformed into exponential decreasing or increasing functions for large values of $|x|$. To preserve the oscillating form of the scattering wave-functions we must make $k = |k| \to |k|e^{-i\theta}$. The latter induces a rotation of the positive real axis in the clockwise direction by the angle 2θ, so that the rotated energy is complex $\varepsilon = E(\cos 2\theta - i \sin 2\theta)$ [1]. Thus, the complex-rotation is such that bound energy states are preserved while the resonance states are now represented by square-integrable functions.

3. Exterior complex scaling

Following [5], we propose the transformation

$$\widetilde{x} = \begin{cases} e^{i\theta}(x+\xi) - \xi, & x \leq -\xi \\ x, & |x| < \xi \\ e^{i\theta}(x-\xi) + \xi, & x \geq \xi \end{cases} \tag{3}$$

The rotated variable $\widetilde{x} = xe^{i\theta}$ is a complex-valued function of x which is continuous in $\mathbb{R}$ and has a derivative with discontinuities at $x = \pm\xi$. Let $\psi(x)$ be a solution to the Schrödinger equation associated with the cut-off potential $V(x) = v(x)\,\Theta\,(\xi - |x|)$. Outside the interaction zone, it can be denoted as ψ_I and ψ_{III} for $x \leq -\xi$ and $x \geq \xi$ respectively. In the interaction zone $|x| < \xi$, we shall write ψ_{II}. The boundary conditions for the transformed solution $\psi(\widetilde{x}(x))$ are as follows

$$\psi_I(\widetilde{x})|_{x=-\xi} = \psi_{II}(\widetilde{x})|_{x=-\xi}, \qquad \psi_{II}(\widetilde{x})|_{x=\xi} = \psi_{III}(\widetilde{x})|_{x=\xi}, \tag{4}$$

$$\left.\frac{d\psi_I(\widetilde{x})}{d\widetilde{x}}\right|_{x=-\xi} = \left.\frac{d\psi_{II}(\widetilde{x})}{d\widetilde{x}}\right|_{x=-\xi}, \qquad \left.\frac{d\psi_{II}(\widetilde{x})}{d\widetilde{x}}\right|_{x=\xi} = \left.\frac{d\psi_{III}(\widetilde{x})}{d\widetilde{x}}\right|_{x=\xi}. \tag{5}$$

To avoid the non-differentiability of $\psi(\widetilde{x})$ at $x = \pm\xi$, let us introduce a twice-differentiable function of x in the form

$$w(x) = \begin{cases} e^{i\theta}(x+\xi) - \xi + w_1(x), & x \leq -\xi \\ x, & -\xi \leq x \leq \xi \\ e^{i\theta}(x-\xi) + \xi + w_2(x), & x \geq \xi \end{cases} \tag{6}$$

where the functions w_1 and w_1 are as smooth as necessary and such that

$$\lim_{x \to -\infty} w_1(x) = 0, \qquad \lim_{x \to +\infty} w_2(x) = 0. \tag{7}$$

Therefore

$$w(x) \to e^{i\theta} x, \quad \text{as } |x| \to \infty. \tag{8}$$

The differentiability requirements on w impose the following conditions on w_1 and w_2,

$$w_1(-\xi) = w_2(\xi) = 0, \qquad \left.\frac{dw_1}{dx}\right|_{x=-\xi} = \left.\frac{dw_2}{dx}\right|_{x=\xi} = 1 - e^{i\theta}, \tag{9}$$

$$\left.\frac{d^2 w_1}{dx^2}\right|_{x=-\xi} = \left.\frac{d^2 w_2}{dx^2}\right|_{x=\xi} = 0, \tag{10}$$

It can be shown that $w_1(x) = (1 - e^{i\theta})(x + \xi)(1 - (x + \xi))e^{x+\xi}$ and $w_2(x) = (1 - e^{i\theta})(x - \xi)(1 + x - \xi)e^{-(x-\xi)}$ satisfy the equations (7), (9) and (10). After some straightforward calculations one arrives at the differential operator

$$\frac{d^2}{dw^2} = (1 - V_2(x))\frac{d^2}{dx^2} - V_1(x)\frac{d}{dx}, \tag{11}$$

where the functions

$$V_1(x) = \begin{cases} \dfrac{w_1''}{(e^{i\theta} + w_1')^3}, & x \le -\xi, \\ 0, & |x| < \xi, \\ \dfrac{w_2''}{(e^{i\theta} + w_2')^3}, & x \ge \xi, \end{cases} \qquad V_2(x) = \begin{cases} 1 - \dfrac{1}{(e^{i\theta} + w_1')^2}, & x \le -\xi \\ 0, & |x| < \xi \\ 1 - \dfrac{1}{(e^{i\theta} + w_2')^2}, & x \ge \xi \end{cases} \tag{12}$$

are continuos in $\mathbb{R}$ since w is twice differentiable. Then, the complex-scaled Hamiltonian can be written as

$$H_\theta = -\frac{d^2}{dw^2} + V(w) = -\frac{d^2}{dx^2} + V_2(x)\frac{d^2}{dx^2} + V_1(x)\frac{d}{dx} + V(w(x)). \tag{13}$$

Notice the kinetic– and flux–like terms defined by the position-dependent coefficients $V_2(x)$ and $V_1(x)$, the latter respectively such that $\lim_{x\to\pm\infty} V_2(x) = 1 - e^{-i\theta}$ and $\lim_{x\to\pm\infty} V_1(x) = 0$. Besides, in the interaction zone, the Hamiltonians H_θ and H are identical because the transformation leaves invariant the function $v(x)$. In Fig 1 we show the behavior of the functions (12) outside the interaction zone.
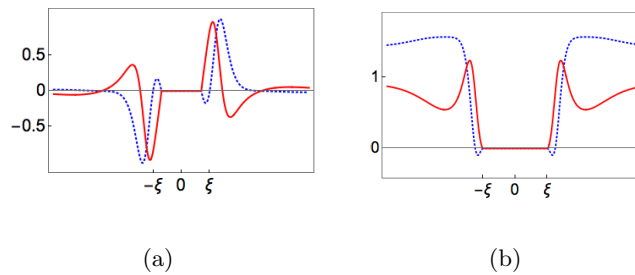

(a)   (b)

Figure 1. (Color online) Real (dotted-blue) and imaginary (continuous-red) parts of the functions V_1 (a) and V_2 (b) defined in (12) for $\theta = 1$. Notice that both functions are equal to zero in the interaction zone $[-\xi, \xi]$.

3.1. Examples

To obtain the transformed resonances of concrete problems, given a Hamiltonian, we only have to substitute the function (6) in the corresponding eigenfunction. For instance, consider the semi-harmonic barrier V_b defined by

$$
V_b(x) = \begin{cases} v_2, & x \in (-\xi, -b), \\ x^2, & x \in (-b, b), \\ v_1, & x \in (b, \xi), \\ 0, & \text{otherwise}, \end{cases}
\tag{14}
$$

where $b, v_1, v_2 > 0$ [7]. The behavior of the new complex-valued potential is defined by the combination of (14) and (12), compare Figs. 1 and 2.
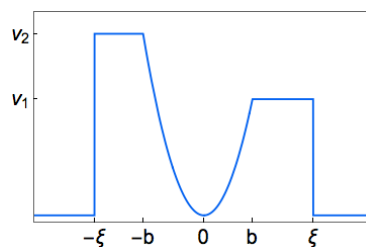

Figure 2. The semi-harmonic potential defined in (14).

In the panel of Fig. 3 we show the results of the exterior complex scaling for two different values of θ. In the upper row ($\theta = 0.05$), two poles in the fourth quadrant of complex k-plane have been rotated up to a position which is very close to the real axis, see Fig. 3(a). The wave-function of the resonance which is closest to the real axis is plotted in Fig. 3(b). Such a function is still not square-integrable, see the corresponding squared modulus in Fig. 3(c). In turn, the kinetic– and flux–like terms defined by V_1 and V_2 in (13) are shown in figures 3(d) and 3(e). For a greater value of θ, namely $\theta = 0.77$, in Fig. 3(f) we appreciate that both resonances have been rotated to the first quadrant of the k-plane. As a result, the above described wave-function is now square-integrable, see Figs. 3(g) and 3(h). Besides, as indicated in Figs. 3(i) and 3(j), the kinetic– and flux–like terms are not oscillating any more and show extremal behavior in the vicinities of $x = \pm\xi$ only.

4. Concluding remarks

We have studied the complex scaling method for cut-off potentials. We have shown that performing the transformation outside the interval where the discontinuities of the potential lie, the complex scaling can be done if the transformed variable is well behaved at the cut-off. We have shown that additional terms are present in the scaled Hamiltonian which can be interpreted as diffusion and flux terms, and that in the case of cut-off potentials they are the unique change in the scaled Hamiltonian, so that they carry all the physical information about the complex scaling. Our results are in agreement with those reported in e.g. [8]. The applicability of our approach is shown with a concrete cut-off potential. The study of the physical information of the diffusion and flux terms is part of work under progress.
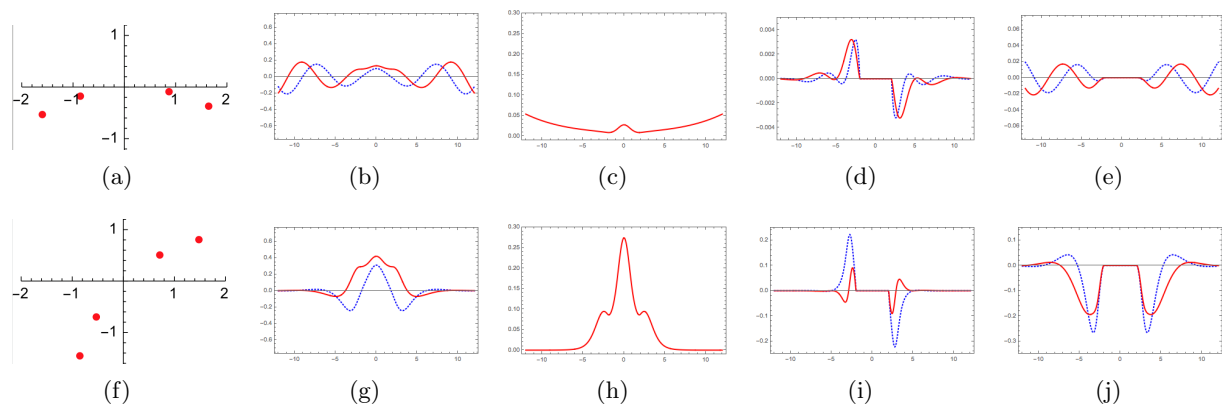
Figure 3. Results of the exterior complex-scaling method applied to the semi-harmonic barrier potential (14) with $v_1 = v_2 = b^2$, $b = 1$, $\xi = 2$, for $\theta = 0.05$ (upper row) and $\theta = 0.77$ (lower row). In both cases, from left to right, the columns correspond to the poles in the complex k-plane that define the resonances, the real (dotted-blue) and imaginary (continuous-red) parts of the wave-function belonging to the resonance which is closest to the real axis, the corresponding squared modulus, the real (dotted-blue) and imaginary (continuous-red) parts of the kinetic– and the flux–like terms defined by the functions V_1 and V_2 in (13).

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