

A Power Series Representation for the Characteristic Equation of Gamow-Siegert Eigenstates

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Abstract. In this work we consider a quantum system described by a stationary Schrödinger equation and obtain an explicit representation for the characteristic equation of its Gamow-Siegert eigenstates in the form of a power series of the energy parameter. This representation is valid for both analytical or numerical calculations. We show that determining resonances reduces to calculating the roots of a polynomial equation. The effectiveness of this approach is demonstrated through several numerical examples.

1. Introduction

Solutions of the Schrödinger equation associated to complex energies and satisfying the purely outgoing wave conditions are called Gamow-Siegert functions, which describe the resonance states of quantum systems. These functions were first used in [1] for describing the spontaneous alpha-decay of nuclei, and later Siegert [2] obtained a dispersion formula where the *radioactive* states were represented by resonance terms. Let $|\Psi\rangle$ be a Gamow-Siegert function associated to the complex energy $\epsilon = E - i\Gamma/2$ ($E > 0$, $\Gamma > 0$) and possessing the complex wave-number $k = \sqrt{2m\epsilon}/\hbar$, then $|\Psi\rangle$ describes states possessing an exponential decay behaviour

$$|\langle\Psi(q,0)|\Psi(q,t)\rangle|^2 = e^{-\Gamma t/\hbar}.$$

Several formalisms have been used for describing resonance states, including Darboux (supersymmetric) transformations [3–6], rigged Hilbert spaces [7–10], the S -matrix [11], the transfer matrix [5], the complex-scaling technique [12], and squeezing operators [13], among others (see, *e.g.*, [14–16] and references therein for a complete review of techniques used in quantum mechanics for analysing resonances). On the other hand, the theory of quantum resonances has been used for analysing leaky modes [17] in electromagnetic waveguides via suitable analogies between quantum mechanics and electromagnetism (see, *e.g.*, [18, 19]).

In the present work we apply the spectral parameter power series method [20] (SPPS for short) for obtaining explicitly the characteristic equation that describes the resonance states. This characteristic equation is given by the Taylor series of an analytic function of the complex variable λ , being λ the complex energy of a quantum particle. This series can be truncated for its numerical implementation. Then, analysing resonances reduces to determining zeros (or approximately, polynomial roots) of the characteristic equation. This approach provides an



effective way for addressing resonance states in Schrödinger operators with almost arbitrary potential functions.

The outline of this work is as follows. In Section 1 we obtain a general solution to a one-dimensional Schrödinger equation equipped with an arbitrary short range potential. In Section 2 we obtain the characteristic equation that defines the resonance states. In Section 3 we obtain a power series representation of the characteristic equation, and use it in some numerical examples. Finally, in Section 4 we give some concluding remarks.

2. General solution of the Schrödinger equation with a short range potential

Let us consider the differential expression

$$\ell(u) := -\frac{d^2 u(x)}{dx^2} + V(x)u(x), \quad V(x) = \begin{cases} V_1, & -\infty < x < h_1, \\ V_2(x), & h_1 < x < h_2, \\ V_3, & h_2 < x < +\infty, \end{cases}$$

in $\mathbb{R} \setminus \{h_1, h_2\}$, corresponding to a stationary Schrödinger operator ($\hbar^2 = 1 = 2m$) in its coordinate representation. The function V_2 represents a short range potential satisfying certain smoothness conditions. At the points of discontinuity the boundary conditions

$$[u(x)]_{x=h_j} = 0, \quad [u'(x)]_{x=h_j} = 0, \quad j = 1, 2, \quad (1)$$

define the behaviour of the functions on which ℓ acts. Here the notation $[f]_{x_0} := f(x_0 + 0) - f(x_0 - 0)$ represents the jump of f at the point x_0 .

Let us search for a general solution of the equation $\ell(\psi) = \lambda\psi$ in $(-\infty, \infty)$, where λ is a parameter corresponding to the energy of a quantum particle. If ψ_1 and ψ_2 are two linearly independent solutions of the equation in (h_1, h_2) , then the piecewise function

$$\psi(x; \lambda) = \begin{cases} a_1 e^{i\kappa_1(x-h_1)} + a_2 e^{-i\kappa_1(x-h_1)}, & -\infty < x < h_1, \\ b_1 \psi_1(x; \lambda) + b_2 \psi_2(x; \lambda), & h_1 \leq x \leq h_2, \\ c_1 e^{i\kappa_3(x-h_2)} + c_2 e^{-i\kappa_3(x-h_2)}, & h_2 < x < \infty \end{cases} \quad (2)$$

with $\kappa_1(\lambda) = (\lambda - V_1)^{1/2}$, $\kappa_3(\lambda) = (\lambda - V_3)^{1/2}$, satisfies the differential equation in $\mathbb{R} \setminus \{h_1, h_2\}$. By $a_1, a_2, b_1, b_2, c_1, c_2$ we denote arbitrary constants. Conditions (1) applied from right to left give the constants a_1, a_2, b_1, b_2 in terms of c_1, c_2 as follows

$$b_1 = \frac{1}{W} (c_1 \beta_{22} + c_2 \beta_{12}), \quad b_2 = -\frac{1}{W} (c_1 \beta_{21} + c_2 \beta_{11}); \quad (3a)$$

$$a_1 = \frac{1}{2i\kappa_1} (b_1 \alpha_{11} + b_2 \alpha_{12}), \quad a_2 = -\frac{1}{2i\kappa_1} (b_1 \alpha_{21} + b_2 \alpha_{22}), \quad (3b)$$

where the coefficients α_{ij}, β_{ij} ($i, j = 1, 2$) are defined by

$$\alpha_{ij} := (-1)^{i+1} i\kappa_1 \psi_j(h_1; \lambda) + \psi'_j(h_1; \lambda), \quad \beta_{ij} := (-1)^{i+1} i\kappa_3 \psi_j(h_2; \lambda) + \psi'_j(h_2; \lambda),$$

and $W = W[\psi_1, \psi_2](x)$ is the Wronskian of ψ_1, ψ_2 . Here the prime $'$ represents the derivative with respect to x .

Consider the Schrödinger equation $\ell(\psi) = \lambda\psi$ with $\lambda \in \mathbb{R}$ and suppose that $V_1, V_3 \in \mathbb{R}$. Scattering states are described by bounded solutions such that $\lambda > \max\{V_1, V_3\}$, while bound states are described by solutions belonging to an appropriate functional space (*e.g.*, the Hilbert space $L^2(\mathbb{R})$) such that $\lambda < \min\{V_1, V_3\}$. In this work, we are interested in the Gamow-Siegert

states possessing complex energies. For $\lambda \in \mathbb{C}$ the operation $(\lambda - V_j)^{1/2}$ ($j = 1, 3$) leads to two branches defined by

$$(\lambda - V_j)^{1/2} = \sqrt{|\lambda - V_j|} e^{i \frac{\theta_j + 2\pi k}{2}}, \quad \theta_j = \arg(\lambda - V_j) \quad (k = 0, 1; j = 1, 3).$$

The appropriate selection of a branch according to the constraints of the problem defines a proper Riemann sheet in the complex λ -plane in which $\kappa_j(\lambda)$ ($j = 1, 3$) is unambiguously defined. Once a branch is chosen, general solution (2)-(3) is well-defined provided that $\kappa_1 \neq 0$.

3. Solutions satisfying purely outgoing wave conditions

Let \mathcal{H} be an operator defined by the expression $\mathcal{H}\psi := \ell(\psi)$, with domain $\text{Dom}(\mathcal{H})$ consisting of functions ψ satisfying continuity conditions (1), and the purely outgoing wave conditions

$$\lim_{x \rightarrow -\infty} (\psi'(x; \lambda) + i\kappa_1 \psi(x; \lambda)) = 0, \quad \lim_{x \rightarrow +\infty} (\psi'(x; \lambda) - i\kappa_3 \psi(x; \lambda)) = 0. \quad (4)$$

Solutions in $\text{Dom}(\mathcal{H})$ of the equation $\mathcal{H}\psi = \lambda\psi$ are constructed from general solution (2)-(3) as follows. Asymptotic condition as $x \rightarrow +\infty$ is satisfied if $c_2 = 0$. The resulting solution describes the dispersion of quantum waves generated by a source of particles to the left of the interaction potential V_2 . The remaining constant c_1 is chosen so that the incoming wave $e^{i\kappa_1(x-h_1)}$ has unit amplitude, more precisely

$$\psi(x; \lambda) = \begin{cases} e^{i\kappa_1(x-h_1)} + (\tilde{a}_2/\tilde{a}_1) e^{-i\kappa_1(x-h_1)}, & -\infty < x < h_1, \\ (\beta_{22}/\tilde{a}_1) \psi_1(x; \lambda) - (\beta_{21}/\tilde{a}_1) \psi_2(x; \lambda), & h_1 \leq x \leq h_2, \\ (W/\tilde{a}_1) e^{i\kappa_3(x-h_2)}, & h_2 < x < \infty, \end{cases}$$

$$\tilde{a}_1 = \frac{1}{2i\kappa_1} (\beta_{22}\alpha_{11} - \beta_{21}\alpha_{12}), \quad \tilde{a}_2 = -\frac{1}{2i\kappa_1} (\beta_{22}\alpha_{21} - \beta_{21}\alpha_{22}).$$

Let $R := \tilde{a}_2/\tilde{a}_1$ and $T := W/\tilde{a}_1$ be the amplitudes of the reflected and transmitted waves, respectively, and let $\mathbb{R} := |R|^2$ and $\mathbb{T} := |T|^2$ be the corresponding reflection and transmission coefficients, which satisfy $\mathbb{T}(\lambda) + \mathbb{R}(\lambda) = 1$ for every $\lambda \in \mathbb{C}$. In order to fulfil asymptotic condition (4) as $x \rightarrow -\infty$, the term $R(\lambda) e^{-i\kappa_1(x-h_1)}$ must dominate over $e^{i\kappa_1(x-h_1)}$ for some complex energies λ_n , that is, $e^{i\kappa_1 x} = o(Re^{-i\kappa_1 x})$ as $x \rightarrow -\infty$, $\lambda \rightarrow \lambda_n$, using Landau's notation. This is fulfilled if

$$\lim_{\lambda \rightarrow \lambda_n} e^{-2i\kappa_1 h_1} \left(\frac{\alpha_{11}\beta_{22} - \alpha_{12}\beta_{21}}{\alpha_{22}\beta_{21} - \alpha_{21}\beta_{22}} \right) = 0.$$

Since $e^{-2i\kappa_1 h_1} \neq 0$ for every $\lambda \in \mathbb{C}$, the limit is satisfied if $\lambda_n \in \mathbb{C}$ is a zero of the equation $\varrho(\lambda) = 0$, where $\varrho(\lambda) := \alpha_{11}(\lambda)\beta_{22}(\lambda) - \alpha_{12}(\lambda)\beta_{21}(\lambda)$. Let $\lambda_n = E_n - i\Gamma_n/2$ ($E_n > 0$, $\Gamma_n > 0$) be a zero of $\varrho(\lambda) = 0$ such that $\text{Re}[\kappa_1(\lambda_n)] > 0$ and $\text{Im}[\kappa_1(\lambda_n)] < 0$, (these conditions define the *correct* direction in which an outgoing wave should propagate [3]) then λ_n represents the complex energy of a resonance state $\psi(x; \lambda_n) =: \psi_n(x) \in \text{Dom}(\mathcal{H})$. The generalised eigenfunction ψ_n associated to the complex eigenvalue λ_n is a Gamow-Siegert eigenstates of the Hamiltonian \mathcal{H} . As usual, E_n is the energy of the resonance state and Γ_n is the inverse of its lifetime. Note that the zeros of $\varrho(\lambda) = 0$ coincide with the poles of the transmission amplitude

$$T(\lambda) = \frac{2i\kappa_1(\lambda)W}{\alpha_{11}(\lambda)\beta_{22}(\lambda) - \alpha_{12}(\lambda)\beta_{21}(\lambda)},$$

which is a meromorphic function of the complex variable λ . The function ϱ can be written in terms of ψ_1 and ψ_2 as follows

$$\begin{aligned} \varrho(\lambda) &= (\psi'_1(h_1; \lambda) + i\kappa_1(\lambda)\psi_1(h_1; \lambda)) (\psi'_2(h_2; \lambda) - i\kappa_3(\lambda)\psi_2(h_2; \lambda)) \\ &\quad - (\psi'_2(h_1; \lambda) + i\kappa_1(\lambda)\psi_2(h_1; \lambda)) (\psi'_1(h_2; \lambda) - i\kappa_3(\lambda)\psi_1(h_2; \lambda)). \end{aligned}$$

In the next section we will obtain a series representation of this formula by means of the SPPS method [20], which is valid for a large class of interaction potentials V_2 . It is worth noting that no general formula exists for obtaining ψ_1 and ψ_2 for, say, every continuous function V_2 , thereby a numerical method should be employed (*e.g.*, the shooting method or the WKB method [21], [22, pp. 484–539], [23]). Numerical methods give approximations of ψ_1 and ψ_2 (see, *e.g.*, [24, Part III], and [25] for a review of the most commonly used numerical methods to solve ODEs), but the SPPS method gives exact solutions of Sturm-Liouville problems in the form of uniformly convergent power series of the spectral parameter, as is shown next.

4. SPPS form of the characteristic equation for the Gamow-Siegert eigenstates

The dispersion equation $\varrho(\lambda) = 0$ for the Gamow-Siegert eigenstates is constructed from two linearly independent solutions ψ_1, ψ_2 of Sturm-Liouville equation

$$-\psi''(x) + V_2(x)\psi(x) = \lambda\psi(x), \quad h_1 < x < h_2 \quad (5)$$

Let ψ_0 be a non-vanishing particular solution of the associated homogeneous equation (*i.e.*, when $\lambda = 0$) satisfying the regularity conditions $\psi_0^2, \psi_0^{-2} \in \mathcal{C}[h_1, h_2]$, then the power series [20]

$$\psi_1(x; \lambda) = \psi_0(x) \sum_{k=0}^{\infty} (-\lambda)^k \tilde{X}^{(2k)}(x), \quad \psi_2(x; \lambda) = \psi_0(x) \sum_{k=0}^{\infty} (-\lambda)^k X^{(2k+1)}(x) \quad (6)$$

with $\tilde{X}^{(n)}, X^{(n)}$ defined by the recursive integration procedure $\tilde{X}^{(0)}(x) \equiv 1, X^{(0)}(x) \equiv 1$,

$$\tilde{X}^{(n)}(x) = \begin{cases} \int_{x_0}^x \tilde{X}^{(n-1)}(s) \psi_0^2(s) ds, & \text{odd } n, \\ \int_{x_0}^x \tilde{X}^{(n-1)}(s) \psi_0^{-2}(s) ds, & \text{even } n; \end{cases} \quad X^{(n)}(x) = \begin{cases} \int_{x_0}^x X^{(n-1)}(s) \psi_0^{-2}(s) ds, & \text{odd } n, \\ \int_{x_0}^x X^{(n-1)}(s) \psi_0^2(s) ds, & \text{even } n, \end{cases} \quad (7)$$

satisfy equation (5), being x_0 an arbitrary point in $[h_1, h_2]$. It is shown in [20] that series (6) converge uniformly in $[h_1, h_2]$. Hence, differentiation term by term leads to the series

$$\psi_1' = \frac{\psi_0'}{\psi_0} \psi_1 + \frac{1}{\psi_0} \sum_{k=1}^{\infty} (-\lambda)^k \tilde{X}^{(2k-1)}, \quad \psi_2' = \frac{\psi_0'}{\psi_0} \psi_2 + \frac{1}{\psi_0} \sum_{k=0}^{\infty} (-\lambda)^k X^{(2k)}.$$

Let $x_0 = h_1$ then, according to recursive procedure (7), ψ_1 and ψ_2 satisfy the initial conditions

$$\psi_1(h_1; \lambda) = \psi_0(h_1), \quad \psi_1'(h_1; \lambda) = \psi_0'(h_1); \quad \psi_2(h_1; \lambda) = 0, \quad \psi_2'(h_1; \lambda) = 1/\psi_0(h_1).$$

By choosing ψ_0 such that $\psi_0(h_1) = 1$ and $\psi_0'(h_1) = i$ (see Appendix A on the construction of such a particular solution), the characteristic equation takes the series representation

$$i(1 + \kappa_1(\lambda)) \left(\theta(\lambda) \sum_{k=0}^{\infty} (-\lambda)^k X^{(2k+1)}(h_2) + \sum_{k=0}^{\infty} (-\lambda)^k X^{(2k)}(h_2) \right) - \left(\theta(\lambda) \sum_{k=0}^{\infty} (-\lambda)^k \tilde{X}^{(2k)}(h_2) + \sum_{k=1}^{\infty} (-\lambda)^k \tilde{X}^{(2k-1)}(h_2) \right) = 0, \quad (8)$$

where $\theta(\lambda) := (\psi_0'(h_2) - i\kappa_3(\lambda)\psi_0(h_2))\psi_0(h_2)$.

Remark 1. According to recursive integration procedure (7) one can see that the interaction potential V_2 is not explicitly invoked in the calculation of the formal powers $\tilde{X}^{(n)}$ and $X^{(n)}$. However, this information is implicitly carried on in the particular solution ψ_0 . If ψ_0 is obtained with the SPPS method (see Appendix A), then the condition $V_2 \in \mathcal{C}[h_1, h_2]$ should be fulfilled. This extends the applicability of our method to a large class of potentials.

Without losing generality, let $V_1 = V_3 = 0$, so that $\kappa_1^2 = \kappa_3^2 = \lambda =: \kappa^2 \in \mathbb{C}$. In this case, the characteristic equation can be written in terms of the complex variable κ as $\tilde{\varrho}(\kappa) = 0$, where

$$\tilde{\varrho}(\kappa) := i(1 + \kappa) \left(\tilde{\theta}(\kappa) \sum_{k=0}^{\infty} (-\kappa)^{2k} X^{(2k+1)}(h_2) + \sum_{k=0}^{\infty} (-\kappa)^{2k} X^{(2k)}(h_2) \right) - \left(\tilde{\theta}(\kappa) \sum_{k=0}^{\infty} (-\kappa)^{2k} \tilde{X}^{(2k)}(h_2) + \sum_{k=1}^{\infty} (-\kappa)^{2k} \tilde{X}^{(2k-1)}(h_2) \right),$$

and $\tilde{\theta}(\kappa) := (\psi'_0(h_2) - i\kappa\psi_0(h_2))\psi_0(h_2)$. This is the Taylor series of an analytic function $\tilde{\varrho}$ defined in the complex κ -plane. If κ_n is a zero of $\tilde{\varrho}(\kappa) = 0$ then $\lambda_n = \kappa_n^2$ is a zero of the characteristic equation (8). Hence, in order for λ_n to be a complex energy of a resonance state it is necessary that $\text{Re}(\kappa_n) > 0$ and $\text{Im}(\kappa_n) < 0$. Numerically, the previous series should be truncated up to a M -th term. Let $\tilde{\varrho}_M$ be the truncated version of $\tilde{\varrho}$. Then, approximate zeros of the equation $\tilde{\varrho}(\kappa) = 0$ can be found from the polynomial roots of $\tilde{\varrho}_M(\kappa) = 0$. In other words, the calculation of resonances for a one-dimensional quantum system reduces to calculating polynomial roots.

Next we present some numerical examples using *Wolfram Mathematica*. For the truncated version $\tilde{\varrho}_M$ of the characteristic equation we take $M = 200$. This implies calculating a finite set of formal powers according to recursive integration procedure (7). Each integration is carried out by segmenting the interval $[h_1, h_2]$ into 2000 segments on which the integrand is interpolated by cubic splines. Exact integration is then performed on the resulting interpolated integrands. For calculating polynomial roots we employ the instruction `FindRoot`, using machine precision.

Example 1. Consider a rectangular potential defined by $V_2(x) \equiv V_0$ on the symmetric support $[-h, h]$, see Figure 1.a. With the settings $V_0 = 10$ and $h = 1$ we calculate the transmission coefficient $\mathbb{T}(\epsilon)$ on the interval $\epsilon \in [0, 80]$ of real energies. In Figure 1.b the transmission coefficient shows a series of maxima corresponding to $|\mathbb{T}(\epsilon_n)| = 1$. The values ϵ_n shown in Table 1 are the transparency energies of the potential V .

Example 2. With the settings of Example 1 we calculate the transmission coefficient $\mathbb{T}(\lambda)$ in a region $\Omega = \{\lambda \in \mathbb{C} : 0 < \text{Re}(\lambda) < 100, -60 < \text{Im}(\lambda) < 10\}$ of the complex λ -plane, see Figure 2. Here we observe a series of peaks corresponding to the poles of the transmission coefficient $\mathbb{T}(\lambda)$. Some of the complex energies λ_n of this quantum system are shown in Table 1.

Remark 2. Piecewise constant potentials are important since more complex potentials can be represented in terms of them. Their simplicity can lead to closed-form characteristic equations that can be solved graphically or using standard numerical methods (e.g., Newton method). Other potentials can be approached by performing Darboux transformations on the solutions corresponding to piecewise constant potentials (see, e.g., [4, 6]). In this work the analysis begins from a non-vanishing particular solution ψ_0 associated to the potential V_2 , from which we calculate a finite set of formal powers $\tilde{X}^{(n)}$, $X^{(n)}$ that compose the truncated characteristic equation $\tilde{\varrho}_M(\kappa) = 0$, and calculate its polynomial roots. On the other hand, the transmission coefficient, which is usually approximated as a superposition of Breit-Wigner distributions (see, e.g., [3, 5]), here is totally characterized by its poles, which are the zeros of $\tilde{\varrho}(\kappa) = 0$.

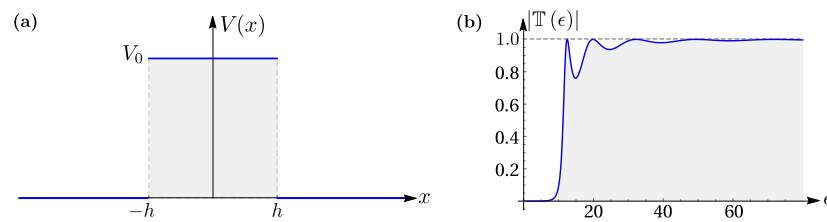


Figure 1. (a) Rectangular potential of Example 1. (b) Plot of the transmission coefficient.

Table 1. Some transparency energies and complex energies for the potential of Example 1.

n	Transparency energy ϵ_n	Complex energy $\lambda_n = E_n - i\Gamma_n/2$
1	12.467401810269243	11.882874871230369 - i 1.2842071483079915
2	19.869815644509725	17.967206726724196 - i 4.9820599537268042
3	32.204502676194192	28.893263517977555 - i 10.532816267432139
4	49.436758521132234	44.892105206950130 - i 17.344759864814847
5	71.565365406214943	65.978437727543150 - i 25.052640345112376

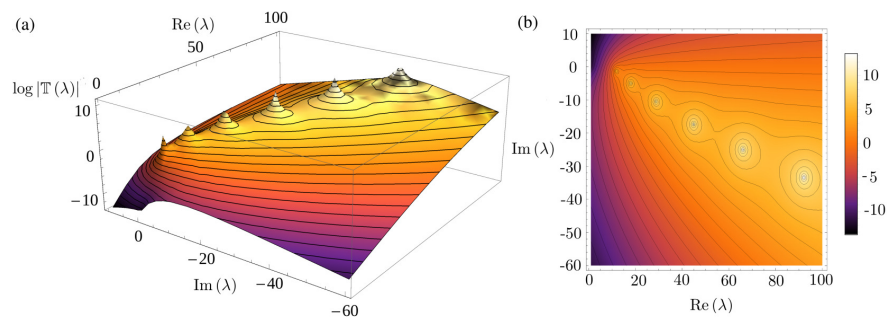


Figure 2. (a) Peaks representing the poles of the transmission coefficient $\mathbb{T}(\lambda)$ of Example 2. (b) Distribution of complex energies in the region Ω .

Example 3. In order to show the applicability of our method to a more interesting potential, let us consider a truncated version of the modified Pöschl-Teller potential, Figure 3.a,

$$V_2(x) = 10 \frac{\mu(\mu-1)}{\cosh^2(x)}, \quad -1 \leq x \leq 1.$$

By setting $\mu = 3$ and $h = 1$, the transmission coefficient $\mathbb{T}(\epsilon)$ evaluated on the interval $\epsilon \in [0, 160]$ of real energies is shown in Figure 3.b. Some transparency energies for this problem calculated from the polynomial roots of $\tilde{q}_M(\kappa) = 0$, are shown in Table 2.

Example 4. As a continuation of Example 4 we calculate the transmission coefficient $\mathbb{T}(\lambda)$ in a region $\Omega = \{\lambda \in \mathbb{C} : 0 < \text{Re}(\lambda) < 180, -60 < \text{Im}(\lambda) < 10\}$ of the complex λ -plane, see Figure 4. Here we observe that two complex energies (λ_1 and λ_2) are very close each other, forming a kind of cluster. In Table 2 we observe the complex energies λ_n calculated for this potential and the closeness of the two mentioned energies.

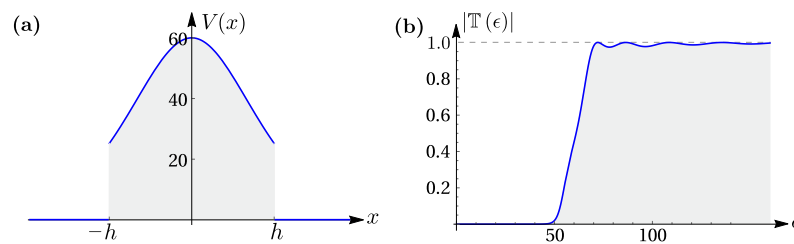


Figure 3. (a) Pöschl-Teller potential of Example 4. (b) Plot of the transmission coefficient.

Table 2. Some transparency energies and complex energies for the potential of Example 3.

n	Transparency energy ϵ_n	Complex energy $\lambda_n = E_n - i\Gamma_n/2$
1	72.00775933091033	53.80659491247304 - i 5.796460655368762
2	85.01644361908951	54.57397005390005 - i 8.329055510961702
3	108.00016333744483	68.08250284745327 - i 8.590087191115057
4	135.00003458628376	105.04504696926546 - i 20.82541895927201
5	150.00060076698233	131.29281605305934 - i 27.47415336739937

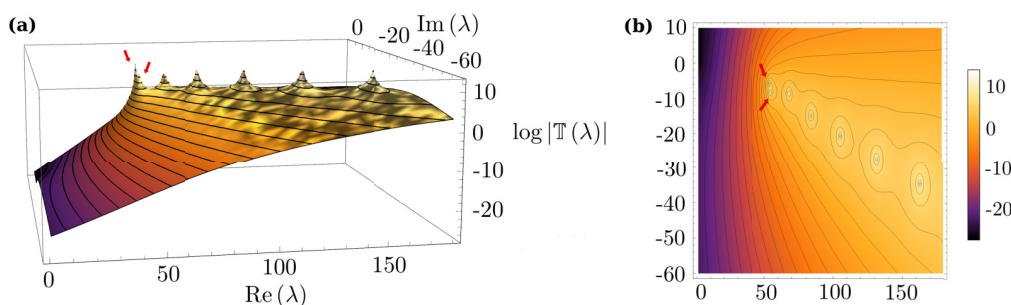


Figure 4. (a) Peaks representing the poles of the transmission coefficient $T(\lambda)$ of Example 4. (b) Clustering of the complex energies λ_1 and λ_2 in the region Ω .

5. Concluding remarks

In this work we considered a one-dimensional Schrödinger equation with a short range potential V_2 defined in a region $[h_1, h_2]$, satisfying the smoothness condition $V_2 \in \mathcal{C}[h_1, h_2]$. We obtained an explicit representation of the characteristic equation for its Gamow-Siegert eigenstates in the form of a power series of the complex energy λ . From a numerical point of view, such series should be truncated up to some M -th term. Thus, the problem of finding the complex energies of the Gamow-Siegert eigenstates of the Hamiltonian \mathcal{H} reduces to calculating the zeros of equation (8) or equivalently to finding the polynomial roots of the equation $\tilde{q}_M(\kappa) = 0$. This constitutes an effective way of analysing the resonances of a quantum system. It is worth mentioning that no approximation nor simplification was used for obtaining the characteristic equation, in addition, the smoothness condition $V_2 \in \mathcal{C}[h_1, h_2]$ allows to apply the present theory to problems having quite arbitrary potentials. Finally, possessing such a series representation for the characteristic equation allows us to analyse other interesting phenomena such as the degeneration of resonances, which roughly consists in determining the multiplicity of the zeros

of equation (8) by means of the standard techniques of complex analysis such as the argument principle or Rouché's theorem.

Appendix A. On the construction of the particular solution ψ_0

The SPPS method can also be used for constructing a non-vanishing particular solution ψ_0 of equation (5) for $\lambda = 0$. Let φ_1 and φ_2 be two linearly independent solutions, then the solution $\psi_0 = \varphi_1 + i\varphi_2$ does not vanish in $[h_1, h_2]$ since φ_1 and φ_2 alternate their zeros according to Sturm's oscillation theorem. Let φ_0 be a non-vanishing particular solution of $-\varphi'' = 0$ in (h_1, h_2) satisfying the conditions $V_2\varphi_0^2, \varphi_0^{-2} \in \mathcal{C}[h_1, h_2]$, then the series

$$\varphi_1(x) := \varphi_0(x) \sum_{k=0}^{\infty} \tilde{Y}^{(2k)}(x), \quad \varphi_2(x) := \varphi_0(x) \sum_{k=0}^{\infty} Y^{(2k+1)}(x) \quad (\text{A.1})$$

with $\tilde{Y}^{(n)}, Y^{(n)}$ defined by the recursive integration procedure $\tilde{Y}^{(0)}(x) \equiv 1$ and $Y^{(0)}(x) \equiv 1$,

$$\tilde{Y}^{(n)}(x) := \begin{cases} \int_{x'_0}^x \tilde{Y}^{(n-1)}(s) V_2(s) \varphi_0^2(s) ds, & \text{odd } n, \\ \int_{x'_0}^x \tilde{Y}^{(n-1)}(s) \frac{ds}{\varphi_0^2(s)}, & \text{even } n, \end{cases} \quad Y^{(n)}(x) := \begin{cases} \int_{x'_0}^x Y^{(n-1)}(s) \frac{ds}{\varphi_0^2(s)}, & \text{odd } n, \\ \int_{x'_0}^x Y^{(n-1)}(s) V_2(s) \varphi_0^2(s) ds, & \text{even } n, \end{cases}$$

satisfy equation (5) for $\lambda = 0$ in $[h_1, h_2]$. The point x'_0 is an arbitrary point in $[h_1, h_2]$. In particular, taking $\varphi_0 \equiv 1$ and choosing $x'_0 = h_1$ simplify significantly the work. According to the SPPS method [20], series (A.1) converge uniformly on $[h_1, h_2]$, and differentiation term by term gives an expression for the derivative ψ'_0 , that is

$$\psi'_0(x) = \sum_{k=0}^{\infty} \left(\tilde{Y}^{(2k+1)}(x) + iY^{(2k)}(x) \right).$$

The solution ψ_0 thus constructed satisfies the initial conditions $\psi_0(h_1) = 1, \psi'_0(h_1) = i$.

References

- [1] Gamov G 1928 *Z. Phys.* **51** 204
- [2] Siegert A J F 1939 *Phys. Rev.* **56** 750
- [3] Fernández-García N and Rosas-Ortiz O 2008 *Ann. Phys.* **323** 1397
- [4] Fernández-García N and Rosas-Ortiz O 2008 *J. Phys.: Conf. Series* **128** 012044
- [5] Orozco-Cortés L F and Fernández-García N 2014 *J. Phys.: Conf. Series* **512** 012027
- [6] Rosas-Ortiz O, Fernández-García N and Cruz y Cruz S G 2008 *AIP Conf. Proc.* **1077** 31
- [7] Gadella M 1983 *J. Math. Phys.* **24** 1462
- [8] Gadella M 1983 *J. Math. Phys.* **24** 2142
- [9] Gadella, M 1984 *Physica A* **124A**,317
- [10] De la Madrid R 2004 *J. Phys. A: Math. Gen.* **37** 8129
- [11] Moiseyev N 2009 *J. Phys. Chem. A* **113** 7660
- [12] Rosas-Ortiz O and Muñoz R 2003 *J. Phys. A: Math. Gen.* **36** 8497
- [13] Fernández D J and Rosu H C 2001 *Phys. Scr.* **64** 177
- [14] Brändas E and Elander N eds 1989 *Resonances. The Unifying Route Towards the Formulation of Dynamical Processes. Foundations and Applications in Nuclear, Atomic and Molecular Physics.* (Lecture Notes in Physics vol 325) eds Araki H *et al* (Berlin: Springer).
- [15] Kukulin V I, Krasnopol'sky V M and Horáček J 1989 *Theory of Resonances. Principles and Applications* (Reidel Texts in the Mathematical Sciences Vol. 3) (Netherlands: Springer)
- [16] Moiseyev N 2011 *Non-Hermitian Quantum Mechanics* (Cambridge: Cambridge University Press)
- [17] Snyder A W 1974 *Appl. Phys.* **4** 273
- [18] Cruz y Cruz S G and Razo R 2015 *J. Phys.: Conf. Series* **624** 012018

- [19] Cruz y Cruz S G and Rosas-Ortiz O 2015 *Adv. Math. Phys.* **2015** 281472
- [20] Kravchenko V V and Porter R M 2010 *Math. Method Appl. Sci.* **33** 459
- [21] Bahar E 1967 *J. Math. Phys.* **8** 1735
- [22] Bender C M and Orszag S A 1978 *Advanced Mathematical Methods for Scientists and Engineers* (New York: McGraw Hill)
- [23] Cao Z, Zham L and Chen Y 1996 *Proc. SPIE* **2891** 289
- [24] Ascher U M, Mattheij R M M and Russell R D 1995 *Numerical Solution of Boundary Value Problems for Ordinary Differential Equations* (Philadelphia: SIAM)
- [25] Butcher J C 2003 *Numerical Methods for Ordinary Differential Equations* (West Sussex: John Wiley & Sons)