IOCMA 2026 Conference

The 2nd International Online Conference on Mathematics and Applications

10–12 June 2026 | Online

MDPI

Complex eigenvalues of the Schrödinger equation with a Gaussian barrier

J. Garcia

La Plata Institute of Physics, National University of La Plata and National Scientific and Technical Research Council,
113 Diagonal and 64 Street - La Plata (1900), Buenos Aires, Argentina

jgarcia@fisica.unlp.edu.ar

Introduction

The Schrödinger equation with an exponential potential $-\psi'' + \lambda e^{-r}\psi = E\psi$ exhibits different sets of complex eigenvalues that are uncovered by performing a complex rotation of the independent variable by different rotation angles [1]. It can be solved analytically in terms of the modified Bessel functions, and it was recently shown that solutions belonging to the different sets have similar eigenvalues, being closer to each other when the potential strength parameter λ increases [2].

The purpose of the present work is to investigate whether the Schrödinger equation with a Gaussian barrier presents similar properties. Since it cannot be solved analytically, this study is numerical in nature.

Schrödinger equation

We treat the Schrödinger equation with a Gaussian barrier potential

$$-\frac{1}{2}\psi''(x) + V(x)\psi(x) = \epsilon\psi(x), \qquad V(x) = v_0 e^{-x^2} \tag{1}$$

with $v_0 > 0$ being the barrier strength parameter.

Eq. (1) can be written as

$$\hat{H}\psi = \epsilon\psi,$$

where $\hat{H} = -d^2/dx^2 + v_0 \exp(-x^2)$ is the Hamiltonian operator. $\hat{H}$ is parity-invariant, and therefore the solutions $\psi(x) = (-1)^s\psi(-x)$, where $s = 0$ or 1 for even or odd solutions, respectively. For the sake of brevity, in the present work we focus only on even states ($s = 0$).

Complex rotation

Since $V(x) \to 0$ as $x \to \pm\infty$, Eq. (1) admits two linearly independent solutions

$$\psi(x) \sim e^{\pm ikx},$$

with $k = \sqrt{\epsilon}$. In order to obtain these eigenfunctions, we perform a complex rotation of the form $x \to xe^{i\theta}$; the transformed Schrödinger equation reads

$$-\frac{1}{2}e^{-2i\theta}\psi''(x) + v_0 e^{-e^{2i\theta}x^2} = \epsilon\psi(x),$$

and $\psi(x) \sim \exp\left[ie^{i\theta}kx\right]$; in this case, if $\Re[ik\exp i\theta] < 0$, then $|\psi(x)| \to 0$ as $x \to \infty$. The complex-rotated potential can be written as

$$V(x) = \exp(-r^2\cos 2\theta)\left[\cos(r^2\sin 2\theta) - i\sin(r^2\sin 2\theta)\right].$$

It is seen that for $\theta < \pi/4$, $\Re[V(x)] \to 0$ for $x \to \pm\infty$, but, $\pi/4 < \theta < 3\pi/4$, $\Re[V(x)]$ oscillates with increasing frequency. $\theta_c = \pi/4$ demarks a Stokes line.

Methodology

Rayleigh-Ritz with complex rotation method

The Rayleigh-Ritz method consists in writing the wavefunction as a linear combination of basis functions: $\psi(x) \approx \sum_{n=0}^{N} c_n\phi_n(x)$; by the variational theorem, the linear coefficients that yield the best approximation to ψ are obtained by diagonalizing the matrix $\mathbf{H}$, with elements $H_{ij} = \int_{-\infty}^{\infty}\phi_i(x)\hat{H}\phi_j(x)\,dx$ [3, 4].

In the present work we resort to the scaled Harmonic Oscillator basis set, $\phi_n(x;\gamma) = N_n(\gamma)H_n(\gamma x)e^{-\frac{\gamma^2 x^2}{2}}$, in which $N_n(\gamma)$ is a normalization constant, and we employ the γ parameter for tuning the basis set, as well as to absorb the complex rotation angle θ: $\gamma = |\gamma|e^{-i\theta}$.

Riccati-Padé method (RPM)

The RPM [5] consists of the expansion of the logarithmic derivative of $\psi(x)$, $f(x) = \frac{s}{x} - \frac{\psi'(x)}{\psi(x)}$, where $s = 0(1)$ for even (odd) states, in a Taylor series about the origin, $f(x) = \sum_{j=0}^{\infty} f_j x^{2j+1}$ where the f_j coefficients depend on ϵ. The quantization condition $H_D^d = |f_{i+j+d-1}|_{i,j=1}^{D} = 0$ leads to values that approximate the resonances as D increases.

The RPM yields both bound states (real eigenvalues) and resonances, without explicitly resorting to the complex rotation.

Main Results

We vary θ from 0 to $\pi/2$, $|\gamma|$ from 1 to 10, and N up to $N = 200$, keeping the complex eigenvalues that persist for small variations of θ and increasing N. In the following table, we show some of the eigenvalues obtained for different barrier strengths v_0, indicating the values of θ and $|\gamma|$.

			$v_0 = 1/2$				
$\|\gamma\| = 1/2$	$\theta = 0.24\pi$	$\|\gamma\| = 5$	$\theta = 0.32\pi$	$\|\gamma\| = 5$	$\theta = 0.34\pi$	$\|\gamma\| = 5$	$\theta = 0.44\pi$
$\Re[\epsilon]$	$-\Im[\epsilon]$	$\Re[\epsilon]$	$-\Im[\epsilon]$	$\Re[\epsilon]$	$-\Im[\epsilon]$	$\Re[\epsilon]$	$-\Im[\epsilon]$
0.232559	0.547368	0.009438	0.295878	0.160699	0.462987	0.312572	0.512182
		0.248205	0.598284	-0.014956	0.723231	-1.566870	2.937743
		-0.419357	1.685718	-0.419467	3.250284	-5.311457	6.052534
		-0.190064	3.601034	-1.464115	6.209895	-10.621786	9.755768
		-0.698412	6.293792	-2.984662	10.157908	-17.363566	13.981433
			$v_0 = 1$				
$\|\gamma\| = 1$	$\theta = 0.24\pi$	$\|\gamma\| = 3$	$\theta = 0.32\pi$	$\|\gamma\| = 3$	$\theta = 0.34\pi$	$\|\gamma\| = 3$	$\theta = 0.44\pi$
$\Re[\epsilon]$	$-\Im[\epsilon]$	$\Re[\epsilon]$	$-\Im[\epsilon]$	$\Re[\epsilon]$	$-\Im[\epsilon]$	$\Re[\epsilon]$	$-\Im[\epsilon]$
0.804571	0.745199	-0.084467	0.333038	-0.196450	0.575187	0.811583	0.715132
		0.807638	0.744370	0.801287	0.753337	-1.177095	3.925410
		-0.477864	1.663686	-0.126051	3.571241	-5.220159	7.854617
		0.117954	3.784105	-0.919989	6.529278	-10.974254	12.433782
		-0.280848	6.489701	-2.198379	10.777277	-18.280834	17.595852
			$v_0 = 2$				
$\|\gamma\| = 1$	$\theta = 0.24\pi$	$\|\gamma\| = 3$	$\theta = 0.32\pi$	$\|\gamma\| = 4$	$\theta = 0.34\pi$	$\|\gamma\| = 3$	$\theta = 0.44\pi$
$\Re[\epsilon]$	$-\Im[\epsilon]$	$\Re[\epsilon]$	$-\Im[\epsilon]$	$\Re[\epsilon]$	$-\Im[\epsilon]$	$\Re[\epsilon]$	$-\Im[\epsilon]$
1.818338	1.008100	-0.137916	0.347663	-0.302155	0.579207	1.811559	1.005093
		-0.612032	1.655685	1.819058	1.008061	-0.267848	5.329551
		1.818214	1.008068	0.065897	4.139009	-4.606194	10.372051
		0.381959	4.192409	-0.080101	6.793286	-10.827578	16.119165
		0.361298	6.724728	-1.218584	11.469501	-18.744166	22.511406
			$v_0 = 5$				
$\|\gamma\| = 1$	$\theta = 0.24\pi$	$\|\gamma\| = 4$	$\theta = 0.31\pi$	$\|\gamma\| = 3$	$\theta = 0.34\pi$	$\|\gamma\| = 3$	$\theta = 0.44\pi$
$\Re[\epsilon]$	$-\Im[\epsilon]$	$\Re[\epsilon]$	$-\Im[\epsilon]$	$\Re[\epsilon]$	$-\Im[\epsilon]$	$\Re[\epsilon]$	$-\Im[\epsilon]$
4.811689	1.583790	-0.191178	0.365492	-0.414246	0.600658	4.811949	1.583967
2.777298	8.108392	-0.827218	1.677776	-0.769364	4.930972	2.648232	8.149582
		-0.149148	4.963372	4.811688	1.583796	-2.039688	15.369747
		4.811689	1.583790	2.776547	8.147097	-8.879095	23.332074
		2.773938	8.118825	0.074101	12.680366	-17.643779	32.011489

For $\theta < \pi/4$, we find a finite amount of resonances (only one or two for the v_0 values shown here). For $\theta > \pi/4$, we find different sets of complex eigenvalues that depend on the values of $|\gamma|$ and θ; these appear to be infinite in quantity, but here we only show five of them for each v_0 value. We have colored the sets of eigenvalues that are close to the set of resonances that appear for $\theta < \pi/4$. The eigenvalues reported here were also computed with the RPM, the results of both methods coinciding up to the last reported digit.

Conclusions

Our results suggest that the Gaussian barrier exhibits two classes of resonances. The first, obtained for $\theta < \pi/4$, consists of a finite set with $0 < \Re\epsilon < v_0$. The second, obtained for $\theta > \pi/4$, appears to form multiple infinite sets with no restrictions on the values of ϵ; some of them have energies that are close to those of the first class, and the coincidence is stronger when v_0 is increased. It is important to remark here that the eigenvalues obtained by means of the Rayleigh-Ritz method with complex rotation were independently confirmed by the RPM method, which involves a different kind of quantization condition, and no explicit complex rotation. Therefore, it is safe to say that the complex eigenvalues computed here are not spurious.

The findings of this work for the Gaussian barrier are consistent with those of the radial exponential potential [2], and it appears that this is a general property of potentials that involve the exponential function.

References

[1] Atabek O and Lefebvre R, *Il Nuovo Cimento B* **76**, 176–188 (1983).

[2] Garcia J, *Phys. Scr.* **99**, 035208 (2024).

[3] Balslev E and Combes J M, *Comm. Math. Phys.* **22**, 280–294 (1971).

[4] Yaris R, Bendler J, Lovett R A, Bender C M and Fedders P A, *Phys. Rev. A* **18**, 1816–1825 (1978).

[5] Fernández F M, Ma Q and Tipping R, *Phys. Rev. A* **39** 1605–1609 (1989).

[6] Moiseyev N, Certain P R and Weinhold F, *Mol. Phys.* **36** 1613–1630 (1978).

[7] Rittby M, Elander N and Brändas E, *Phys. Rev. A* **26** 1804–1807 (1982).

[8] Fernandez F M and Garcia J, *J. Math. Chem.* **55** 623–631 (2016).