Resonances for symmetric two-barrier potentials

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Abstract
We describe a method for the accurate calculation of bound-state and resonance energies for one-dimensional potentials. We calculate the shape resonances for symmetric two-barrier potentials and compare them with those coming from the Siegert approximation, the complex scaling method and the box-stabilization method. A comparison of the Breit–Wigner profile and the transmission coefficient about its maximum illustrates that the better the agreement, the sharper the resonance.

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

1. Introduction

In a recent paper, Rapedius [1] showed how to calculate resonance positions and widths by means of the Siegert approximation (SA). He applied it to two exactly solvable models and also to the transmission through a double barrier. In the latter nontrivial example he compared the approximate SA resonances with the more accurate ones provided by complex scaling (CS). In this interesting pedagogical paper, Rapedius showed that the SA is suitable for narrow resonances. He also described the difference between Siegert and transmission resonances. The former are complex eigenvalues of the Schrödinger equation whereas the latter are related to the maxima of the transmission coefficient.

Somewhat earlier Dutt and Kar [2] had discussed scattering through smooth double barriers constructed by means of Gaussian functions. They compared the accurate transmission coefficient calculated numerically with analytical expressions derived by means of the WKB method. The agreement is remarkable for all values of the energy of the incident particle.

The physical interest in double-barrier potentials arises from models for fission barriers [3, 4] as well as in the study of chemical reaction thresholds [5] and simple molecular collisions [6]. In such cases sharp resonances are associated with states trapped between the two barriers [4, 5] and exhibit Lorentzian or Breit–Wigner (BW) profile [6]. In addition to its remarkably
accurate results [4] the WKB method is suitable for proving that the resonances are of BW type [8, 9]. Square wells and barriers have also proved suitable for a pedagogical discussion of bound states, virtual states and resonances [10].

The purpose of this paper is to illustrate the relation between Siegert and transmission resonances in a somewhat more detailed way by means of the symmetrical two-barrier potential discussed by Rapedius [1]. The Schrödinger equation for this potential is not exactly solvable but one can calculate the Siegert resonances accurately by means of the Riccati–Padé method (RPM) [11, 12]. It is also possible to obtain the transmission coefficient as a function of the energy by means of the Wronskian method [13, 14] and thus to compare its resonance peaks with the BW expression for different barrier heights. This paper is expected to be a useful complement to those earlier pedagogical discussions on the subject [1, 2, 10] and a suitable approach to the problem for courses of quantum mechanics at advanced undergraduate or graduate level.

In section 2, we derive the SA in a way that differs from that followed by Rapedius [1]. Like this author, we introduce the Siegert and transmission resonances that will be discussed and compared in later sections. In section 3, we outline the main ideas of the RPM for symmetric one-dimensional potentials. In section 4, we calculate the Siegert resonances by means of the RPM and the transmission coefficient by means of the Wronskian method. We can thus compare the peak of the transmission coefficient with the BW profile for several barrier heights. Finally, in section 5 we summarize the main results and draw conclusions.

2. The Siegert approximation method

Rapedius [1] developed the SA from the time-dependent Schrödinger equation. Since this equation is not used in the calculation of either the Siegert or the transmission resonances, we think that it may be fruitful to derive the SA entirely from the time-independent Schrödinger equation.

In order to simplify and facilitate both the algebra and the numerical calculations in this paper, we first convert the Schrödinger equation into a dimensionless eigenvalue equation. In this way, one removes all the physical constants and reduces the number of model parameters to a minimum. Although we have already discussed this well-known procedure in earlier papers [13–15], we think that it is worthwhile to insist on the advantages of working with proper dimensionless equations in physics.

The time-independent Schrödinger equation for a particle of mass $m$ that moves in one dimension ($-\infty < X < \infty$) under the effect of a potential $V(X)$ is

$$\frac{-\hbar^2}{2m} \psi''(X) + V(X)\psi(X) = E\psi(X) ,$$

where a prime indicates the derivative with respect to the coordinate $X$. If we define the dimensionless coordinate $x = X/L$, where $L$ is an appropriate length scale (or length unit), then we obtain the dimensionless eigenvalue equation

$$-\frac{1}{2} \varphi''(x) + v(x)\varphi(x) = \epsilon\varphi(x)$$

$$\varphi(x) = \sqrt{L}\psi(Lx), \quad v(x) = \frac{mL^2}{\hbar^2}V(Lx), \quad \epsilon = \frac{mL^2E}{\hbar^2} .$$

The length unit $L$ that renders both $\epsilon$ and $v(x)$ dimensionless is arbitrary, and we can choose it in such a way that makes the Schrödinger equation as simple as possible, as shown in the first example of section 4.
For the time being we just assume that the potential tends to zero,
\[
\lim_{|x| \to \infty} v(x) = 0,
\]
(3)
faster than \(|x|^{-1}\) and that the particle approaches the interaction region from the left. Therefore, the boundary conditions are
\[
\begin{align*}
\lim_{x \to -\infty} \varphi(x) &= \varphi_-(x) = A e^{ikx} + B e^{-ikx} \\
\lim_{x \to \infty} \varphi(x) &= \varphi_+(x) = C e^{ikx},
\end{align*}
\]
(4)
where \(k = \sqrt{2\epsilon}\).

It follows from the Schrödinger equation (2) and its complex conjugate that
\[
(q^* q^* - q^* q)' = 2(e^* - \epsilon)|q|^2.
\]
(5)
If \(\epsilon\) is real then the Wronskian
\[
W(q^* q, q) = q'^* q - q'^ q = \text{constant}
\]
leads to
\[
|A(\epsilon)|^2 - |B(\epsilon)|^2 = |C(\epsilon)|^2
\]
or \(T(\epsilon) + R(\epsilon) = 1\), where \(T(\epsilon) = |C(\epsilon)|^2/|A(\epsilon)|^2\) and \(R(\epsilon) = |B(\epsilon)|^2/|A(\epsilon)|^2\) are the transmission and reflection coefficients, respectively.

Following Rapoport [1], we call transmission resonance to an energy value \(\epsilon = \epsilon_T\) for which \(T(\epsilon)\) exhibits a local maximum. In the particular case where the potential is symmetric about the origin \(v(-x) = v(x)\), the maximum has a unit value \(T(\epsilon_T) = 1\) [8]; consequently, \(R(\epsilon_T) = 0\), \(|A(\epsilon_T)|^2 = |C(\epsilon_T)|^2\) and \(|B(\epsilon_T)|^2 = 0\). The boundary conditions for such particular energy value are
\[
\psi_T^\pm(x) = ik_T \psi_T^\pm(x)
\]
and
\[
|\psi_T^+|^2 = |A_T|^2 = |C_T|^2 = |\psi_T^-|^2,
\]
(8)
where the subscript \(T\) indicates that \(\epsilon = \epsilon_T\). For concreteness, we assume that the potential is symmetric from now on. If it were symmetric about another point \(x = x_0 \neq 0\), we would simply shift the coordinate origin from \(x = 0\) to \(x = x_0\).

A resonance (or Siegert) eigenstate is a solution to the Schrödinger equation that behaves asymptotically as a purely outgoing wave [7, 8, and references therein]:
\[
\lim_{x \to -\infty} \varphi_S(x) = \varphi_-(x) = B_S e^{-ik_S x} \\
\lim_{x \to \infty} \varphi_S(x) = \varphi_+(x) = C_S e^{ik_S x},
\]
(9)
where the subscript \(S\) indicates that \(\epsilon = \epsilon_{res}\) which is a complex eigenvalue \(\epsilon_{res} = \epsilon_R + i\epsilon_I\). The real part is the resonance position and the imaginary part is related to the resonance width \(\Gamma = -2\epsilon_I > 0\). For practical purposes, it is customary to assume that these boundary conditions are approximately valid for a sufficiently large coordinate value \(|x| = a\). Therefore, if we integrate equation (5) between \(-a\) and \(a\), we obtain
\[
(q^* q^* - q^* q)^{[a]}_{-a} = i(k_S + k_T^2)(|\varphi_S^+|^2 + |\varphi_S^-|^2)
= -4i\epsilon_I \int_{-a}^{a} |\varphi_S|^2 dx.
\]
(10)
The Siegert states for a symmetrical potential are either even or odd; therefore \(|\varphi_S^+|^2 = |\varphi_S^-|^2\).

In the case of a sufficiently narrow resonance \(|\epsilon_I| \ll \epsilon_R\), we may safely carry out the additional approximation that \(\epsilon_{res} \approx \epsilon_R \approx \epsilon_T\).
Since the Siegert state is strongly localized in the well between the barriers located at $x = \pm b$ [1], we can also write
\[
\int_{-a}^{d} |\psi_S|^2 \, dx \approx \int_{-b}^{b} |\psi_T|^2 \, dx \approx \int_{-b}^{b} |\psi_T|^2 \, dx.
\]
Finally, from the equations above we obtain an expression for the resonance width
\[
\Gamma = \frac{k_T |\psi_T(a)|^2}{\int_{0}^{b} |\psi_T|^2 \, dx}
\]
already derived by Rapedius [1] by means of the time-dependent Schrödinger equation.

A more rigorous, general and elegant derivation of the results above was given by Whitton and Connor [16] many years ago by means of a Wronskian analysis. Those authors called the $S$ and $T$ boundary conditions ‘outward moving waves only’ and ‘forward moving waves only’, respectively. Rapedius [1] also showed an expression for the nonsymmetric case $v(-x) \neq v(x)$ that we do not consider here. The general expressions of Whitton and Connor [16] do in fact apply to both the symmetric and nonsymmetric case. Note that the energies for the forward-moving-waves-only boundary conditions are real for a symmetric potential but they may be complex for a nonsymmetric one [16].

It is clear from all the assumptions made above that the SA equation (12) applies only to sufficiently narrow resonances. In fact, Rapedius [1] illustrated this point by comparing SA results with those provided by the more accurate CS. In section 4, we propose an alternative comparative discussion of Siegert and transmission resonances.

3. The Riccati–Padé method (RPM)

In order to compare Siegert and transmission resonances, we need sufficiently accurate complex eigenvalues of the Schrödinger equation with purely outgoing-wave boundary conditions. There are many suitable methods for this purpose; for example, Rapedius [1] discussed the SA and CS ones. In what follows, we outline the RPM that yields remarkably accurate results for narrow and broad resonances [11, 12] (a pedagogical approach to the RPM for bound states is available elsewhere [17]). We think that the RPM may be a suitable practical tool for a quantum mechanics course because the derivation of its main equations and their implementation in a computer program are both straightforward.

Suppose that we want to obtain the eigenvalues of the dimensionless Schrödinger equation (2) with a symmetric potential $v(-x) = v(x)$ (without loss of generality we assume that $v(0) = 0$). We restrict ourselves to those eigenstates that are either even $\psi(-x) = \psi(x)$ or odd $\psi(-x) = -\psi(x)$ (both bound and resonance states satisfy this criterion). We define the regularized logarithmic derivative of the eigenfunction
\[
f(x) = \frac{s}{x} \frac{\psi'(x)}{\psi(x)},
\]
where $s = 0$ or $s = 1$ for even or odd states, respectively. It satisfies the Riccati equation
\[
f'(x) + \frac{2s}{x} f(x) - f(x)^2 + 2v(x) - 2\epsilon = 0.
\]
If we can expand $v(x)$ in a Taylor series about $x = 0$,
\[
v(x) = \sum_{j=1}^{\infty} v_j x^{2j},
\]
then we can also expand \( f(x) \) about the same point as
\[
f(x) = x \sum_{j=0}^{\infty} f_j(\epsilon) z^j, \quad z = x^2.
\] (16)

Note that the term \( s/x \) in equation (13) removes the pole at origin in the case of odd states \( \varphi^{\text{odd}}(0) = 0 \). The expansion of equation (14) in a Taylor series about the origin leads to a recurrence relation for the coefficients \( f_j \) that enables us to obtain as many coefficients \( f_j(\epsilon) \) as necessary:
\[
f_n = \frac{1}{2n + 2s + 1} \left( \sum_{j=0}^{n-1} f_j f_{n-j-1} + 2\epsilon \delta_{n0} - 2v_n \right), \quad n = 1, 2, \ldots.
\] (17)

Since \( f(x) \) has poles at the zeros of \( \varphi(x) \), we look for a rational approximation of the form
\[
f(x) \approx x \left[ \frac{M}{N} \right](z) = \frac{\sum_{j=0}^{M} a_j z^j}{\sum_{j=0}^{N} b_j z^j} + O(z^{M+N+2}).
\] (18)

Because we can arbitrarily choose \( b_0 = 1 \), we are left with \( M + N + 1 \) coefficients \( a_j \) and \( b_j \) of the rational function and the unknown energy as independently adjustable parameters. Therefore we require that the rational approximation (Padé approximant) yields \( M + N + 2 \) exact coefficients of the Taylor series for \( f(x) \) as explicitly indicated in equation (18). When \( M \geq N \) we easily derive the following equations:
\[
\begin{align*}
\sum_{k=0}^{\min(j,N)} b_k f_{j-k} &= a_j, \quad j = 0, 1, \ldots, M \\
\sum_{k=0}^{N} b_k f_{j-k} &= 0, \quad j = M + 1, M + 2, \ldots, M + N + 1.
\end{align*}
\] (19)

We can view the second set of equations as a system of \( N + 1 \) homogeneous equations with \( N + 1 \) unknowns \( b_N, b_{N-1}, \ldots, b_0 \). Therefore, there will be a nontrivial solution only if \( \epsilon \) is a root of
\[
H_D^D(\epsilon) = \begin{vmatrix}
\hat{f}_{M-N+1} & \hat{f}_{M-N+2} & \cdots & \hat{f}_{M+1} \\
\hat{f}_{M-N+2} & \hat{f}_{M-N+3} & \cdots & \hat{f}_{M+2} \\
\vdots & \vdots & \ddots & \vdots \\
\hat{f}_{M+1} & \hat{f}_{M+2} & \cdots & \hat{f}_{M+N+1}
\end{vmatrix} = 0,
\] (20)

where \( d = M - N = 0, 1, \ldots \) and \( D = N + 1 = 2, 3, \ldots \) is the dimension of the Hankel determinant \( H_D^D(\epsilon) \). As \( D \) increases, sequences of roots \( \epsilon^{(D,d)} \) of the Hankel determinant converge towards the allowed energies of the Schrödinger equation. This sort of quantization condition applies to bound states and resonances \([11, 12, 17]\). We simply identify convergent sequences of real and complex roots \( \epsilon^{(D,d)} \) of the Hankel determinants \( H_D^D(\epsilon) \) for \( D = 2, 3, \ldots, D_m \) and estimate the error of the calculation as \( |w^{(D_0)} - w^{(D_0-1)}| \), where \( w^{(D)} \) stands for the real or complex part of \( \epsilon^{(D,d)} \). We thus truncate the results to the last stable digit.
Table 1. Lowest resonances for the potential (21) with $v_0 = 1/2$ and $\lambda = 0.1$.

| $n$ | $\epsilon_R$ | $-\epsilon_i$ |
|-----|---------------|--------------|
| 0   | 0.460 147 276 539 333 563 60 | 9.620 388 319 820 192 9683 $\times 10^{-7}$ |
| 1   | 1.280 420 353 468 282 1470 | 1.673 713 594 583 040 4 $\times 10^{-3}$ |
| 2   | 1.853 108 635 175 053 3910 | 6.724 025 510 387 261 334 $\times 10^{-2}$ |
| 3   | 2.232 325 276 245 551 1600 | 0.339 898 556 891 856 507 13 |
| 4   | 2.567 615 869 399 468 602 | 0.819 402 813 170 296 0163 |
| 5   | 2.887 957 554 267 041 665 | 1.409 344 599 863 779 927 |

4. Results and discussion

As a first illustrative example, we consider the symmetrical double barrier $V(X) = V_0X^2 e^{-\alpha X^2}$, where $V_0$, $\alpha > 0$, discussed by Rapedius [1]. The Schrödinger equation for this potential is not exactly solvable but it is sufficiently simple for pedagogical purposes. In this case the dimensionless potential is given by

$$v(x) = v_0 x^2 e^{-\lambda x^2},$$

$$v_0 = \frac{mL^4}{\hbar^2} V_0, \quad \lambda = \alpha L^2.$$  \hspace{1cm} (21)

Note that without loss of generality we can treat this problem as a one-parameter model because we may have either $v_0 = 1$ when $L^2 = \hbar^2 / m V_0$ or $\lambda = 1$ when $L^2 = 1 / \alpha$. However, we write $v(x)$ as a two-parameter potential following Rapedius [1]. This potential exhibits a well centred at $x = 0$ and two barriers of height $v_b = v_0 / (e \lambda)$ symmetrically located at $x = \pm b$, $b = 1 / \sqrt{\lambda}$.

For comparison purposes we first consider the potential parameters $v_0 = 1/2$ and $\lambda = 0.1$ already chosen by Rapedius [1]. Table 1 shows the first six resonances obtained from Hankel sequences with $D \leq 20$ and $d = 0$. The first three of them agree with those calculated by means of SA and CS [1]. Present results are supposed to be accurate to the last digit and, consequently, much more accurate than the SA and CS ones shown by Rapedius [1]. However, it is worth mentioning that the CS results can in principle be made as accurate as desired by increasing the dimension of the basis set [19]. As stated above (and already shown in table 1) the RPM is suitable for both sharp and broad resonances. However, the accuracy of the RPM for a given determinant dimension $D$ decreases with the resonance ‘quantum number’ $n$ because the Hankel sequences for higher resonances appear at greater values of $D$.

The RPM is extremely accurate but it is not as general as other approaches (like, for example, CS) because it only applies to separable Schrödinger equations. However, one-dimensional and separable models are widely discussed in most courses on quantum mechanics.

It is not difficult to calculate the transmission probability $T(\epsilon)$ for the potential (21) by means of the Wronskian method [13, 14] and thus compare the Siegert $\epsilon_{res}$ and transmission $\epsilon_T$ resonances discussed by Rapedius [1]. More precisely, we compare the actual transmission coefficient $T(\epsilon)$ and the BW shape

$$T(\epsilon) \approx \frac{\epsilon_T^2}{(\epsilon - \epsilon_R)^2 + \epsilon_T^2}$$ \hspace{1cm} (22)

in a neighbourhood of the maximum of $T(\epsilon)$ at $\epsilon = \epsilon_T \approx \epsilon_R$. Connor [8] has already shown that $T(\epsilon_T) = 1$ for a symmetric potential and that equation (22) is a reasonable approximation for isolated sharp resonances.
Resonances for symmetric two-barrier potentials

Figure 1. Potential function (blue) and quasi-stable energy (red) for $v_0 = 2, 5, 10, 15$.

Table 2. Lowest resonance for the potential (21) and several potential parameters.

| $v_0$ | $v_b$ | $\epsilon_R$ | $-\epsilon_I$ |
|-------|-------|---------------|---------------|
| 2     | 0.7358| 0.559 371 184 582 527 329 95 | 0.158 305 251 142 711 355 25 |
| 5     | 1.839 | 1.108 215 762 992 029 5074  | 0.078 972 583 905 329 832 058 |
| 10    | 3.679 | 1.781 676 382 586 911 3601  | 0.023 794 309 337 967 155 927 |
| 15    | 5.518 | 2.304 251 933 177 486 8362  | 0.007 347 829 662 205 245 864 |

Table 2 shows the lowest resonance for $v_0 = 2, 5, 10, 15$ and $\lambda = 1$ calculated by means of the RPM exactly as discussed above. We have rounded off all the results to the first unstable digit. The second column displays the approximate values of the barrier heights $v_b = v_0/e$. Note that $|v_b - \epsilon_R|$ increases with $v_0$, that is to say, the resonance moves deeper into the well between the barriers as $v_0$ increases. At the same time it becomes narrower and therefore more stable (its decay rate $\Gamma = -2\epsilon_I$ decreases). Figure 1 shows the potential and the location of the lowest resonance (horizontal line) for each case and illustrates graphically the behaviour just discussed.

Figure 2 shows the transmission probability $T(\epsilon)$ calculated by means of the Wronskian method [13, 14] and the BW profile (22) with the values of $\epsilon_R$ and $\epsilon_I$ given in table 2. It clearly illustrates that $T(\epsilon)$ becomes sharper about the maximum as $\Gamma$ decreases. In addition to it, we appreciate the well-known fact that the BW profile gives a better description of the peak of the transmission coefficient if the resonance is sharper. In other words, as the potential parameter increases from $v_0 = 2$ to $v_0 = 15$ and $\Gamma$ decreases, the BW profile (22) becomes increasingly more accurate in the neighbourhood of the maximum.
Figure 2. Numerical transmission probability (solid line, blue) and Lorentzian profile (dashed line, red) for \( v_0 = 2, 5, 10, 15 \).

The BW profile is suitable for isolated resonances, and closely spaced broad resonances may overlap. In such a case, \( T(\epsilon) \) becomes rather too distorted for the BW profile to fit satisfactorily. Figure 3 shows the two first resonances for several values of \( v_0 \). The resonance positions are indicated by symbols and their widths by error bars. We clearly appreciate that the resonances overlap for \( v_0 = 2 \) and \( v_0 = 3 \), in which cases the BW profile is unsuitable. The magnitude of the overlap diminishes with \( v_0 \) as the gap between the resonances increases and their widths decrease.

Klaiman and Moiseyev [18] have recently proposed an improved profile based on the same information required for the BW one. The KM profile is nonsymmetric and it is peaked at \( |\epsilon_{\text{res}}| > \epsilon_R \) which corrects the fact that typically \( \epsilon_R < \epsilon_T \) as shown in figure 2. We do not show the KM profile here because the correction is mild for the present model. The reason is that \( \epsilon_I \ll \epsilon_R \) and \( |\epsilon_{\text{res}}| \approx \epsilon_R \) for the isolated resonances (say \( v_0 \geq 4 \)).

Once we have the complex energy eigenvalue we can easily calculate the Siegert state by numerical integration or any other approach. For example, its Taylor expansion about the origin

\[
\varphi(x) = \sum_{j=0}^{\infty} c_j x^{2j+s}
\]

provides a suitable approximate analytical expression. It is not difficult to verify that the coefficients of this series are given by the recurrence relation

\[
c_{j+1} = \frac{2}{(2j+s+1)(2j+s+2)} \left[ \sum_{k=0}^{j} v_k c_{j-k} - \epsilon c_j \right], \quad j = 0, 1, \ldots
\]
Figure 3. Real (symbols) and imaginary (error bars) parts of the first (blue, circles) and second (red, squares) resonance.

Figure 4. Potential (blue) and $|\phi(x)|^2$ (red) for $v_0 = 1/2$ and $\lambda = 0.1$.

where we arbitrarily choose $c_0 = 1$. The Taylor expansion (23) converges for all values of $x$ but in practice we can only add a finite number $M$ of terms and the resulting partial sum for $|\phi(x)|^2$ tends to infinity as $x \to \infty$. For this reason the partial sum will be valid only in a finite interval $-x_M < x < x_M$ that we should choose judiciously. Figure 4 shows $v(x)$ for $v_0 = 1/2$ and $\lambda = 0.1$ and $|\phi(x)|^2$ for $M = 24$. This figure is similar to the one shown by Rapedius [1] for the same potential on a wider abscissas interval. We clearly see that the Siegert state is so strongly localized in the well between the two barriers that $|\phi(x)|^2 \approx 0$ for $|x| > b$ which justifies one of the assumptions made in section 2.

Some time ago Korsch and Glück [19] proposed a pedagogical approach to the calculation of the eigenvalues of the Schrödinger equation by means of the matrix representation of the
Table 3. Bound state and resonances for the potential (25).

| $\varepsilon_R$ | $-\varepsilon_I$ |
|-----------------|-----------------|
| 0.502 040 362 1419 | 0 |
| 1.420 970 945 714 693 2076 | 5.826 528 088 554 03 $\times 10^{-5}$ |
| 2.127 197 077 522 495 9319 | 1.544 731 284 180 518 3109 $\times 10^{-2}$ |
| 2.584 582 859 853 100 1914 | 0.173 750 719 162 199 280 95 |
| 2.924 421 929 737 7486 | 0.564 794 965 582 576 499 |
| 3.255 486 140 023 381 540 | 1.111 531 600 024 699 481 6 |
| 3.557 216 626 556 9298 | 1.755 506 234 676 9250 |
| 3.824 329 026 868 890 | 2.487 445 153 227 8992 |
| 4.055 433 668 209 184 | 3.298 644 201 453 19 |
| 4.249 963 938 764 321 | 4.183 165 827 588 71 |
| 4.407 748 386 304 | 5.136 436 406 966 |
| 4.528 814 027 868 | 6.154 809 667 01 |

coordinate and momentum. Among other illustrative examples they considered the one-dimensional potential

$$v(x) = \left(\frac{x^2}{2} - J\right) e^{-\lambda x^2} + J$$

which supports one bound state and many resonances when $J = 0.8$ and $\lambda = 0.1$. Note that this potential-energy function reduces to a particular case of equation (21) when $J = 0$. Those authors calculated the bound-state energy by a straightforward application of the matrix method and the first two resonances by means of the box-stabilization method [19]. The application of the RPM to this problem is straightforward and one simply looks for converging sequences of real and complex roots of the Hankel determinants in order to obtain the energies of the bound-state and resonances, respectively. Table 3 shows the eigenvalues estimated from Hankel determinants of dimension $D \leq 20$. Also in this case we see that the RPM results are remarkably accurate.

5. Conclusions

One of the purposes of this paper is to compare the Siegert and transmission resonances in an alternative way to that discussed by Rapedius [1]. To this end we calculated accurate Siegert resonances by means of the RPM and the transmission coefficient by means of the Wronskian method [13, 14] for the two-barrier potential (21). The chosen model is nontrivial but sufficiently simple for the straightforward application of both approaches. In this way, we can compare the shape of $T(\epsilon)$ about its maximum at $\epsilon = \epsilon_T$ (transmission resonance) with the BW profile (22) constructed by means of the complex eigenvalues $\epsilon_{\text{res}} = \epsilon_R + i\epsilon_I$ (Siegert resonance). The comparison illustrates the well-known fact that the BW profile fits sharp isolated resonances more accurately. This conclusion complements the Rapedius observation that the SA becomes less accurate as the resonance width increases [1]. In addition to it, we have argued that in the present example, the KM profile [18] mildly improves on the BW one because the lowest resonance is rather too sharp when it can be considered sufficiently isolated from the next resonance.

We have derived the SA from the time-independent Schrödinger equation in a way that is more consistent with the methods for the calculation of the resonances described in this and
Rapedius’ papers. The Wronskian approach is most suitable for the discussion of the problem and enables the decomposition of the resonance widths into the sum of partial widths [16] which we have omitted here.

We have shown that the RPM is a powerful tool for the location of resonances in one-dimensional quantum-mechanical problems (more precisely, it applies to separable Schrödinger equations). The RPM is a local approach based on the expansion of the logarithmic derivative of the wavefunction about a chosen point, and for this reason it may not be the most convenient method for a pedagogical illustration of the main features of the Siegert states (for example, the discussion of the boundary conditions). However, it provides remarkably accurate results and the derivation of its main equations offers no difficulty. In addition to it, the recipe for its application is simple and easy to encode into a computer program, especially in most available computer algebra systems. We think that the RPM may be a valuable tool for teaching purposes because it allows the students to obtain accurate bound-state and resonance energies and compare them with those provided by other approaches like SA, CS or the matrix method [1, 19].

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