Determination of resonances by the optimized spectral approach

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Abstract
The Rayleigh–Ritz procedure for determining bound states of the Schrödinger equation relies on spectral representation of the solution as a linear combination of the basis functions. Several possible extensions of the method to resonance states have been considered in the literature. Here we propose the application of the optimized Rayleigh–Ritz method to this end. The method uses a basis of the functions containing adjustable nonlinear parameters, the values of which are fixed so as to make the trace of the variational matrix stationary. Generalization to resonances proceeds by allowing the parameters to be complex numbers. Using various basis sets, we demonstrate that the optimized Rayleigh–Ritz scheme with complex parameters provides an effective algorithm for the determination of both the energy and lifetime of the resonant states for various one-dimensional and spherically symmetric potentials. The method is computationally inexpensive since it does not require iterations or predetermined initial values. The convergence rate compares favorably to other approaches.

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(Some figures may appear in colour only in the online journal)

1. Introduction
Resonance phenomena appear in many fields of quantum physics: from unstable elementary particles to resonances in atomic or molecular systems and to collective excitations in the condensed phase. They are described as long-lived states of a system that have enough energy to undergo a decay process. Wavefunctions of resonant configurations resemble bound states over a period of time, called the decaying lifetime, when they are captured in a small area of space. Like the bound states, they may be treated as eigenstates of the Hamiltonian that are associated with the natural frequencies of the system. The difference lies in the complex character of the resonance eigenvalues which is related to the purely outgoing boundary
condition they fulfil. Such an approach to resonances was started by Gamow in the paper on α-decay of radioactive nuclei [1] and further developed by Siegert [2]. It has been shown that the problem of non-square integrability of their eigenfunctions can be rigorously overcome by enlarging the functional space to a rigged Hilbert space [3, 4]. On the other hand, the complex scaling idea [5] has enabled development of practical approaches where the resonant states are treated on the same footing as the bound states [6, 7]. One of the most practical methods is the Rayleigh–Ritz (RR) determination of the eigenstates of a complex-scaled Hamiltonian.

In this work, we discuss the determination of the resonances by the optimized RR scheme [8] which proved successful for bound states [9–11]. The method uses a basis of functions with adjustable nonlinear parameters, the values of which are fixed so as to make the trace of the RR matrix stationary. Generalization to resonances proceeds straightforwardly by allowing nonlinear parameters to be complex numbers. Through the study of several systems with different potentials we demonstrate the efficiency of our method in finding both the energy and lifetime of the resonant states.

The plan of our work is as follows. In section 2, the optimized RR method is described and its extension to resonances is discussed. The calculations of the resonance parameters are presented in section 3 for one-dimensional potentials, and in section 4 for the spherically symmetric case in D dimensions. Section 5 is devoted to conclusion.

2. The method

The Schrödinger equation

\[
\hat{H} \psi(x) = \varepsilon \psi(x),
\]

in the vast majority of cases cannot be solved exactly and has to be dealt with approximately. One of the classical methods for calculating numerically accurate solutions is the linear Rayleigh–Ritz procedure.

2.1. Rayleigh–Ritz determination of bound states

The RR method for solving the Schrödinger equation (1) is based on the variational principle which says that the Rayleigh quotient

\[
R[\Phi] = \frac{\langle \Phi(x) | \hat{H} | \Phi(x) \rangle}{\langle \Phi(x) | \Phi(x) \rangle},
\]

achieves a minimum when \( \Phi(x) \) fulfils equation (1) with boundary conditions \( \psi(x \to \pm \infty) \to 0 \). This allows determination of bound-state wavefunctions by approximating them by finite linear combinations

\[
\Phi(x) = \sum_{j=0}^{M-1} c_j \phi_j^A(x),
\]

where the functions \( \phi_j^A(x) \) are taken from an orthonormal basis in the function space. The variational principle yields the matrix equation for the linear parameters \( c_j \) in the form

\[
\sum_{j=0}^{M-1} (H_{jm}^A - \varepsilon \delta_{jm}) c_j = 0, \quad m = 0, 1, \ldots, M - 1,
\]

where the matrix elements of the Hamiltonian are

\[
H_{jm}^A = \langle \phi_j^A | \hat{H} | \phi_m^A \rangle = \int_{-\infty}^{\infty} \phi_j^A(x) \hat{H} \phi_m^A(x) \, dx.
\]
Diagonalization of the RR matrix provides $M$th order approximations to the $M$ of the lowest energy states. Systematically increasing the matrix dimension $M$, we increase the number of determined bound states, wherein their approximate energies approach the exact results from above. The convergence of the method depends heavily on the choice of the basis set \{$\phi^j_0(x)$, $j = 0, 1, \ldots$\}. It appears advantageous to make the functions of the basis adaptable to the problem under study by allowing their dependence on nonlinear parameters (A), the values of which can be conveniently adjusted in each order approximation. To ensure a fast convergence of the particular eigenvalue (usually the ground-state energy), the values of nonlinear parameters are chosen by trial and error or determined in numerically demanding optimization procedures \[12\]. Another option, that does not need any starting values or iterations, is to fix the nonlinear parameters according to the principle of minimal sensitivity \[13\], i.e. so that the approximation to a physical quantity would depend as weakly as possible on infinitesimal changes of their values. In the optimized RR method, proposed by one of us \[8\], the sum of $M$ bound-state energies is chosen as the physical quantity, the $M$th order approximation to which is given by the trace of the RR matrix $\text{Tr} H^M_A = \sum_{j=0}^{M-1} \langle \phi^j_0 | \hat{H} | \phi^j_0 \rangle$. The stationarity of the trace requirement

$$\frac{\delta}{\delta A} \text{Tr} H^M_A = 0,$$

is used to fix the values of nonlinear parameters, and a diagonalization of the so-optimized matrix determines a set of $M$ approximate eigenstates which are mutually orthogonal. The method is computationally less demanding although its convergence for a particular state may be slower than that achieved with nonlinear parameters iteratively optimized for that state. In the case of bound states, the effectiveness of our method has been demonstrated for various potentials and various basis sets \[8–11\]. Here we extend its application to resonant states.

2.2. Rayleigh–Ritz determination of resonant states

Most frequently, the resonances manifest themselves as sharp peaks in the collision cross sections which are well described by the two parameter Breit–Wigner formula. The resonance energy $\varepsilon$ and the half-width of the peak $\Gamma$ may be related to the complex eigenvalues $\varepsilon = E - i \Gamma / 2$,\n
$$\varepsilon = E - i \Gamma / 2,$$

of the Schrödinger equation (1), allowing $\Gamma$ to be interpreted as the inverse of the resonance lifetime. In finite range potentials, the wavefunction of a resonant state exhibits asymptotic behavior of the form

$$\psi_{\text{rez}}(x \to \pm \infty) \approx e^{\pm ik_{\text{rez}}x},$$

where

$$k_{\text{rez}} = |k_{\text{rez}}| e^{-i \alpha_{\text{rez}}},$$

with $0 < \alpha_{\text{rez}} < \pi / 2$, corresponds to the position of wave vector $k_{\text{rez}}$ in the fourth quarter of the complex plane. Since the resonant wavefunctions $\psi_{\text{rez}}(x)$ do not belong to the $L^2$ Hilbert space, the hermicity property does not hold for them. The corresponding eigenvalues of the Hamiltonian are thus complex numbers that are hidden on a higher Riemann sheet of the complex energy plane.

2.2.1. Complex scaling. The complex scaling transformation

$$U(\theta) : x \mapsto xe^{i\theta},$$

(10)
allows the treatment of resonant states in analogy to bound states. The corresponding complex-rotated Hamiltonian
\[ \hat{H}_\theta = U(\theta)\hat{H}U^{-1}(\theta), \] (11)
satisfies the eigenequation
\[ \hat{H}_\theta \psi_\theta(x) = \varepsilon_\theta \psi_\theta(x), \] (12)
and its spectrum is described by the Balslev–Combes theorem. For dilatation analytic potentials [5], among which are the Coulomb and Yukawa potentials in addition to the finite range ones, the theorem states that the real bound-state eigenvalues, the complex resonance eigenvalues and the thresholds are the same as those of the original Hamiltonian, but the eigenvalues of the continuous spectrum are rotated about the thresholds by an angle \(2\theta\) into the lower energy half-plane, exposing complex resonance eigenvalues. The complex scaling transformation (10) turns the function \(\psi_{\text{rez}}(x)\) into a normalizable one, if the real parameter \(\theta\) is such that \(0 < \theta < \alpha_{\text{rez}} < \pi/2\). In this case, the resonances can be determined as the eigenstates of the non-Hermitian Hamiltonian \(\hat{H}_\theta\) by using bound-state-like strategies. Here we use the optimized RR method with a complex basis to this end.

2.2.2. Complex basis. Since the resonance eigenvalues are complex numbers, their spectrum is determined by stationarity rather than minimization condition. This requires that the Rayleigh quotient
\[ R[\Phi] = \frac{\langle \Phi(x)|\hat{H}_\theta|\Phi(x) \rangle}{\langle \Phi(x)|\Phi(x) \rangle}, \] (13)
be stationary at the square integrable solutions of the complex rotated Hamiltonian (11). With the solution \(\Phi(x)\) approximated by a finite linear combination of the real functions (3), the same secular equation is obtained as for bound states (4) but with the matrix element \(H^{\alpha}_{jm}\) replaced by
\[ H^{A,\theta}_{jm} = \int_{-\infty}^{\infty} \phi_{\alpha j}(x)\hat{H}_\theta \phi_{\alpha m}(x) \, dx. \] (14)
It has been observed [14] that changing the variable \(x\) to \(xe^{-i\theta}\) and using Cauchy’s theorem to distort the integration contour back to the real axis, the matrix elements turn into
\[ H^{A,\theta}_{jm} = \int_{-\infty}^{\infty} \phi_{\alpha j}(xe^{-i\theta})\hat{H}_\theta \phi_{\alpha m}(xe^{-i\theta}) \, dx. \] (15)
The complex scaling is thus equivalent to working with the original Hamiltonian and using the basis functions with coordinates rescaled with factor \(e^{-i\theta}\) [6, 14]. Note, however, that instead of the ordinary scalar product of the Hilbert space \(\langle f|g \rangle = \int_{-\infty}^{\infty} f(x)g(x) \, dx\), the c-scalar product \(\langle f|g \rangle = \int_{-\infty}^{\infty} f(x)g(x) \, dx\) is to be used in the complex basis approach [15]. The advantage of the complex basis approach is that it applies also for non-dilatation analytic potentials [16–18]. Moreover, generalization to many-body systems allows introducing different scaling parameter for each degree-of-freedom, which makes the method more flexible than that of the complex-scaled Hamiltonian. In the case when the nonlinear parameter \(A\) is the scale parameter, so that
\[ \phi_{\alpha j}(x) = \frac{1}{\sqrt{A}} \phi_{j} \left( \frac{x}{A} \right), \] (16)
the RR matrix element (15) may be written as
\[ H^{\alpha}_{jm} = \int_{-\infty}^{\infty} \phi_{\alpha j}(x)\hat{H}\phi_{\alpha m}(x) \, dx, \] (17)
where \(\alpha = Ae^{i\theta}\) and may be simply obtained by replacing the real parameter \(A\) in (5) by a complex parameter \(\alpha\).
2.2.3. Optimized RR method for resonances. In this work, we generalize the optimized RR method [8] to the case of resonant states by using the complex basis approach. Dealing with the unscaled Hamiltonian \( \hat{H} \), we choose a basis set of real functions \( \{ \phi_j(x), j = 0, 1, \ldots \} \) so that the matrix elements \( \langle \phi_m | \hat{H} | \phi_n \rangle \) are given by analytic expressions. In the \( M \)th order calculation, we fix the value of the parameter \( \alpha \) to be equal to the complex solution of the stationarity of the trace condition (6) and after a single diagonalization of the \( M \)-dimensional symmetric complex matrix we obtain a set of \( M \) approximate eigenvalues. The number of calculated eigenvalues and their accuracy may be increased by increasing \( M \), which permits quantification of the precision of the obtained results. In order to demonstrate the effectiveness of our method, we consider several very different systems described by one-dimensional and radial Schrödinger equations, using various basis sets of functions with adjustable scale parameters. In some cases it turns out to be advantageous to introduce additional parameters that are not the scaling parameters. Our calculations have been carried out with the use of the Mathematica package. The algorithmic formulation of the optimized RR scheme allows an arbitrary precision calculation by taking advantage of the computer algebra abilities to deal with exact numbers.

3. One-dimensional Schrödinger equations

3.1. Harmonic oscillator basis: \( \text{RR}^{\Omega \mu}_{\text{opt}} \) method

First, we consider the case of reflection symmetric potentials \( V(x) = V(-x) \). We use the \( \text{RR}^{\Omega \mu}_{\text{opt}} \) method with the basis of the harmonic oscillator (HO) eigenfunctions

\[
\phi_{\mu}^{\Omega}(x) = \left( \frac{\sqrt{\Omega}}{\sqrt{\pi} 2^j j!} \right)^{1/2} H_j(\sqrt{\Omega}x)e^{-\frac{x^2}{2}},
\]

where the square root of the oscillator frequency \( \Omega \) plays the role of an inverse scaling parameter. The functions \( H_j(\sqrt{\Omega}x) \) are Hermite polynomials. Due to reflection symmetry, the even-(odd-) parity states may be obtained by diagonalization of the Hamiltonian matrix in the basis of the first \( M \) even (odd) functions, which substantially reduces the computational cost.

3.1.1. Quartic resonance potential. A simple example of a resonant system is the inverse quartic anharmonic oscillator with a Hamiltonian

\[
\hat{H} = -\frac{1}{2} \frac{d^2}{dx^2} + V(x) = -\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2} x^2 - \frac{\lambda}{2} x^4,
\]

where the units \( \hbar = 1 \) and \( m = 1 \) are used. In the case of \( \lambda > 0 \), the potential \( V(x) \) is not bounded from below and the system possesses only resonant states, the lowest energies of which are marked on figure 1 for \( \lambda = 0.02 \). The lifetime of the resonances increases with decreasing \( \lambda \), and the \( \text{RR}^{\Omega \mu}_{\text{opt}} \) calculations require using larger basis sets to obtain a satisfactory accuracy. Our numerical approximations to \( \epsilon_0 \) and \( \epsilon_2 \) for \( \lambda = 0.02 \), which is the most demanding case considered in the literature [19], are presented in table 1 as a function of the dimension of the RR matrix \( M \). Here and in the following tables the results are accurate to the number of figures shown. The best accuracy is obtained for the lowest resonance, and for all states it quickly improves with increasing \( M \). We can see that the literature results of the Riccati–Padé method [19] are reproduced with RR matrix of dimension \( M = 25 \); for larger \( M \), more accurate values are easily obtained. The imaginary part of \( \epsilon_2 \) is larger than that of \( \epsilon_0 \), and we observed its further increase for higher resonances, which confirms that the lifetime decreases with increasing resonance energy.
Figure 1. The first five resonance energies Re \( \varepsilon \) for the potential \( V(x) = \frac{1}{2} x^2 - 0.01 x^4 \).

Table 1. Optimal values of the parameter \( \Omega \) and the energies and widths of the two lowest even resonances for the Hamiltonian (19) with \( \lambda = 0.02 \) calculated by the RR\(_{opt}\) method.

| \( M \) | \( \Omega_{opt} \) | \( E_0 \) | \( E_2 \) | \( \Gamma_0 \) | \( \Gamma_2 \) |
|--------|-----------------|--------|--------|--------|--------|
| 20     | 0.723–0.754 I   | 0.492  | 2.393  | 5.109 \times 10^{-14} |
|        | 213 834 482 627 7005 | 483 626 | 213 834 627 7005 | 2.842 \times 10^{-9} |
| 25     | 0.759–0.835 I   | 0.492  | 2.393  | 5.109 \times 10^{-14} |
|        | 213 834 482 627 700 | 362 194 884 888 72 | 2.842 \times 10^{-9} |
| 30     | 0.791–0.937 I   | 0.492  | 2.393  | 5.109 \times 10^{-14} |
|        | 213 834 482 627 700 421 36 | 324 213 834 482 627 700 | 2.842 \times 10^{-9} |
| 35     | 0.821–1.010 I   | 0.492  | 2.393  | 5.109 \times 10^{-14} |
|        | 213 834 482 627 700 421 36 | 324 213 834 482 627 700 | 2.842 \times 10^{-9} |

As an additional test of accuracy of our method, we can use the hypervirial theorem [20] which states that the expectation value of the commutator \( \langle \psi | [\hat{H}, \hat{\Lambda}] | \psi \rangle \) should vanish for any operator \( \hat{\Lambda} \) if \( \psi \) is an exact eigenstate. Choosing the operator \( \hat{\Lambda} = x \frac{d^2}{dx^2} \), it has been shown [21] for bound states that the expectation value of the commutator calculated with approximate wavefunctions provides a good measure of their accuracy. Using the same operator \( \hat{\Lambda} = x \frac{d^2}{dx^2} \), we calculated the parameter

\[
\eta = \frac{1}{\Phi_1(\chi)} \langle \hat{H}, \hat{\Lambda} \rangle \Phi_1(\chi),
\]

(20)
to test the accuracy of the resonant wavefunctions as determined by the RR\(_{opt}\) method. Table 2 demonstrates how quickly the values of \( \eta \) decrease with increasing number of basis functions \( M \) in the case of the lowest resonant state of the Hamiltonian (19).

3.1.2. Triple-well oscillator. The sextic oscillator Hamiltonian

\[
\hat{H} = -\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2} x^2 - g^2 x^4 + \frac{g^4}{2} x^6,
\]

(21)
where the triple-well potential \( V(x) = \frac{1}{2} x^2 - g^2 x^4 + \frac{g^4}{2} x^6 \) is bounded from below and increases to infinity at \( |x| \to \infty \), describes an interesting system which supports only bound states. It has been shown [22, 23] that the complex scaling transformation turns the asymptotically
divergent solutions of this problem into square integrable ones that are associated with complex
eigenvalues which describe the rates of tunneling between the potential wells. The eigenvalues
\( \epsilon_0 \) and \( \epsilon_4 \) determined with the RR\( \Omega \)/opt method for various matrix dimensions
\( M \) are presented in table 3 for \( g = 0.08 \) and in table 4 for \( g = 0.3 \). We observe that with increasing \( g \), the imaginary part of the eigenvalue grows, i.e. the resonance lifetime decreases, and the accuracy of the method improves. Comparison with the best published results for \( \epsilon_0 \), obtained by the Ricatti–Padé method [19], shows that in the most unfavorable case of \( g = 0.08 \) we attain the same level of accuracy with the matrix of dimension \( M = 60 \), while \( M = 30 \) is sufficient in the case of \( g = 0.3 \).

3.2. Shifted harmonic oscillator basis: RR\( \Omega,t \)/opt method

Discussing problems with the resonant potential that is not symmetric about the origin, it is advantageous to use the RR\( \Omega,t \)/opt method with additional complex parameter \( t \) that shifts the argument of the HO basis functions

\[
\phi_j^{\Omega,t}(x) = \left( \frac{\sqrt{\Omega}}{\sqrt{\pi} \sqrt{j!}} \right)^{1/2} H_j(\sqrt{\Omega}(x-t)) e^{-\frac{(x-t)^2}{\Omega}}.
\]  

(22)

We apply the above basis to determine the spectrum of the cubic anharmonic Hamiltonian

\[
\hat{H} = -\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2} x^2 + \gamma x^3,
\]  

(23)

for an exemplary value of \( \gamma = 0.1 \). In table 5, the complex energies of the lowest resonant state are presented with the corresponding optimal values of the nonlinear parameters \( \Omega_{opt} \) and \( \epsilon_{opt} \) for various dimensions \( M \) of the RR matrix. The best previously published results [24] are reproduced with the RR matrix of dimension \( M = 40 \). By increasing \( M \), we easily obtain more accurate eigenvalues. It is interesting to note that although the shift parameter is not a scale parameter, its value determined by the stationarity of the trace condition turns out to be complex and this appears crucial for a fast convergence of the optimized RR scheme.

3.3. Trigonometric basis: RR\( \Omega,t \)/opt method

Another convenient basis is provided by the set of trigonometric (TRIG) functions that satisfy the Dirichlet boundary condition at \( x = \pm L \), where the width of the box \( L \) serves as a scaling parameter. The even functions are of the form

\[
\phi_j^e(x) = \frac{1}{\sqrt{L}} \cos \left[ \left( j + \frac{1}{2} \right) \frac{\pi x}{L} \right],
\]  

(24)
Table 3. Optimal values of the parameter $\Omega$ and the energies and widths of the even resonances for the Hamiltonian (21) with $g = 0.08$ calculated by the RR$^{\Omega}_{\text{opt}}$ method.

| $M$  | $\Omega_{\text{opt}}$ | $E_0$                      | $E_4$ | $\Gamma_0$ | $\Gamma_4$               |
|------|----------------------|---------------------------|-------|------------|---------------------------|
| 40   | 0.5161–0.8673 I      | 0.495 128 229 770 753 001 569 295 4656 |       |            | $10^{-28}$                |
|      |                      | 4.289 620 313 836 233 300 694 90 4.289 620 313 836 233 300 694 90 4.289 620 313 836 233 300 694 90 |       |            | $4 \times 10^{-20}$     |
| 50   | 0.5162–1.0001 I      | 0.495 128 229 770 753 001 569 295 465 687 4446 |       |            | $1.2 \times 10^{-32}$               |
|      |                      | 4.289 620 313 836 233 300 694 904 739 4.289 620 313 836 233 300 694 904 739 4.289 620 313 836 233 300 694 904 739 |       |            | $4.180 046 \times 10^{-20}$               |
| 60   | 0.5163–1.1171 I      | 0.495 128 229 770 753 001 569 295 465 687 4446 417 9669 |       |            | $1.169 941 74 \times 10^{-32}$               |
|      |                      | 4.289 620 313 836 233 300 694 904 738 818 061 623 7064 4.289 620 313 836 233 300 694 904 738 818 061 623 7064 4.289 620 313 836 233 300 694 904 738 818 061 623 7064 |       |            | $4.180 045 611 813 252 125 \times 10^{-20}$               |
| 70   | 0.5163–1.2230 I      | 0.495 128 229 770 753 001 569 295 465 687 4446 617 966 881 040 |       |            | $1.169 941 743 985 5 \times 10^{-32}$               |
|      |                      | 4.289 620 313 836 233 300 694 904 738 818 061 623 7064 4.289 620 313 836 233 300 694 904 738 818 061 623 7064 4.289 620 313 836 233 300 694 904 738 818 061 623 7064 |       |            | $4.180 045 611 813 252 125 \times 10^{-20}$               |
Table 4. Same as in table 3 but for $g = 0.3$.

| $M$ | $\Omega_{opt}$ | $E_0$  | $\Gamma_0$ | $E_4$  | $\Gamma_4$ |
|-----|-----------------|--------|------------|--------|------------|
| 10  | 0.5159–1.7799 I | 0.4078 | 0.029 4002 | 2.6095 | 4.7968     |
| 20  | 0.5163–2.5792 I | 0.4078 | 0.029 4002 | 4.7967 | 530 29     |
| 30  | 0.5163–3.1840 I | 0.4078 | 0.029 4002 | 4.7967 | 530 29     |
| 40  | 0.5164–3.6909 I | 0.4078 | 0.029 4002 | 4.7967 | 530 29     |
| 50  | 0.5164–4.1363 I | 0.4078 | 0.029 4002 | 4.7967 | 530 29     |
Table 5. Optimal values of nonlinear parameters and the energy and width of the lowest resonance state for the Hamiltonian (23) with $\gamma = 0.1$ calculated by the RR$_{\Omega}$ method.

| $M$  | $t_{\text{opt}}$ | $\Omega_{\text{opt}}$ | $E_0$    | $\Gamma_0$ |
|------|------------------|----------------------|---------|------------|
| 20   | −0.67–2.26 i     | 1.02–0.66 i          | 0.484 32 | 0.000 0161 |
| 30   | −0.54–2.78 i     | 1.11–0.75 i          | 0.484 315 997 00 | 0.000 016 1204 |
| 40   | −0.43–3.20 i     | 1.18–0.81 i          | 0.484 315 997 004 117 | 0.000 016 120 419 000 |
| 50   | −0.34–3.55 i     | 1.24–0.86 i          | 0.484 315 997 004 117 5430 | 0.000 016 120 419 000 133 57 |
| 60   | −0.25–3.86 i     | 1.29–0.90 i          | 0.484 315 997 004 117 543 023 | 0.000 016 120 419 000 133 5639 |

and the odd ones are given by

$$
\phi_{L,j}^\Lambda(x) = \frac{1}{\sqrt{L}} \sin \left[ \left( j + 1 \right) \frac{\pi x}{L} \right].
$$

We use the TRIG basis to find the eigenvalues of the Hamiltonian with an inverted Gaussian potential with quartic perturbation

$$
\hat{H} = -\frac{1}{2} \frac{d^2}{dx^2} - 5e^{-0.1x^2} - \frac{\lambda}{2} x^4.
$$

The energies and widths presented in tables 6 and 7 show that already with matrices of dimension $M = 20$ we reach the accuracy of the literature results [25]. We observe that the energy of the resonant state does not change much with decreasing $\lambda$, while its width decreases rapidly to zero, switching to the bound state at $\lambda = 0$.

4. Radial Schrödinger equation in $D$-dimensional space

For spherically symmetric problems in $D$-dimensional space, the solution of the Schrödinger equation factorizes into the angular part given by hyperspherical harmonics and the radial part $R(r)$ that fulfils

$$
\left[ -\frac{1}{2} \frac{d^2}{dr^2} - \frac{(D-1)}{2r} \frac{d}{dr} + \frac{l(l+D-2)}{2r^2} + V(r) \right] R(r) = ER(r).
$$

(27)

By substituting $R(r) = r^{(l-D)/2} u(r)$, the radial equation is brought to the one-dimensional Schrödinger form

$$
\hat{H}_r u(r) = \left[ -\frac{1}{2} \frac{d^2}{dr^2} + \frac{\Lambda(\Lambda+1)}{2r^2} + V(r) \right] u(r) = Eu(r),
$$

(28)

where $\Lambda = l + D/2 - 3/2$.

4.1. Radial harmonic oscillator basis: RR$_{\Omega}$ method

For determining the resonant spectrum of radial anharmonic oscillators, it is convenient to use the basis of the spherically symmetric HO eigenfunctions that are given by

$$
\phi_{J/\Lambda}^\Omega(r) = \sqrt{\frac{(2j+\Lambda+\Lambda)}{\Gamma(j+\Lambda+\Lambda/2)}} r^{\Lambda+1} e^{-\frac{r^2}{2}} L_j^{\Lambda+\frac{1}{2}}(r^2 \Omega),
$$

(29)

where the functions $L_j^{\Lambda+\frac{1}{2}}(r^2 \Omega)$ are Laguerre polynomials. As an example, we consider the case of two dimensions, where $\Lambda = l - 1/2$. We determine the resonances in the inverted Mexican hat potential with the radial Hamiltonian given by

$$
\hat{H} = -\frac{1}{2} \frac{d^2}{dr^2} + \frac{l^2 - \frac{1}{4} - \frac{1}{2} r^2 + \frac{1}{2} r^4}{2r^2} - \frac{g}{2} r^4.
$$

(30)
Table 6. Optimal values of the parameter $L$ and the energies and widths of the two lowest resonances for the Hamiltonian (26) with $\lambda = 0.08$ calculated by the $R\mathcal{R}_{\text{opt}}$ method.

| $M$ | $L_{\text{opt}}$ | $E_0$ | $E_1$ | $\Gamma_0$ | $\Gamma_1$ |
|-----|------------------|-------|-------|------------|------------|
| 20  | 5.114 + 2.888 I  | -4.566 565 509 377 7188 | | | 0.017 706 894 105 4286 |
|     | 5.155 + 2.915 I  | -3.838 103 508 910 8826 | | | 0.274 321 590 467 8811 |
| 30  | 5.840 + 3.348 I  | -4.566 565 509 377 718 816 870 2314 | | | 0.017 706 894 105 428 619 830 2607 |
|     | 5.872 + 3.367 I  | -3.838 103 508 910 882 658 606 3027 | | | 0.274 321 590 467 881 124 323 36 |
| 40  | 6.427 + 3.699 I  | -4.566 565 509 377 718 816 870 231 336 773 358 4 | | | 0.017 706 894 105 428 619 830 260 744 952 78 |
|     | 6.454 + 3.715 I  | -3.838 103 508 910 882 658 606 302 626 356 831 | | | 0.274 321 590 467 881 124 323 361 759 999 012 |
| 50  | 6.924 + 3.989 I  | -4.566 565 509 377 718 816 870 231 336 773 358 361 540 6723 | | | 0.017 706 894 105 428 619 830 260 744 952 784 024 460 349 |
|     | 6.947 + 4.003 I  | -3.838 103 508 910 882 658 606 302 626 356 830 430 463 41 | | | 0.274 321 590 467 881 124 323 361 759 999 012 391 368 05 |
| $M$ | $L_{opt}$  | $E_{0}$  | $E_{1}$  | $\Gamma_{0}$ | $\Gamma_{1}$ |
|-----|-----------|----------|----------|--------------|--------------|
| 20  | 7.202 + 4.098 I | −4.523 482 872 19 |  | 2.068 2 × 10^−7 |  |
| 30  | 8.261 + 4.726 I | −4.523 482 872 186 005 7186 |  | 2.068 22 142 91 × 10^−7 |  |
| 40  | 9.089 + 5.218 I | −4.523 482 872 186 005 718 608 260 15 |  | 2.068 22 142 909 129 854 23 × 10^−7 |  |
| 50  | 9.788 + 5.630 I | −4.523 482 872 186 005 718 608 260 144 363 4245 |  | 2.068 22 142 909 129 854 222 1588 × 10^−7 |  |
|  | 9.821 + 5.649 I | −3.623 316 934 353 133 789 895 383 842 752 28 |  | 0.000 687 607 656 914 005 718 608 260 144 363 4244 |  |

Table 7. Same as table 6, but for $\lambda = 0.01$
Figure 2. Bardsley potential \( V(r) = 7.5r^2e^{-r} \).

Table 8. Optimal values of the parameter \( \Omega \) and the energies and widths of the lowest resonances with \( l = 0 \) and \( l = 1 \) for the Hamiltonian (30) with \( g = 0.1 \), calculated by the RR\( _{\Omega} \) method for increasing dimension \( M \).

| \( M \) | \( \Omega_{\text{opt}} \) | \( E_{0j}^0 \) | \( E_{0j}^1 \) | \( \Gamma_{0j}^0 \) | \( \Gamma_{0j}^1 \) |
|-----|-----|-----|-----|-----|-----|
| 10  | 0.8982–1.1917 \( i \) 0.856 745 041 | 0.856 745 041 | 0.045 436 67 |
|     | 0.9095–1.2172 \( i \) 1.568 182 93 | 1.568 182 93 | 0.346 824 42 |
| 15  | 1.0000–1.4142 \( i \) 0.856 745 041 145 83 | 0.856 745 041 145 83 | 0.045 436 670 7026 |
|     | 1.0090–1.4333 \( i \) 1.568 182 929 694 | 1.568 182 929 694 | 0.346 824 423 557 63 |
| 20  | 1.0832–1.5874 \( i \) 0.856 745 041 145 827 3172 | 0.856 745 041 145 827 3172 | 0.045 436 670 702 590 7851 |
|     | 1.0907–1.6029 \( i \) 1.568 182 929 693 699 2519 | 1.568 182 929 693 699 2519 | 0.346 824 423 557 637 908 916 |
| 25  | 1.1545–1.7316 \( i \) 0.856 745 041 145 827 317 214 2177 | 0.856 745 041 145 827 317 214 2177 | 0.045 436 670 702 590 785 072 3740 |
|     | 1.1611–1.7448 \( i \) 1.568 182 929 693 699 251 881 382 | 1.568 182 929 693 699 251 881 382 | 0.346 824 423 557 637 908 915 711 4 |
| 30  | 1.2174–1.8564 \( i \) 0.856 745 041 145 827 317 214 217 717 9279 | 0.856 745 041 145 827 317 214 217 717 9279 | 0.045 436 670 702 590 785 072 373 905 48 |
|     | 1.2233–1.8681 \( i \) 1.568 182 929 693 699 251 881 381 495 503 | 1.568 182 929 693 699 251 881 381 495 503 | 0.346 824 423 557 637 908 915 711 315 930 |

where \( g > 0 \). The above Hamiltonian has been studied before in [26] by the RR method with the same basis (29), but iteratively adjusting the value of \( \Omega \) in each order so as to obtain the best convergence for a single selected state. Our results obtained with \( \Omega \) being fixed \textit{a priori} from the trace condition (6) are presented in table 8. The comparison shows that our method automatically provides a fast convergence in determining a number of resonances with different quantum number \( n \) in one run.

4.2. Radial trigonometric basis: RR\( _{\Omega} \) method

For studying problems with \( \Lambda = 0 \), it appears convenient to use the basis of antisymmetric trigonometric functions

\[
\phi^L_j(x) = \sqrt{\frac{2}{L}} \sin \left[ (j + 1) \frac{\pi x}{L} \right],
\]

(31)
Table 9. Optimal values of the parameter $L$ and the energies and widths of a few resonances for the Hamiltonian (30) with $V_0 = 7.5$, calculated by the RR$_{opt}$ method for increasing dimension $M$.

| $M$   | $L_{opt}$ | $E_0$     | $\Gamma_0$ | $E_8$     | $\Gamma_8$ | $E_9$     | $\Gamma_9$ |
|-------|-----------|-----------|-------------|-----------|-------------|-----------|-------------|
| 100   | $-0.841 + 6.661i$ | 3.4264   | 0.025 549 | $-3.7$    | 40          | $-6.9$    | 45          |
|       |           |           |             |           |             |           |             |
| 120   | $-1.099 + 6.804i$ | 3.426 3903 | 0.025 548 96 | $-3.75$   | 40.01       | $-6.801$  | 45.527     |
|       |           |           |             |           |             |           |             |
| 140   | $-1.319 + 6.920i$ | 3.426 390 310 15 | 0.025 548 961 18 | $-3.754$ 144 | 40.009 0149 | $-6.800$ 30 | 45.526 3 |
|       |           |           |             |           |             |           |             |
| 160   | $-1.511 + 7.018i$ | 3.426 390 310 1482 | 0.025 548 961 185 80 | $-3.754$ 122 | 40.009 0149 | $-6.800$ 303 89 | 45.526 310 15 |
|       |           |           |             |           |             |           |             |
| 180   | $-1.680 + 7.102i$ | 3.426 390 310 148 2505 | 0.025 548 961 185 791 | $-3.754$ 122 607 | 40.009 014 9933 | $-6.800$ 303 886 379 | 45.526 310 150 00 |

where $L$ represents the confinement radius. We apply the above basis to calculate the resonant states of the Bardsley [27], presented in figure 2, the Hamiltonian of which reads

$$\hat{H} = -\frac{1}{2} \frac{d^2}{dr^2} + V_0 r^2 e^{-r}.$$  (32)

In [28], the very accurate results obtained using the Jost-function method are presented for nine lowest resonances. We show our results for the first and ninth states in table 9. The convergence rate decreases with increasing resonance width but with matrices of dimension $N = 160$ we automatically reproduce all the results of [28]. Our results for the next resonance $(E_9, \Gamma_9)$ are also presented in the table.

5. Conclusion

We applied the optimized RR method with complex nonlinear parameters to determine the resonance states in various one-dimensional potentials. The expansion bases were adapted to the considered problems so that the RR matrix elements were given by analytic expressions. The values of nonlinear parameters were fixed by requiring that the trace of the truncated matrix be stationary. We have shown that the basis of the HO eigenfunctions with frequency $\Omega$ optimized by the stationarity of the trace condition is efficient in determining the resonance spectrum in anharmonic potentials. In the case of nonsymmetric about the origin potentials, an additional complex shift parameter $r$ has proved to be useful to obtain quick convergence. The trigonometric basis with optimized boundary period parameter $L$ appears convenient, especially in the case of potentials described by exponential functions. Effectiveness of a similar approach in determining resonances of the radial Schrödinger equation has also been shown. The advantage of the optimized RR scheme is that a set of resonances is determined automatically in one run without the necessity of specifying any starting value. The computational cost of our method is much lower than in the case of iterative optimization of nonlinear parameters. The method appears especially effective in the cases where only
resonant modes exist. For the class of resonant potentials considered in this work, it is highly competitive with existing methods, the results of which are easily recovered in our approach.

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