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On two different kinds of resonances in one-dimensional quantum-mechanical models

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Abstract We apply the Riccati–Padé method and the Rayleigh–Ritz method with complex rotation to the study of the resonances of a one-dimensional well with two barriers. The model exhibits two different kinds of resonances and we calculate them by means of both approaches. While the Rayleigh–Ritz method reveals each set at a particular interval of rotation angles the Riccati–Padé method yields both of them as roots of the same Hankel determinants.

Keywords Bound states · Resonances · Pre-dissociation · Riccati–Padé · Rayleigh–Ritz · Complex rotation

1 Introduction

Many years ago Moyseyev et al. [1] discussed the application of complex rotation to the calculation of resonances. As a simple, nontrivial illustrative example they chose the potential $V(x) = \left(\frac{1}{2}x^2 - J\right)\exp\left(-\lambda x^2\right) + J$ that exhibits "pre-dissociating resonances analogous to those found in diatomic molecules". The same model was chosen by other authors to test different approaches for the calculation of resonances [2–4] and a controversy about the behaviour of $\Re E$ versus $\Im E$ arose [5,6]. The discrepancy between the results of Rittby et al. [3,4] and Korsch et al. [5] was shown to be caused by the choice of the rotation angle θ with respect to the critical angle θ_{crit} [6]. The set of resonances that one obtains with complex-rotation angles $\theta < \pi/4$ is different from the one that comes from greater angles $\theta > \pi/4$. Epifanov [7] and Abramov et

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al. [8] also chose this model for resonance calculations. The latter authors stated that their results broadly agreed with those of Rittby et al. [4]. For the commonly chosen parameters are $J = 0.8$, $\lambda = 0.1$ the potential supports only one bound state with energy $E_0 < J$ and many resonances.

On studying the performance of the Riccati–Padé method (RPM) for the calculation of bound states and resonances Fernández [9] found an apparently strange resonance located quite close to the only bound state of the model. This resonance had in fact been reported by Rittby et al. [6] and labelled as the KLM pole 0^+.

The purpose of this paper is to investigate if the RPM yields both sets of poles REB and KLM [6] or just one kind. To this end we carry out extremely accurate RPM calculations and compare them with the results provided by the Rayleigh–Ritz method with complex rotation.

2 The model

In this paper we study the spectrum of the dimensionless Hamiltonian operator $H = p^2 + V(x)$, where $p = -i d/dx$ and

$$V(x) = \left(x^2 - 2J\right) e^{-\lambda x^2} + 2J, \quad J, \lambda > 0. \tag{1}$$

Note that this Hamiltonian, which is the one chosen by Fernández [9] , is exactly twice the one mentioned above [2–8]. The potential (1) exhibits a minimum $V(0) = 0$ at origin and two barriers of height

$$V(\pm x_b) = \frac{e^{-2J\lambda-1}}{\lambda} + 2J, \quad x_b = \sqrt{\frac{2J\lambda + 1}{\lambda}}, \tag{2}$$

located at $x = \pm x_b$. In addition to it, $\lim_{|x|\to\infty} V(x) = 2J$ is the threshold of the continuum spectrum. That is to say: we expect bound states for $0 < E < 2J$ and unbound states for $\Re E > 2J$. It is well known that there is always a bound state $\psi_0(x)$ with energy E_0 for all values of $J > 0$. The Hellmann–Feynman theorem tells us that the bound states satisfy

$$0 < \frac{\partial E}{\partial J} = 2\left\langle 1 - e^{-\lambda x^2} \right\rangle < 2. \tag{3}$$

The energies of the bound states increase with J more slowly than the threshold $2J$ and as J increases more bound states appear.

The Taylor expansion of $V(x)$ about the origin

$$V(x) = (2J\lambda + 1) x^2 - \lambda (J\lambda + 1) x^4 + \frac{\lambda^2 (2J\lambda + 3)}{6} x^6 + \cdots \tag{4}$$

suggests that if $\lambda \ll 1$ the bound-state eigenvalues are approximately given by $E_n \approx \sqrt{2J\lambda + 1}(2n + 1)$, $n = 0, 1, \ldots$, provided that $E_n \ll 2J$. In other words, the

harmonic approximation is valid in the limit of sufficiently small λ and sufficiently large J.

3 The Riccati–Padé method

The dimensionless Schrödinger equation for a one-dimensional model reads

$$\psi''(x) + [E - V(x)] \psi(x) = 0, \tag{5}$$

where E is the eigenvalue and $\psi(x)$ is the eigenfunction that satisfies some given boundary conditions. For example, $\lim_{|x|\to\infty} \psi(x) = 0$ determines the discrete spectrum and the resonances are associated to outgoing waves in each channel (for example, $\psi(x) \sim A e^{ikx}$).

In order to apply the RPM we define the regularized logarithmic derivative of the eigenfunction

$$f(x) = \frac{s}{x} - \frac{\psi'(x)}{\psi(x)}, \tag{6}$$

that satisfies the Riccati equation

$$f'(x) + \frac{2sf(x)}{x} - f(x)^2 + V(x) - E = 0, \tag{7}$$

where $s = 0$ or $s = 1$ for even or odd states, respectively. If $V(x)$ is a polynomial function of x or it can be expanded in a Taylor series about $x = 0$ then one can also expand $f(x)$ in a Taylor series about the origin

$$f(x) = x \sum_{j=0}^{\infty} f_j(E) x^{2j}. \tag{8}$$

On arguing as in earlier papers (see, for example [9] and references therein) we conclude that we can obtain approximate eigenvalues to the Schrödinger equation from the roots of the Hankel determinant

$$H_D^d(E) = \begin{vmatrix} f_{d+1} & f_{d+2} & \cdots & f_{d+D} \\ f_{d+2} & f_{d+3} & \cdots & f_{d+D+1} \\ \vdots & \vdots & \ddots & \vdots \\ f_{d+D} & f_{d+D+1} & \cdots & f_{d+2D-1} \end{vmatrix} = 0, \tag{9}$$

where $D = 2, 3, \ldots$ is the dimension of the determinant and d is the difference between the degrees of the polynomials in the numerator and denominator of the rational approximation to $f(x)$. In those earlier papers we have shown that there are sequences of roots $E^{[D,d]}$, $D = 2, 3, \ldots$ of the determinant $H_D^d(E)$ that converge towards the bound states and resonances of the quantum-mechanical problem. We have at our disposal many sequences, one for each value of d, but it is commonly

sufficient to choose $d = 0$. For this reason, in this paper we restrict ourselves to the sequences of roots $E^{[D]} = E^{[D,0]}$ (unless stated otherwise).

The Hankel determinants (9) are polynomial functions of E with real coefficients. Therefore, since both E and E^* are roots we simply show the absolute value of the imaginary part of the complex eigenvalues calculated by means of the RPM.

It has been shown that the quantization condition (9) is consistent with moving a zero of $\psi(x)$ towards infinity either along the real axis [10,11] or along a ray $xe^{i\beta}$ on the complex coordinate plane [12]. In order to appreciate the latter statement clearer consider the canonical transformation

$$UxU^{-1} = \gamma x, \quad UpU^{-1} = \gamma^{-1}p, \tag{10}$$

that is commonly called scaling or dilatation transformation. If γ is real, then U is unitary and $U^{-1} = U^\dagger$ (the adjoint of U). The coefficients $\tilde{f}_j$ of the Taylor expansion of $\tilde{f}(x) = f(\gamma x)$ about $x = 0$ are given by $\tilde{f}_j = \gamma^{2j+1}f_j$ and the corresponding Hankel determinants are related by $H_D^d(\tilde{f}) = \gamma^{D(2D+2d+1)}H_D^d(f)$. It is clear from this expression that the roots of the Hankel determinant $H_D^d(f)$ are also those of $H_D^d(\tilde{f})$.

4 Results and discussion

We first comment on a particular feature of the RPM that was already discussed in earlier papers(see, for example, [9]). The canonical transformation (10) with $\gamma = e^{i\theta}$ leads to

$$UHU^{-1} = e^{-2i\theta}\left[p^2 + e^{2i\theta}V(e^{i\theta}x)\right]. \tag{11}$$

When $\theta = \pi/2$ then

$$UHU^{-1} = -H_{CR}, \quad H_{CR} = p^2 + \left(x^2 + 2J\right)e^{\lambda x^2} - 2J. \tag{12}$$

The Hamiltonian H_{CR} exhibits discrete spectrum for all $E > 0$ and, according to the discussion of the preceding section, the application of RPM to H yields also the eigenvalues of $-H_{CR}$. For example, from a sequence of negative roots $E^{[D]}$, $2 \le D \le 7$, we obtained $-E_0^{CR} = -1.144507971437882$. Note that in this case the RPM is moving the zero of $\psi(x)$ towards infinity along the imaginary axis ($UxU^{-1} = ix$).

Some time ago, Rittby et al. [3,4] calculated the resonances for the potential (1) with $J = 0.8$ and $\lambda = 0.1$ finding a curious oscillation in the plot of $\Re E$ versus $\Im E$ and that $\Re E < E_{threshold}$. Korsch et al. [5] argued that such oscillation was due to numerical instabilities or to a limited range of variation of the complex-rotation angle and presented alternative results for $\Re E$ versus $\Im E$ that exhibited a smoother behaviour with a maximum. The discrepancy was found to be more noticeable between the resonances with high quantum number. In a reply to this comment Rittby et al. [6] showed that one obtains either one set of results or the other depending on the angle of rotation of the coordinate in the complex plane. They obtained their earlier results when $\theta < \theta_{crit}$ and those of Korsch et al. [5] when $\theta > \theta_{crit}$, where $\theta_{crit} = \frac{\pi}{4}$ is

Table 1 Resonances of type a (REB poles) for the potential well (1) with $J = 0.8$ and $\lambda = 0.1$

n	$\Re E$	$|\Im E|$
0	1.00408072428393443017	
1	2.84194190210246090571	0.00011653325419685182
2	4.25439414535445676474	0.03089463756140796363
3	5.16916573799994004827	0.34750141927735930069
4	5.84884378317999747884	1.12958996483545345776
5	6.51097253363998538888	2.22306318914049287816
6	7.11443165024522044127	3.51101211133329168976
7	7.64865900791597156098	4.97489236442085409173
8	8.11086942948812965998	6.59728208929395179151
9	8.49991012723345008717	8.36633927847726677570
10	8.81554505392263084583	10.27290632674290915601

the angle at which the asymptotic limit of $V(e^{i\theta}x)$ ceases to exist. More precisely, the real part of $V(e^{i\theta}x)$ exhibits an oscillation of increasing magnitude when $\theta \geq \frac{\pi}{4}$.

It follows from the discussion above that there are two sets of eigenvalues that for brevity we decided to call type a and type b. The former appear at complex-rotation angles $\theta < \frac{\pi}{4}$ and the latter at $\theta > \frac{\pi}{4}$. They are obviously the REB and KLM poles discussed by Rittby et al. [6] and reported in their Tables 1 and 2, respectively. The RPM yields both sets of resonances but those of type a, including the bound state that is probably the REB pole 0^+, appear at considerably larger determinant dimensions. For example, from determinants of order $115 \leq D \leq 132$ we estimated

$$E_{16}^a = 9.19265185 - 24.2859880i, \tag{13}$$

while, on the other hand, from determinants of dimension $D \leq 34$ we obtained

$$E_{16}^b = 9.178238697954503583761 - 24.263016247192105546239i. \tag{14}$$

For even solutions $\psi(-x) = \psi(x)$ there is always a bound state and from roots of Hankel determinants of order $D \leq 34$ we obtained

$$E_0^{bs} = 1.004080724283934. \tag{15}$$

As stated above, this bound state is probably the REB pole 0^+ that was supposed to exhibit a very small imaginary part ($\sim 10^{-14}$) [6]. It was also reported in a table of another paper by the same authors [4]. Close to this bound state lays the resonance E_0^b that one easily obtains by means of the RPM. From determinants of dimension $D \leq 34$ we obtained

$$E_0^b = 1.00408072630157046939561459261599 4014289250$$
$$-0.29347127189074777146724772150589 36 \times 10^{-8}i. \tag{16}$$

Table 2 Resonances of type *b* (KLM poles) for the potential well (1) with $J = 0.8$ and $\lambda = 0.1$

n	$\Re E$	$|\Im E|$
0	1.00408072630157046940	0.00000000293471271891
1	2.84194189142938641479	0.00011653056177108158
2	4.25439415504499186371	0.03089462568361036622
3	5.16916571970620038273	0.34750143832439856191
4	5.84884385847547449718	1.12958993116515299773
5	6.51097228004676307937	2.22306320004939896286
6	7.11443232530273964386	3.51101246935385004749
7	7.64865805373778059202	4.97489030645579846012
8	8.11086733641836896565	6.59728840290639287908
9	8.49992787752865274035	8.36633165517743824541
10	8.81549677260886623210	10.27287881393211008638
11	9.05762805573781967843	12.30961933401526496646
12	9.22657497347881017987	14.47051165461491434216
13	9.32269370788061645446	16.75044181031167253591
14	9.34639100651463929862	19.14500056419140530520
15	9.29809501050649218041	21.65033039282456000024
16	9.17823869795450358376	24.26301624719210554624
17	8.98725046024366224546	26.98000499389483811828
18	8.72554882720201232788	29.79854439102831848701
19	8.39353964985405639416	32.71613581097854432033
20	7.99161475460693463976	35.73049690934641949224
21	7.52015148083891622536	38.83953166339397165944
22	6.97951274517891567252	42.04130598427444775492
23	6.37004741335819685837	45.33402762088381309024
24	5.69209084394630221200	48.71602942021668615706
25	4.94596551967542290825	52.18575524932345994550
26	4.13198171411806152281	55.74174805382654044018
27	3.25043816167984493764	59.38263965038260687933
28	2.30162271167951448456	63.10714194024298827641
29	1.28581295544208483457	66.91403929790148766545
30	0.20327682052002685664	70.80218193928122646417
31	−0.94572687055748570093	74.77048011249426351515
32	−2.16094787755166857383	78.81789898404686559215
33	−3.44214405508360832566	82.94345411668353883653
34	−4.78908089905121521519	87.14620745346424210130
35	−6.20153112503278609622	91.42526373731795161905
36	−7.67927427662588964625	95.77976730707267051567
37	−9.22209636161676757971	100.20889922046949752260
38	−10.82978951390703259870	104.71187466241100492439

Table 2 continued

n	$\Re E$	$|\Im E|$
39	-12.50215167920702077572	109.28794060304091487333
40	-14.23898632261633438011	113.93637367548645768060

It is worth noting that $\left|\Im E_0^b\right|$ is of the order of $\left|\Re E_0^b - E_0^{bs}\right|$.

The first odd resonance of type b is embedded in the continuum:

$$E_1^b = 2.84194189142938641479284813290283093$$
$$-0.11653056177108158006256047430109 \times 10^{-3}i. \qquad (17)$$

By means of the RPM we calculated some of the REB poles (Table 1) and all the KLM poles (Table 2). Resonances of type a with larger quantum number n are very difficult to obtain by means of the RPM because they appear at rather too large determinant dimensions. However, the results shown in these tables are more accurate than those reported by Rittby et al. [3,4,6] and Korsch et al. [5] (note that our results are twice those in references [3–6]).

Resonances in the discrete spectrum also appear for odd solutions provided that J is large enough. For example, when $J = 2$ we have one odd bound state with energy

$$E_1^{bs} = 3.203701434562602, \qquad (18)$$

and its partner resonance

$$E_1^b = 3.203701485896181395655563226675496312$$
$$-0.83665793634597482016260533385 \times 10^{-8}i, \qquad (19)$$

both obtained from determinants of dimension $D \leq 34$. In this case we also appreciate that $\left|\Im E_1^b\right|$ is of the order of $\left|\Re E_1^b - E_1^{bs}\right|$. Note that $\Re E_1^b$ increased with J but not as fast as $2J$ and, consequently, it crossed the threshold from the continuum to the discrete spectrum. Our numerical results suggest that the resonances also satisfy the bound-state condition $0 < \partial \Re E^{res}/\partial J < 2$ and that $\partial \left|\Im E^{res}\right|/\partial J < 0$.

For the same potential parameters we have the ground state

$$E_0^{bs} = 1.117002075677124853805, \qquad (20)$$

and its partner resonance

$$E_0^b = 1.11700207583211644471335770311286477$$
$$-0.99992858940384812992313357 \times 10^{-10}i, \qquad (21)$$

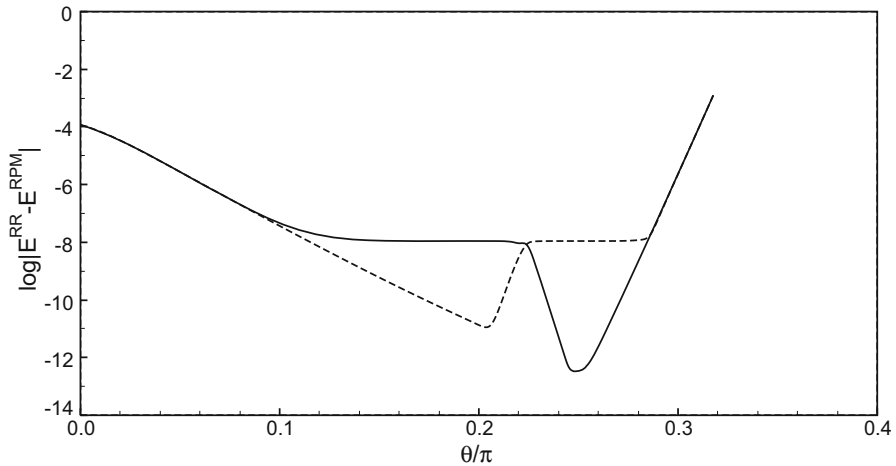obtained from determinants of dimension $D \leq 34$.

Fig. 1 $\log \left| E^{RR}(\theta) - E^{RPM} \right|$ for the REB (*dash line*) and KLM (*solid line*) poles when $\lambda = 0.1$ and $J = 0.8$
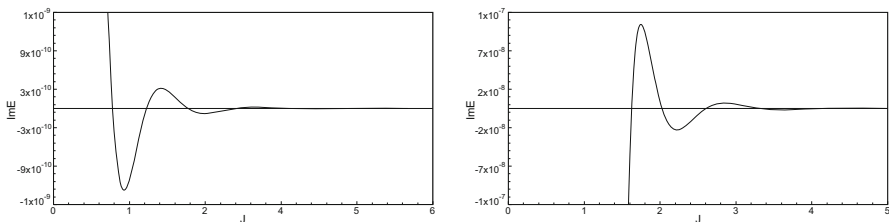

Fig. 2 $\Im E$ versus J for the first (*left*) and second (*right*) resonances of type b (KLM poles)

For small J it is easier to obtain the resonance in the discrete part of the spectrum than the partner bound state by means of the RPM. This behaviour tends to be exactly the opposite as J increases.

According to the results of Rittby et al. [6] (see also present Tables 1 and 2) the REB and KLM poles with the same quantum number are almost identical if the resonance number n is small enough. As n increases the members of each pair move apart. Present results suggest that if J increases a pair of complex eigenvalues crosses the threshold $2J$ into the discrete spectrum. The eigenvalue of type a becomes the energy of a bound state ($\Im E^a = 0$ when $\Re E^a < 2J$) while the eigenvalue of type b becomes its accompanying resonance.

In order to test the RPM results we have carried out a Rayleigh–Ritz calculation with complex-rotation (see, for example, reference [1] and references therein) and the basis set of the harmonic oscillator $H_{HO} = p^2 + x^2$. Fig. 1 shows $\log \left| E^{RR}(\theta) - E^{RPM}_{REB} \right|$ and $\log \left| E^{RR}(\theta) - E^{RPM}_{KLM} \right|$ for $J = 0.8$, $\lambda = 0.1$ and $N = 80$ basis functions. This figure shows that the optimal angles satisfy $\theta_{REB} < \pi/4 < \theta_{KLM}$. A more extensive calculation with several values of N suggests that both optimal complex-rotation angles increase with N in such a way that while the REB one remains smaller that $\pi/4$ the KLM one becomes clearly greater than such critical angle.

An interesting property of the resonances of type b (KLM poles) emerged during the calculation. If we look for stable eigenvalues roughly in the interval $0.85 < \theta < 0.95$ then $\Im E^b$ oscillates as shown in Fig. 2 for the first two ones E_0^b and E_1^b. On the other hand, $\Im E^a$ is always negative when $0.65 < \theta < 0.78$. As argued above, the latter eigenvalues become real when crossing the continuum threshold $\Re E = 2J$ and the rate of convergence of the Rayleigh–Ritz method becomes remarkably small about such point.

There is no doubt that the one-dimensional potential (1) exhibits two kinds of resonances (REB and KLM poles) that the complex-rotation method reveals at two different intervals of rotation angles. What is most interesting is that the RPM yields both sets of eigenvalues as roots of the same Hankel determinants. The only difference is that the KLM poles appear in Hankel determinants of smaller dimension and we can calculate them more accurately when J is relatively small. Exactly the opposite is commonly true for sufficiently large values of J. The RPM yields both sets of eigenvalues because the roots of the Hankel determinants are invariant under complex-rotation of the coordinate. Since the resonances of type a become bound states when they pass from $\Re E^a > 2J$ to $\Re E^a < 2J$ one may interpret them as the usual metastable states and bound states. It only remains to know if the resonances of type b have any useful physical meaning.

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