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The accurate calculation of resonances in multiple-well oscillators

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Abstract
Quantum–mechanical multiple-well oscillators exhibit curious complex eigenvalues that resemble resonances in models with continuum spectra. We discuss a method for the accurate calculation of their real and imaginary parts.

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1. Introduction

Some time ago, Benassi *et al* [1] discussed the occurrence of complex eigenvalues, or 'resonances', in some quantum–mechanical multiple-well oscillators, and calculated them for a particular example. Recently Killingbeck [2] showed that the Hill-series method yields quite accurate results for both the real and imaginary parts of those eigenvalues if one introduces a complex parameter in the exponential factor of the expansion. In principle, one has to tune up this parameter in order to obtain an acceptable rate of convergence. Such 'complexification' of the well-known Hill-series method had been tried successfully before in perturbation and matrix approaches [3–5]. Complexification is a term coined to indicate the use of, for example, a complex frequency in the treatment of a perturbed harmonic oscillator or a complex atomic number in the case of a perturbed Coulomb problem [2–5].

Moiseyev *et al* [6] have already stressed the physical significance of tunnelling rates in bound systems and obtained the corresponding complex eigenvalues by the complex coordinate method.

The Riccati–Padé method (RPM) is known to be suitable for the accurate calculation of bound states and resonances of simple quantum–mechanical models [7–15]. However, it has only been applied to the most commonplace resonances in the continuum spectrum [11–15]. The purpose of this paper is to investigate if the RPM is also a reasonable alternative to the calculation of the unusual kind of resonances considered by Benassi *et al* [1], Killingbeck [2] and Moiseyev *et al* [6].

In section 2 we outline the RPM and in section 3 we apply it to the three-well oscillator treated explicitly by Benassi *et al* [1], Killingbeck [2] and Moiseyev *et al* [6].

2. The Riccati–Padé method (RPM)

In order to make this paper reasonably self-contained, in this section we outline the RPM in a quite general way. Suppose that a solution to the eigenvalue equation

$$\Psi''(x) + [E - V(x)]\Psi(x) = 0 \tag{1}$$

can be expanded in the form

$$\Psi(x) = x^{\alpha} \sum_{j=0}^{\infty} c_j x^{\beta j}, \alpha, \beta > 0. \tag{2}$$

The power-series expansion for the regularized logarithmic derivative

$$f(x) = \frac{\alpha}{x} - \frac{\Psi'(x)}{\Psi(x)} = x^{\beta-1} \sum_{j=0}^{\infty} f_j x^{\beta j} \tag{3}$$

converges in a neighbourhood of $x = 0$ and the coefficients f_j depend on the eigenvalue E. The function $f(x)$ is a solution to the Riccati equation

$$f'(x) - f(x)^2 + \frac{2\alpha}{x} f(x) + V(x) - E - \frac{\alpha(\alpha-1)}{x^2} = 0. \tag{4}$$

Equations (1)–(4) apply to both one-dimensional ($-\infty < x < \infty$) and central–field ($0 \leqslant x < \infty$) models. If $V(x)$ is a parity–invariant one-dimensional potential, then $\alpha = 0$ for even states, $\alpha = 1$ for odd ones, and $\beta = 2$ for both cases. If $\lim_{x\to 0^+} x^2 V(x) = V_{-2} > 0$, then $\alpha(\alpha - 1) = V_{-2} + l(l + 1)$ removes the singularity at origin in the case of a central–field model, where $l = 0, 1, \ldots$ is the angular momentum quantum number. If $V_{-2} = 0$ then $\alpha = l + 1$.

The RPM consists of rewriting the partial sums of the power series (3) as Padé approximants $x^{\beta-1}[N + d/N](z)$, $z = x^{\beta}$, in such a way that

$$[N + d/N](z) = \frac{\sum_{j=0}^{N+d} a_j z^j}{\sum_{j=0}^{N} b_j z^j} = \sum_{j=0}^{2N+d+1} f_j z^j + O(z^{2N+d+2}). \tag{5}$$

In order to satisfy this condition the Hankel determinant H_D^d, with matrix elements $f_{i+j+d+1}, i, j = 0, 1, \ldots, N$, vanishes, where $D = N + 1 = 2, 3, \ldots$ is the determinant dimension, and $d = 0, 1, \ldots$ is the displacement [7–15]. The main assumption of the RPM is that there is a sequence of roots $E^{[D,d]}$ of the Hankel determinants H_D^d that converges towards a given eigenvalue of the Schrödinger equation (1) as D increases [7–15]. For brevity we call it a Hankel sequence.

Note that one obtains the coefficients f_j from the expansion of the Schrödinger equation (1) or the Riccati equation (4) quite easily, and that unlike the Hill-series method [2] the RPM does not require an adjustable complex parameter. Besides, it is not necessary to take into account the boundary conditions explicitly in order to apply the RPM, and, for that reason, the method provides both bound states and resonances simultaneously [7–15].

Table 1. Convergence of a Hankel sequence $E^{[D,0]}$ towards the lowest complex eigenvalue of the oscillator (6) with $g = 0.14$.

D	Re E	Im E
2	0.969 134 740 629 297 932 08	0
3	0.969 129 330 309 521 446 88	0
4	0.969 129 320 292 846 354 48	0
5	0.969 129 320 066 429 612 26	$3.678\,122\,174\,385\,715\,3252 \times 10^{-10}$
6	0.969 129 320 026 472 271 46	$3.399\,032\,623\,412\,755\,0889 \times 10^{-10}$
7	0.969 129 320 027 109 733 79	$3.380\,103\,869\,829\,339\,2418 \times 10^{-10}$
8	0.969 129 320 027 172 890 39	$3.379\,807\,958\,678\,023\,4680 \times 10^{-10}$
9	0.969 129 320 027 175 184 42	$3.379\,809\,314\,340\,721\,2241 \times 10^{-10}$
10	0.969 129 320 027 175 254 09	$3.379\,809\,539\,728\,076\,7486 \times 10^{-10}$
11	0.969 129 320 027 175 256 22	$3.379\,809\,547\,944\,212\,3313 \times 10^{-10}$
12	0.969 129 320 027 175 256 29	$3.379\,809\,548\,121\,929\,5624 \times 10^{-10}$
13	0.969 129 320 027 175 256 29	$3.379\,809\,548\,121\,902\,9216 \times 10^{-10}$
14	0.969 129 320 027 175 256 29	$3.379\,809\,548\,121\,658\,7093 \times 10^{-10}$
15	0.969 129 320 027 175 256 29	$3.379\,809\,548\,121\,643\,5223 \times 10^{-10}$

Table 2. Complex eigenvalue of the oscillator (6) for several values of g.

g	Re $E(g^2)$	Im $E(g^2)$	Im $E(g^2)g^2\exp(1/(2g^2))$
0.08	0.990 256 459 541 506 003 14	$1.169\,94 \times 10^{-32}$	0.636 209 4894
0.09	0.987 617 651 108 347 304 15	$1.286\,236\,98 \times 10^{-25}$	0.670 050 2315
0.10	0.984 641 588 302 858 826 43	$1.351\,393\,026\,0 \times 10^{-20}$	0.700 657 4893
0.12	0.977 634 914 793 235 291 57	$4.353\,012\,537\,903\,1 \times 10^{-14}$	0.753 046 7190
0.14	0.969 129 320 027 175 256 29	$3.379\,809\,548\,121\,64 \times 10^{-10}$	0.794 491 3345
0.16	0.958 969 970 461 692 078 32	$1.061\,900\,173\,295\,9989 \times 10^{-7}$	0.825 349 2417
0.18	0.946 916 040 677 459 323 55	$5.180\,776\,671\,590\,131\,13 \times 10^{-6}$	0.845 308 4682
0.20	0.932 555 715 824 774 521 80	$7.947\,755\,439\,967\,676\,51 \times 10^{-5}$	0.853 071 6514
0.22	0.915 253 547 480 342 082 73	$5.702\,530\,659\,142\,961\,41 \times 10^{-4}$	0.846 108 8416
0.24	0.894 420 553 209 914 524 96	$2.424\,632\,840\,047\,890\,532 \times 10^{-3}$	0.822 215 8493
0.26	0.870 115 311 574 305 392 25	$7.104\,058\,338\,260\,953\,225 \times 10^{-3}$	0.782 871 5436
0.28	0.843 334 423 923 420 604 12	$1.591\,585\,946\,525\,020\,6010 \times 10^{-2}$	0.734 313 2667
0.30	0.815 607 958 147 339 142 93	$2.940\,021\,689\,215\,348\,5663 \times 10^{-2}$	0.684 447 5376

3. Results and discussion

In what follows we apply the RPM to calculate the curious complex eigenvalue of the triple-well oscillator

$$V(x) = x^2 - 2g^2x^4 + g^4x^6 \tag{6}$$

reported by Benassi *et al* [1], Killingbeck [2], and Moiseyev *et al* [6]. In this case $\beta = 2$ and we choose $\alpha = 0$ for even states as discussed above.

Table 1 shows a Hankel sequence $E^{[D,0]}$ that converges towards the lowest complex eigenvalue when $g = 0.14$. We have kept twenty digits in all entries in order to show how they become stable as D increases. Note the remarkable rate of convergence of the Hankel sequence for both the real and imaginary parts of the eigenvalue.

Table 2 shows the same complex eigenvalue for a range of g-values somewhat wider than those chosen by Benassi *et al* [1] and Killingbeck [2]. We have truncated the results, obtained

Table 3. Lowest resonance of the oscillator (7) for several values of g.

g	Re $E(g^2)$	Im $E(g^2)$	Im $E(g^2)g\exp(1/(3g^2))$
0.08	0.990 173 151 545 681 050 30	$4.666\,679\,51 \times 10^{-22}$	1.554 541 174
0.09	0.987 481 055 483 085 332 16	$2.301\,473\,6620 \times 10^{-17}$	1.543 296 673
0.10	0.984 427 669 765 255 400 84	$5.109\,394\,888\,3947 \times 10^{-14}$	1.530 566 484
0.12	0.977 160 201 918 415 512 16	$1.106\,368\,021\,386\,1671 \times 10^{-9}$	1.500 354 438
0.14	0.968 164 247 842 059 635 13	$4.297\,124\,100\,601\,175\,228 \times 10^{-7}$	1.463 074 727
0.16	0.957 085 006 539 887 060 61	$1.960\,687\,029\,352\,410\,0682 \times 10^{-5}$	1.417 112 487
0.18	0.943 282 187 993 810 381 66	$2.569\,986\,483\,605\,579\,7687 \times 10^{-4}$	1.359 106 75
0.20	0.925 942 461 073 143 182 52	$1.544\,022\,124\,320\,492\,5966 \times 10^{-3}$	1.284 707 315
0.22	0.904 825 085 519 859 510 67	$5.539\,501\,705\,857\,366\,0278 \times 10^{-3}$	1.193 719 284
0.24	0.880 930 111 973 863 668 07	$1.397\,847\,527\,942\,315\,4843 \times 10^{-2}$	1.093 828 654
0.26	0.856 133 537 632 951 427 44	$2.767\,004\,146\,177\,769\,213 \times 10^{-2}$	0.996 493 9951
0.28	0.832 259 899 857 693 637 26	$4.630\,061\,197\,106\,582\,3176 \times 10^{-2}$	0.910 405 5713
0.30	0.810 527 122 179 393 643 97	$6.890\,850\,364\,683\,767\,0242 \times 10^{-2}$	0.839 251 556

Table 4. Convergence of a Hankel sequence $E^{[D,0]}$ towards a real eigenvalue of the oscillator (6) with $g = 0.26$.

D	$E^{[D,0]}$	$E^{[D,1]}$
10	0.824 217 387 531 934 403 91	0.864 108 603 418 729 767 00
11	0.862 935 251 616 532 668 46	0.863 277 048 954 784 210 38
12	0.863 370 278 875 450 570 47	0.863 402 783 728 829 744 35
13	0.863 388 498 890 448 050 32	0.863 387 461 265 452 994 57
14	0.863 388 230 920 394 730 97	0.863 389 276 120 953 456 65
15	0.863 389 022 498 964 652 99	0.863 389 071 537 399 266 67
16	0.863 389 237 523 142 759 41	0.863 389 093 648 338 163 63
17	0.863 389 089 809 862 178 46	0.863 389 091 349 792 846 91
18	0.863 389 091 840 163 698 55	0.863 389 091 580 357 757 25
19	0.863 389 091 538 823 669 76	0.863 389 091 557 979 621 68
20	0.863 389 091 562 044 626 24	0.863 389 091 560 086 318 82

from Hankel determinants with $D \leqslant 15$ and $d = 0$, to the apparently last stable digit. The first digits of our results agree with those given by Benassi *et al* [1] and Killingbeck [2]. We note that Im $E(g^2)g^2\exp(1/(2g^2))$ does not seem to approach a constant for those values of g. It may be that Im $E(g^2)$ attains the WKB asymptotics [1] at smaller values of g.

It is interesting to compare the strange resonance of the potential (6) with the more commonplace one of the potential

$$V_2(x) = x^2 - 2g^2x^4 \tag{7}$$

that was treated earlier by means of the RPM [11]. Table 3 shows the lowest resonance for this model for the same values of g considered before. We appreciate that the imaginary part of this resonance is considerably greater than the previous one and that it seems to approach the WKB asymptotics Im $E^{WKB}(g^2) = [4/(2\pi g^2)]\exp(-1/[3g^2])$ somewhat faster.

The Hankel determinants are polynomial functions of E and their real roots give rise to sequences that converge towards bound-state eigenvalues. Table 4 shows a real sequence that converges towards the bound-state eigenvalue close to the complex one discussed above. The rate of convergence of the real Hankel sequences decreases as g decreases and the real an complex eigenvalue approach each other. Our calculations suggest that the rate of convergence is always greater for the complex eigenvalue. We calculated the real roots for the same values of g shown in table 2. For $g \leqslant 0.16$ the Hankel sequences seem to appear at $D > 20$.

The results of this paper clearly show that the RPM is suitable for the calculation of both real and complex eigenvalues of simple Hamiltonian operators, even in the case of quite small imaginary parts. We believe that this approach is a most useful tool in the numerical investigation of a wide variety of eigenvalue problems. Its main advantages are as follows: great rate of convergence and simple straightforward application that does not require adjustable parameters or explicit consideration of boundary conditions. From a purely practical point of view, we do not believe that the RPM is more efficient than the Hill-series method [2–5], but in our opinion the former approach is interesting by itself because of its most singular features, some of which have already been outlined above.

Present method is not restricted to the Schrödinger equation. We have recently applied a variant of the RPM, which we may call Padé–Hankel method, to nonlinear two-point boundary value problems, obtaining very accurate results for the unknown parameters in several models of physical interest [17].

Finally, we mention that the complex rotation of the coordinate [6] is more general than both the Hill series [2–5] and present RPM which are in principle restricted to separable models.

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