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

\[ \Psi''(x) + (E - V(x))\Psi(x) = 0 \]  

can be expanded in the form

\[ \Psi(x) = x^\alpha \sum_{j=0}^{\infty} c_j x^{\beta j}, \alpha, \beta > 0. \]  

The power-series expansion for the regularized logarithmic derivative

\[ f(x) = \frac{x^\beta - 1}{x^\beta - 1} \sum_{j=0}^{\infty} f_j x^{\beta j} \]  

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

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

Equations (1)–(4) apply to both one-dimensional \(( -\infty < x < \infty )\) and central–field \((0 \leq x < \infty)\) 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

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

In order to satisfy this condition the Hankel determinant \( H_{D,d}^D \), with matrix elements \( f_{j+sD+1}, j = 0, 1, \ldots, N_d \), 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 \( H_{D,d}^D \) 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   | 0.969 134 740 629 297 932 080 | 0            |
| 3   | 0.969 129 330 309 521 446 880 | 0            |
| 4   | 0.969 129 320 292 846 354 480 | 0            |
| 5   | 0.969 129 320 066 429 612 260 | 3.678 122 174 385 715 325 297 932 080 × 10^{-10} |
| 6   | 0.969 129 320 026 472 271 460 | 3.399 032 623 412 755 089 9 × 10^{-10} |
| 7   | 0.969 129 320 027 109 733 790 | 3.380 103 869 829 339 241 8 × 10^{-10} |
| 8   | 0.969 129 320 027 172 890 390 | 3.379 809 548 121 643 522 3 × 10^{-10} |
| 9   | 0.969 129 320 027 175 184 420 | 3.379 809 548 121 929 921 9 × 10^{-10} |
| 10  | 0.969 129 320 027 175 254 090 | 3.379 809 548 121 902 921 6 × 10^{-10} |
| 11  | 0.969 129 320 027 175 256 290 | 3.379 809 548 121 634 522 3 × 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 $E(g^2)g^4 \exp(1/(2g^2))$ |
|------|-------------|-------------|--------------------------------|
| 0.08 | 0.990 256 459 541 506 003 14 | 1.169 94 × 10^{-32} | 0.636 209 4894 |
| 0.09 | 0.987 617 651 108 347 304 15 | 1.286 236 98 × 10^{-25} | 0.670 050 2315 |
| 0.10 | 0.984 641 588 302 858 826 43 | 1.351 393 026 0 × 10^{-20} | 0.700 657 4893 |
| 0.12 | 0.977 634 914 793 235 291 57 | 4.353 012 537 903 1 × 10^{-14} | 0.753 046 7190 |
| 0.14 | 0.969 129 320 027 175 256 29 | 3.379 809 548 121 64 × 10^{-10} | 0.794 491 3345 |
| 0.16 | 0.958 969 970 461 692 078 32 | 1.061 900 173 295 989 898 × 10^{-7} | 0.825 349 2417 |
| 0.18 | 0.946 916 040 677 459 323 55 | 5.180 776 671 590 131 13 × 10^{-6} | 0.845 308 4682 |
| 0.20 | 0.932 555 715 824 774 521 80 | 7.947 755 439 967 676 51 × 10^{-5} | 0.853 071 6514 |
| 0.22 | 0.915 253 547 480 342 082 73 | 7.502 530 659 142 961 41 × 10^{-4} | 0.846 108 8416 |
| 0.24 | 0.894 200 533 209 914 524 96 | 2.424 632 840 047 890 532 × 10^{-3} | 0.822 215 8493 |
| 0.26 | 0.870 115 311 574 305 392 25 | 7.104 058 338 260 953 225 × 10^{-3} | 0.782 871 5436 |
| 0.28 | 0.843 334 423 923 420 604 12 | 1.591 585 946 525 020 601 0 × 10^{-2} | 0.734 313 2667 |
| 0.30 | 0.815 607 958 147 339 142 93 | 2.940 021 689 215 348 566 3 × 10^{-2} | 0.684 447 5576 |

3. Results and discussion

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

$$V(x) = x^2 - 2g^2 x^4 + g^4 x^6$$

reported by Benassi et al \cite{1}, Killingbeck \cite{2}, and Moiseyev et al \cite{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 \cite{1} and Killingbeck \cite{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     | 2.301 473 662 $\times 10^{-17}$  | 1.543 296 673               |
| 0.10 | 0.984 427 669 765 255 400 84     | 5.109 394 888 394 $\times 10^{-14}$ | 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     | 1.561 870 293 524 410 068 2 $\times 10^{-5}$ | 1.417 112 487         |
| 0.18 | 0.943 282 187 993 810 381 66     | 2.569 986 483 605 579 768 7 $\times 10^{-4}$ | 1.359 106 75         |
| 0.20 | 0.925 942 461 073 143 182 52     | 1.544 022 124 320 492 966 $\times 10^{-3}$ | 1.284 707 315        |
| 0.22 | 0.904 825 085 519 859 510 67     | 5.539 501 705 857 366 027 8 $\times 10^{-3}$ | 1.193 719 284       |
| 0.24 | 0.880 930 111 973 863 668 07     | 1.397 847 527 942 315 484 7  $\times 10^{-2}$ | 1.093 828 654         |
| 0.26 | 0.856 133 537 632 951 427 44     | 2.767 004 146 177 769 213 $\times 10^{-2}$ | 0.996 493 995         |
| 0.28 | 0.832 259 999 857 693 637 26     | 4.630 061 197 106 882 317 6 $\times 10^{-2}$ | 0.891 045 571         |
| 0.30 | 0.810 527 122 179 393 643 97     | 6.890 850 364 683 767 024 $\times 10^{-2}$ | 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 | 0.863 389 091 648 338 163 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 $D \leq 15$ 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 $\text{Im } E(g^2)g^2 \exp(1/(2g^2))$ does not seem to approach a constant for those values of $g$. It may be that $\text{Im } E(g^2)$ 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 $V_2(x) = x^2 - 2g^2 x^4$ (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 $\text{Im } E^{WKB}(g^2) = [4/(2\pi g^2)] \exp(-1/(3g^2))$ 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 and 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 \( g \leq 0.16 \) 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.

References

[1] Benassi L, Graffi S and Grecchi V 1979 Phys. Lett. B 82 229
[2] Killingbeck J P 2007 J. Phys. A: Math. Theor. 40 9017
[3] Killingbeck J P, Grosjean A and Jolicard G 2004 J. Phys. A: Math. Gen. 37 7971
[4] Killingbeck J P, Grosjean A and Jolicard G 2005 J. Phys. A: Math. Gen. 38 L695
[5] Killingbeck J P, Grosjean A and Jolicard G 2006 J. Phys. A: Math. Gen. 39 L547
[6] Moiseyev N, Lipkin N, Farrelly D, Atabek O and Lefebvre R 1989 J. Chem. Phys. 91 6246
[7] Fernández F M, Ma Q and Tipping R H 1989 Phys. Rev. A 39 1605
[8] Fernández F M, Ma Q and Tipping R H 1989 Phys. Rev. A 40 6149
[9] Fernández F M 1992 Phys. Lett. A 166 173
[10] Fernández F M and Guardiola R 1993 J. Phys. A: Math. Gen. 26 7169
[11] Fernández F M 1995 J. Phys. A: Math. Gen. 28 4043
[12] Fernández F M 1995 Phys. Lett. A 203 275
[13] Fernández F M 1996 J. Phys. A: Math. Gen. 29 3167
[14] Fernández F M 1996 Phys. Rev. A 54 1206
[15] Fernández F M 1997 Chem. Phys. Lett 281 337
[16] Bender C M and Wu T T 1973 Phys. Rev. D 7 1620
[17] Amore P and Fernández F M 2007 Rational Approximation for Two-Point Boundary Value Problems Preprint 0705.3862