IOPscience iopscience.iop.org

Home Search Collections Journals About Contact us My IOPscience

Eigenvalues from power-series expansions: an alternative approach

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

2009 J. Phys. A: Math. Theor. 42 075201

(http://iopscience.iop.org/1751-8121/42/7/075201)

View the table of contents for this issue, or go to the journal homepage for more

Download details:
IP Address: 171.66.16.156
The article was downloaded on 03/06/2010 at 08:30

Please note that terms and conditions apply.

IOP PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND THEORETICAL

J. Phys. A: Math. Theor. **42** (2009) 075201 (8pp) doi:10.1088/1751-8113/42/7/075201

Eigenvalues from power-series expansions: an alternative approach

Paolo Amore[1] **and Francisco M Fernández**[2,3]

[1] Facultad de Ciencias, Universidad de Colima, Bernal Díaz del Castillo 340, Colima, Colima, Mexico
[2] INIFTA (UNLP, CCT La Plata-CONICET), División Química Teórica, Diag. 113 y 64 (S/N), Sucursal 4, Casilla de Correo 16, 1900 La Plata, Argentina

E-mail: paolo.amore@gmail.com and fernande@quimica.unlp.edu.ar

Received 22 September 2008, in final form 8 December 2008
Published 21 January 2009
Online at stacks.iop.org/JPhysA/42/075201

Abstract
An appropriate rational approximation to the eigenfunction of the Schrödinger equation for anharmonic oscillators enables one to obtain the eigenvalue accurately as the limit of a sequence of roots of Hankel determinants. The convergence rate of this approach is greater than that for a well-established method based on power-series expansions weighted by a Gaussian factor with an adjustable parameter (the so-called Hill-determinant method).

PACS number: 03.65.Ge

1. Introduction

Power-series methods have proved to yield remarkably accurate eigenvalues of simple one-dimensional and central-field quantum-mechanical models [1–11]. There are basically two different approaches: on the one hand, the use of Dirichlet boundary conditions at the endpoints of a sufficiently wide interval [4, 10], on the other, the Hill-determinant method and its variants [1–9, 11]. In this paper we focus our attention on the latter that has been applied to a wide variety of problems, including the vibration–rotation spectra of diatomic molecules [5, 6, 8]. The success of this method commonly depends on the weight function which in many cases is an exponential function with a width parameter that affects the rate of convergence of the approach [1–3].

The purpose of this paper is to discuss an alternative approach that is less dependent on the width parameter or scaling factor. In section 2 we outline a well-known weighted power-series method. In section 3 we develop an alternative approach based on a rational approximation to that power series approach. In section 4 we apply both approaches to the pure quartic

[3] Author to whom any correspondence should be addressed.

 © 2009 IOP Publishing Ltd Printed in the UK

anharmonic oscillator. In section 5 we consider a rational potential with a singular point on the complex coordinate plane. Finally, in section 6 we draw conclusions.

2. Weighted power-series method

Consider the Schrödinger equation

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

where the potential-energy function $V(x)$ can be expanded as

$$V(x) = \sum_{j=1}^{\infty} v_j x^{2j} \tag{2}$$

A well-known approach for the calculation of eigenvalues and eigenfunctions is based on the ansatz

$$\psi(x) = \mathrm{e}^{-ax^2} \sum_{j=0}^{\infty} c_j x^{2j+s}, \tag{3}$$

where $s = 0$ or $s = 1$ for even or odd states, respectively. If this expansion satisfies the Schrödinger equation (1), then the coefficients c_j are polynomial functions of the energy E. It has been shown [1–3] that one can obtain the allowed energies (those consistent with square-integrable solutions) from the roots of

$$c_M(E) = 0, \qquad M = M_0, M_0 + 1, \ldots. \tag{4}$$

The rate of convergence of the sequence of roots $E^{[M]}$ of this equation depends on the adjustable parameter a. If its value is far from optimal, the sequences may not converge at all.

3. The Hankel–Padé method

The Riccati–Padé method is based on a rational approximation to the logarithmic derivative of the eigenfunction $f(x) = s/x - \psi'(x)/\psi(x)$ [12, 13]. An appropriate truncation condition determines the allowed energies to be the roots of Hankel determinants [12, 13]. The convergence rate of the sequences of such roots is remarkable and provides accurate eigenvalues with Hankel determinants of relatively small dimension.

Here we explore an alternative approach based on a rational approximation to $x^{-s}\psi(x)\,\mathrm{e}^{ax^2}$

$$\frac{\sum_{j=0}^{N+d} a_j x^{2j}}{\sum_{j=0}^{N} b_j x^{2j}} = \sum_{j=0}^{2N+d+1} c_j x^{2j}. \tag{5}$$

Note that we require that the Padé approximant with just $2N + d + 1$ adjustable parameters yields $2N + d + 2$ coefficients of the power series (3). As in the case of the Riccati–Padé method [12, 13] it leads to a quantization condition for the energy given by the roots of the Hankel determinants

$$H_D^d(E) = |c_{i+j+d-1}(E)|_{i,j=1}^{D} = 0 \tag{6}$$

where $D = N + 1 = 2, 3, \ldots$ and $d = 0, 1, \ldots$

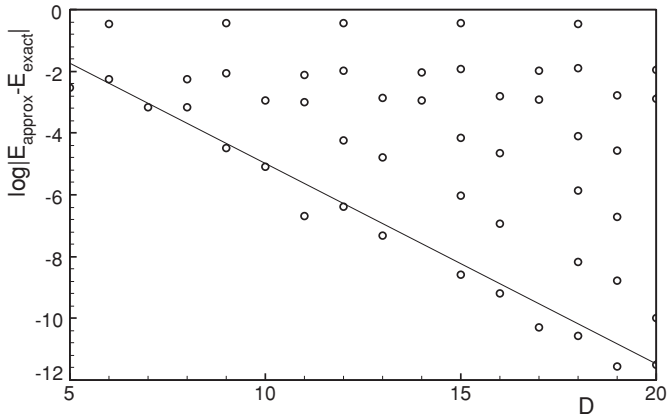

Figure 1. Sequences of roots of $H_D^d(E) = 0$ for the lowest eigenvalue of the quartic anharmonic oscillator (7) when $a = 0$

4. Anharmonic oscillator

As an example consider the anharmonic oscillator

$$V(x) = x^4 \tag{7}$$

The first coefficients are

$$c_1 = a - \frac{E}{2} \qquad c_2 = \frac{a^2}{2} - \frac{Ea}{2} + \frac{E^2}{24} \tag{8}$$

and the first Hankel determinant is

$$H_2^0 = \frac{a}{30} - \frac{a^4}{12} - \frac{E}{60} + \frac{Ea^3}{6} - \frac{E^2a^2}{8} + \frac{7E^3a}{360} - \frac{E^4}{960}. \tag{9}$$

Figure 1 shows several sequences of roots of $H_D^0(E) = 0$ when $a = 0$. We appreciate that the phenomenon of multiple converging sequences of roots present in the RPM [12, 13] also appears in this case. It seems to be related to the Hankel determinant and to the rational approximation (either to the logarithmic derivative or to just a factor of the wavefunction). A straight line in figure 1 marks the sequence with the best convergence rate. One obtains similar sequences for other values of a. Note that the standard method (4) [1–3] does not apply to the case $a = 0$.

Figure 2 shows the logarithmic error $\log|E_{\text{approx}} - E_{\text{exact}}|$ of the sequences of roots of $H_D^0(E) = 0$ and $c_M(E) = 0$ for $a = 1$ in terms of the number of coefficients $M = 2D - 1$ required by the calculation. Straight lines show the overall trend of the logarithmic sequences. We appreciate that the Hankel sequence converges faster than the one for the standard approach. The 'exact' result $E_{\text{exact}} = 1.060\,362\,090\,484\,182\,8996$ is simply a more accurate estimate of the eigenvalue provided by the RPM [12, 13].

Figure 3 shows the variation of the logarithmic error of the roots of $c_M(E) = 0$ with a for three values of M. We appreciate that the optimal value of the adjustable parameter for the quartic oscillator (7) is about $a \approx 2.5$.

It is not necessary to have the 'exact' energy in order to estimate an optimal value of the adjustable parameter. If $E_n^{[k]}$ is the approximation of order k to the nth eigenvalue, we simply monitor the convergence of the sequence in terms of, for example, $\log\left|E_n^{[k+1]} - E_n^{[k]}\right|$, where $k = k_0, k_0 + 1, \ldots$.

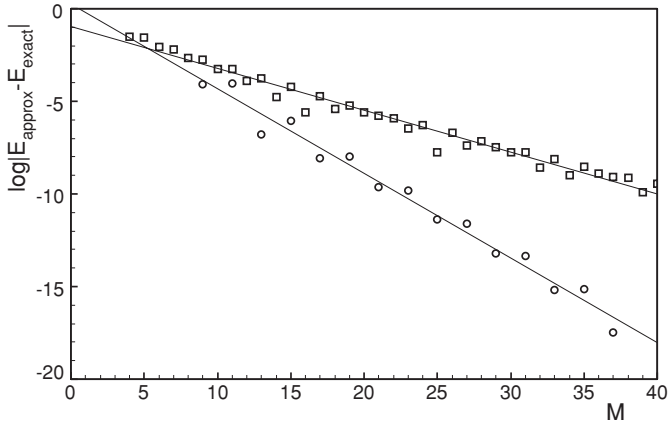

Figure 2. Sequences of roots of $H_D^d(E) = 0$ (circles) and $c_M(E) = 0$ (squares), $M = 2D - 1$, for the lowest eigenvalue of the quartic anharmonic oscillator (7) when $a = 1$

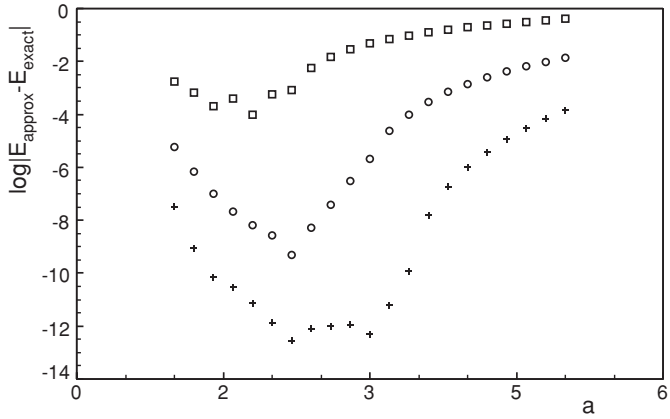

Figure 3. Logarithmic error of the roots of $c_M(E) = 0$ as function of a for $M = 9$ (squares), $M = 19$ (circles) and $M = 29$ (crosses) for the lowest eigenvalue of the quartic anharmonic oscillator (7)

5. Rational potential

Both the straightforward power-series method and the Hankel–Padé approach apply successfully to polynomial potentials as illustrated in the preceding section by means of a simple nontrivial example. In what follows we consider the rational potential

$$V(x) = x^2 + \lambda x^2/(1 + gx^2), \qquad -\infty < \lambda < \infty, \quad g > 0 \tag{10}$$

that has been studied by several authors', [14–57]. Among the approaches applied to this model we mention perturbation theory [15, 22, 24, 30, 52], including the $1/N$ expansion [38, 42, 43], variational methods [14, 16, 34, 55, 57], and in particular the Rayleigh–Ritz method [14, 34, 55, 57]. One can easily obtain exact solutions to the Schrödinger equation with the potential (10) for some values of the parameters λ and g [17, 19–23, 25–28, 35, 37, 39, 41, 43–49, 51, 57] that prove suitable for testing approximate methods.

Table 1. Hankel–Padé estimate of the ground-state eigenvalue of the Schrödinger equation with the rational potential (10) for $\lambda = 1$.

D	$g = 0.1$	$g = 0.2$	$g = 1$
2	1.385	1.353 120	1.21
3	1.380 525	1.353 123	1.23
4	1.380 5318	1.352 9481	1.232
5	1.380 5322	1.352 9489	1.2323
6	1.380 531 81	1.352 948 023	1.232 34
7	1.380 531 800 9377	1.352 952	1.232 348
8	1.380 531 800 938 043	1.352 948 022 755	1.232 3502
9	1.380 531 800 938 0452	1.352 948 037 359	1.232 3506
10	1.380 531 800 938 045 232	1.352 948 022 753 577	1.232 350 69
11	1.380 531 800 938 045 2345	1.352 948 022 753 566	1.232 350 72
12	1.380 531 800 938 045 2344	1.352 948 022 753 570 88	1.232 350 721
13	1.380 531 800 938 045 2344	1.352 948 022 753 570 81	1.232 350 723
14		1.352 948 022 753 570 8289	1.232 350 7233
15		1.352 948 022 753 570 8284	1.232 350 723 37
16		1.352 948 022 753 570 8285	1.232 350 723 39
17		1.352 948 022 753 570 8284	1.232 350 723 403
18		1.352 948 022 753 570 8284	1.232 350 723 405
19			1.232 350 723 4057
20			1.232 350 723 405 95
21			1.232 350 723 406 02
22			1.232 350 723 406 047
23			1.232 350 723 406 054
24			1.232 350 723 406 0566
25			1.232 350 723 406 0574

The power series (2) converges only for $|x| < |x_g|$, where $x_g = \pm \mathrm{i}/\sqrt{g}$ are the two poles of the potential-energy function on the imaginary axis of the complex x-plane. If $g \ll 1$ the eigenfunction is negligible for $|x| > |x_g|$ and the Hill-determinant method may yield reasonable results for the lowest energies and only after judicious truncation of the sequences of roots [5]. On the other hand, the expansion of the wavefunction in a power series of the variable $u = x^2/(1 + gx^2)$ leads to a successful approach for all values of g and λ [50].

Since the Hankel–Padé method is based on a rational approximation to the wavefunction, one expects that it takes into account the singularities properly, succeeding even for moderate values of g. In what follows we compare it with the weighted power-series method (3). First of all, note that $V(x)/x^2 \to 1$ as $|x| \to \infty$ so that we expect $a = 1/2$ to be optimal [3] and choose this width-parameter value from now on. We have verified that the Hankel–Padé approach yields reasonable results for other values of a such as, for example, $a = 0$, $a = 1$ and $a = 3/2$.

Table 1 shows the results of the Hankel–Padé calculation of the ground-state eigenvalue of the Schrödinger equation (1) with the rational potential (10) for $\lambda = 1$ and three values of g. Note that present Hankel–Padé results are more accurate than those obtained earlier by means of the Rayleigh–Ritz variational method [14], and comparable to those provided by a kind of iterative solution of the Rayleigh–Ritz secular equation with an adjustable parameter [34]. There are much more accurate results in the literature; for example, Stubbins and Gornstein [55] obtained $E_0 = 1.380\,531\,800\,938\,045\,234\,389\,950\,060\,09$ and $E_0 = 1.232\,350\,723\,406\,057\,813\,862\,069\,958\,68$ for $g = 0.1$ and $g = 1$, respectively.

Table 2. Hill-determinant estimate of the ground-state eigenvalue of the Schrödinger equation with the rational potential (10) for $\lambda = 1$.

M	$g = 0.1$	$g = 0.2$
2	1.59	1.59
3	1.32	1.26
4	1.41	1.43
5	1.37	1.30
6	1.389	1.42
7	1.375	1.29
8	1.385	1.46
9	1.377	1.22
10	1.384	1.82
11	1.377	1.03
12	1.384	
13	1.376	
14	1.386	
15	1.373	
16	1.391	
17	1.364	
18	1.409	
19	1.337	
20	1.48	
21	1.25	

Table 2 shows results from the Hill-determinant method. A lack of entry means that we did not find any root in the interval $0.5 < E < 1.5$. Note that while the Hankel–Padé approach converges smoothly the Hill-determinant method does not, even for $g = 0.1$. Besides, the latter approach does not give any reasonable result for $g = 1$. For $g = 0.1$ the roots of the Hill-determinant oscillate about the exact eigenvalue, giving the tightest bounds for $9 \leqslant M \leqslant 12$, before the sequence begins to diverge. Averaging the roots for $M = 10$ and $M = 11$ one estimates $E_0 = 1.380\,531\,81$ that is quite close to the exact eigenvalue. However, this strategy is only practical for sufficiently small values of g as discussed above. We have thus verified our earlier supposition that the Hankel–Padé method should correct a possible failure of the power-series approach caused by singular points of the potential-energy function in the complex coordinate plane.

6. Further comments and conclusions

Clearly, the results of the preceding sections show that

- The sequence of roots of the Hankel determinants (6) converges more smoothly than the sequence of roots of equation (4) for polynomial potentials.
- The rate of convergence of the sequence of roots of the Hankel determinants (6) is not so strongly dependent on the value of a as the sequence of roots of the standard approach (4). In fact, the former converges where the latter does not (even when $a = 0$).
- The Hankel–Padé method is preferable for the treatment of potential-energy functions with singularities in the complex coordinate plane that limit seriously the range of applicability of the power series.
- However, from a purely practical point of view it is worth noticing that when both approaches are successful, the calculation of the roots of the Hankel determinants typically requires more CPU time.

- There is more than one sequence of roots of the Hankel determinant (6) that converges towards a given eigenvalue. Present approach shares this curious phenomenon with the RPM [12, 13] and appears to be a feature of the Hankel determinants constructed from the coefficients of the power series coming from either the Riccati equation or the Schrödinger one.

The Schrödinger equation with the simple potential-energy functions discussed above can easily be treated by means of the Rayleigh–Ritz variational method and the basis set of eigenfunctions $\{\phi_n\}$ of the harmonic oscillator $\hat{H} = \hat{p}^2 + \omega^2 x^2$, where ω is an adjustable parameter. The problem reduces to the diagonalization of the Hamiltonian matrix **H** with elements $H_{ij} = \langle \phi_i | \hat{H} | \phi_j \rangle$. The main advantage of this approach is that it provides upper bounds to all the eigenvalues [14, 34, 55, 57]. Besides, in some cases $H_{ij} = 0$ for all $|i-j| > k$, and the resulting secular equation with a band matrix can be treated as a recurrence relation. In this way one does not have to diagonalize a large matrix but simply find the roots of a determinant of much smaller constant dimension [58]. This is precisely the case for the simple examples discussed above. However, this variational method may not be practical if the calculation of the matrix elements of the potential-energy function is too difficult. In that case the power-series methods and its variants may be preferable.

References

[1] Banerjee K 1978 *Proc. R. Soc. Lond.* A **364** 265
[2] Banerjee K, Bhatnagar S P, Choudhry V and Kanwal S S 1978 *Proc. R. Soc. Lond.* A **360** 575
[3] Ginsburg C A 1982 *Phys. Rev. Lett.* **48** 839
[4] Killingbeck J P 1983 *Microcomputer Quantum Mechanics* (Bristol, Boston: Adam Hilger Ltd)
[5] Estrín D A, Fernández F M and Castro E A 1987 *J. Chem. Phys.* **87** 7059
[6] Estrín D A, Fernández F M and Castro E A 1988 *J. Mol. Struct. (Theochem)* **166** 257
[7] Estrín D A, Fernández F M and Castro E A 1988 *Phys. Lett.* A **130** 330
[8] Estrín D A, Fernández F M and Castro E A 1990 *J. Math. Chem.* **5** 177
[9] Estrín D A, Fernández F M and Castro E A 1990 *J. Phys. A: Math. Gen.* **23** 2395
[10] Alhendi H A and Lashin E I 2005 *J. Phys. A: Math. Gen.* **38** 6785
[11] Killingbeck J P 2007 *J. Phys. A: Math. Theor.* **40** 2819
[12] Fernández F M, Ma Q and Tipping R H 1989 *Phys. Rev.* A **39** 1605
[13] Fernández F M, Ma Q and Tipping R H 1989 *Phys. Rev.* A **40** 6149
[14] Mitra A K 1978 *J. Math. Phys.* **19** 2018
[15] Kaushal R S 1979 *J. Phys. A: Math. Gen.* **12** L253
[16] Bessis N and Bessis G 1980 *J. Math. Phys.* **21** 2780
[17] Flessas G P 1981 *Phys. Lett.* A **83** 121
[18] Hautot A 1981 *J. Comput. Phys.* **39** 72
[19] Varma V S 1981 *J. Phys. A: Math. Gen.* **14** L489
[20] Flessas G P 1982 *J. Phys. A: Math. Gen.* **15** L97
[21] Heading J 1982 *J. Phys. A: Math. Gen.* **15** 2355
[22] Lai C S and Lin H E 1982 *J. Phys. A: Math. Gen.* **15** 1495
[23] Whiteheadt R R, Watt A, Flessas G P and Nagarajan M A 1982 *J. Phys. A: Math. Gen.* **15** 1217
[24] Bessis N, Bessis G and Hadinger G 1983 *J. Phys. A: Math. Gen.* **16** 497
[25] Chaudhuri R N and Mukherjee B 1983 *J. Phys. A: Math. Gen.* **16** 4031
[26] Heading J 1983 *J. Phys. A: Math. Gen.* **16** 2121
[27] Znojil M 1983 *J. Phys. A: Math. Gen.* **16** 293
[28] Znojil M 1983 *J. Phys. A: Math. Gen.* **16** 279
[29] Cohen M 1984 *J. Phys. A: Math. Gen.* **17** 2345
[30] Znojil M 1984 *J. Phys. A: Math. Gen.* **17** 3441
[31] Fack V and Berghe G V 1985 *J. Phys. A: Math. Gen.* **18** 3355
[32] Handy C R 1985 *J. Phys. A: Math. Gen.* **18** 3593
[33] Marcilhacy G and Pons R 1985 *J. Phys. A: Math. Gen.* **18** 2441
[34] Fack V, De Meyer H and Vanden Berghe G 1986 *J. Math. Phys.* **27** 1340

[35] Blecher M H and Leach P G L 1987 *J. Phys. A: Math. Gen.* **20** 5923
[36] Fack V and Berghe G V 1987 *J. Phys. A: Math. Gen.* **20** 4153
[37] Roy P and Roychoudhury R 1987 *Phys. Lett.* A **122** 275
[38] Varshni Y P 1987 *Phys. Rev.* A **36** 3009
[39] Gallas J A C 1988 *J. Phys. A: Math. Gen.* **21** 3393
[40] Hodgson R J W 1988 *J. Phys. A: Math. Gen.* **21** 1563
[41] Roy P, Roychoudhury R and Varshni Y P 1988 *J. Phys. A: Math. Gen.* **21** 1589
[42] Roy B, Roychoudhury R and Roy P 1988 *J. Phys. A: Math. Gen.* **21** 1579
[43] Scherrer H, Risken H and Leiber T 1988 *Phys. Rev.* A **38** 3949
[44] Berghe G V and Meyer H E D 1989 *J. Phys. A: Math. Gen.* **22** 1705
[45] Bose S K and Varma N 1989 *Phys. Lett.* A **141** 141
[46] Lakhtakia A 1989 *J. Phys. A: Math. Gen.* **22** 1701
[47] Hislop D, Wolfaard M F and Leach P G L 1990 *J. Phys. A: Math. Gen.* **23** L1109
[48] Roy P and Roychoudhury R 1990 *J. Phys. A: Math. Gen.* **23** 1657
[49] Adhikari R, Dutt R and Varshni Y P 1991 *J. Math. Phys.* **32** 447
[50] Fernández F M 1991 *Phys. Lett.* A **160** 116
[51] Pons R and Marcilhacy G 1991 *Phys. Lett.* A **152** 235
[52] Witwit M R M 1991 *J. Phys. A: Math. Gen.* **24** 5291
[53] Agrawal R K and Varma V S 1993 *Phys. Rev.* A **48** 1921
[54] Handy C R, Hayes H, Stephens D V, Joshua J and Summerour S 1993 *J. Phys. A: Math. Gen.* **26** 263
[55] Stubbins C and Gornstein M 1995 *Phys. Lett.* A **202** 34
[56] Ishikawa H 2002 *J. Phys. A: Math. Gen.* **35** 4453
[57] Saad N, Hall R L and Ciftci H 2006 *J. Phys. A: Math. Gen.* **39** 7745
[58] Fernández F M, Ogilvie J F and Tipping R H 1986 *J. Chem. Phys.* **85** 5850