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High-precision calculation of the eigenvalues for the $x^2+\lambda x^2/(1+gx^2)$ potential

R J W Hodgson

Ottawa-Carleton Institute for Physics, University of Ottawa, Ottawa, Ontario, Canada K1N 9B4

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Abstract. An analytic continuation procedure using a Taylor series is used to produce very accurate wavefunctions and eigenvalues for the one-dimensional anharmonic oscillator governed by the potential $V(x)=x^2+\lambda x^2/(1+gx^2)$.

1. Introduction

Considerable interest has centred on analytical and numerical solutions of the one-dimensional Schrödinger equation with the anharmonic potential

$$V(x)=x^2+\lambda x^2/(1+gx^2). \tag{1}$$

Mitra (1978) has pointed out that this potential is related to certain specific models in laser theory (Haken 1970) as well as zero-dimensional field theory (Risken and Vollmer 1967).

A variety of numerical procedures have been employed to obtain the eigenvalues for the ground state and first few excited states for a range of values of λ and g. The Ritz variational method used in combination with the Givens-Householder algorithm was used by Mitra (1978) to determine the ground state and first two excited states. Problems were encountered for large values of g. Kaushal (1979) used perturbation theory for the restricted class having small g and large λ. The potential was expanded under the condition $gx^2<1$. Bessis and Bessis (1980) avoided the numerical quadrature in the approach of Mitra (1978) by expanding in terms of a basis set of harmonic oscillator functions. They obtained eight-digit accuracy for the ground state and first three excited states for λ and g ranging from 0.1 to 500. Lai and Lin (1982) formed the [6, 6] Padé approximants to the energy perturbation series to obtain an accuracy similar to that of Bessis and Bessis (1980). First-order perturbation theory and direct numerical integration were employed in the calculations by Killingbeck (1979) and Garcia and Killingbeck (1979). Fack and Vanden Berghe (1985) used direct numerical integration of the Schrödinger equation by introducing a finite difference representation of $D^2y(x)$. Finally, Handy (1985) has employed the Hankel-Hadamard moment determinant analysis to obtain upper and lower bounds for the ground and first excited states.

Exact solutions to the above problem have also been presented by Flessas (1981, 1982), Varma (1981), Lai and Lin (1982) and Whitehead *et al* (1982). These are obtained under the restrictive conditions $\lambda<0$, $g>0$ and $\lambda=\lambda(g)$, $E=E(g)$.

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In this paper an analytic continuation approach originally introduced by Holubec and Stauffer (1985) is used to obtain the eigenvalues and eigenfunctions for the potential (1) to very high accuracy. Carrying out the computations on a 32-digit precision computer, it is not too difficult to obtain results accurate to this precision.

2. Analytic continuation

The standard Taylor series approach to the solution of a differential equation (DE) with initial values given at z_0 is to approximate the solution in the neighbourhood of z_0 by a truncated Taylor series. The values of the derivatives at z_0 are determined from successive differentiations of the DE. One then proceeds to construct a new Taylor series about $z_1 = z_0 + h$ using the derivatives of the first series. This process continues to generate an analytic continuation of the solution of the DE along the path $\{z_0, z_1, z_2, \ldots\}$. This technique requires successive differentiation of the DE, and becomes restricted if the DE has singularities anywhere in the complex z plane.

Holubec and Stauffer (1985) have proposed a way around this problem based on the idea of analytically continuing a Frobenius series rather than a Taylor series. The method is applied to second-order linear DE with a regular singularity and with analytic coefficients which are finite polynomials. In practice the method works for arbitrary order and for more general analytic coefficients. The technique was originally applied to second-order linear DE of the form

$$u'' + P(z)u' + Q(z)u = 0 \tag{2}$$

with $P(z)$ and $Q(z)$ finite polynomials.

In order to handle the potential (1) we have modified the method of Holubec and Stauffer (1985) so that we can handle a DE of the form

$$u'' + [P(z)/Q(z)]u = 0 \tag{3}$$

or

$$Q(z)u'' + P(z)u = 0. \tag{4}$$

Working with the Schrödinger equation

$$u'' - V(z)u = Eu \tag{5}$$

with $V(z)$ having the form (1), $P(z)$ and $Q(z)$ are both finite polynomials

$$P(z) = E + (Eg - \lambda - 1)z^2 - gz^4 \tag{6}$$

$$Q(z) = 1 + gz^2. \tag{7}$$

Naturally this approach will not work if we are close to points such that $Q(z) = 0$.

The general solution u is expanded in a Taylor series about the point z_0 as

$$u = \sum_{i=0}^{N_t} c_i (z - z_0)^i. \tag{8}$$

The polynomial coefficients $P(z)$ and $Q(z)$ must be expanded in a similar manner:

$$P(z) = \sum_{i=0}^{p} \tilde{P}_i (z - z_0)^i \tag{9}$$

$$Q(z) = \sum_{i=0}^{q} \tilde{Q}_i (z - z_0)^i. \tag{10}$$

By substituting these expansions for u and for P and Q into the DE, and by setting the coefficients of the different powers of $(z-z_0)$ to zero, we arrive at a set of recurrence relations to generate the coefficients c_i.

For the potential form (1) the complete expansions for $P(z)$ and $Q(z)$ become

$$P(z) = E + (Eg - 1 - \lambda)z_0^2 - gz_0^4 + \{2(Eg - 1 - \lambda)z_0 - 4gz_0^3\}(z - z_0) + \{Eg - 1 - \lambda - 6gz_0^2\}(z - z_0)^2 - 4gz_0(z - z_0)^3 - g(z - z_0)^4 \quad (11)$$

$$Q(z) = 1 + gz_0^2 + 2gz_0(z - z_0) + g(z - z_0)^2. \quad (12)$$

These lead to the general recurrence relation for the c_i coefficients,

$$(k+2)(k+1)\tilde{Q}_0 c_{k+2} + (k+1)k\tilde{Q}_1 c_{k+1} + k(k-1)\tilde{Q}_2 c_k + \sum_{i=0}^{4} \tilde{P}_i c_{k-i} = 0 \quad (13)$$

which is valid for $k \geqslant 0$ with the understanding that $c_k = 0$ if $k < 0$. The initial values $c_0 = u(z_0)$ and $c_1 = u'(z_0)$ are used to start the series.

If we start from the origin, we can use the above results with $z_0 = 0$. In the general case a Frobenius series is used, with the appropriate characteristic exponent. For the oscillator problem under examination here, the characteristic exponent is 0, and so the regular Taylor series about $z_0 = 0$ suffices.

3. Results

We have applied the analytic continuation procedure as described to compute the first few eigenvalues with the same boundary condition as employed by Fack and Vanden Berghe (1985), namely that the Dirichlet boundary condition $u(R) = 0$ is imposed with $R = 10.0$. We have also examined the effect of varying R. The eigenvalues are determined by starting at the origin with $z_0 = 0$ and using the Taylor series to compute the values of u and u' at the first step $z = h$. The range for z is subdivided into N_s equal parts, so that $h = R/N_s$. Then z_0 is set to h and the series (8) used to compute u and u' at $2h$. In this way the wavefunction is generated out to $z = R$. All of this is done using an initial guess for the eigenvalue E. The value of E is then adjusted until the value of $u(R)$ is as close to zero as is possible within the precision of the calculations.

In practice we first find two values of E which lie on either side of the correct eigenvalue, such that they produce values for $u(R)$ having opposite signs. We then use the secant method to generate a new guess for E, and repeat the process until we converge on the correct value. The iterates for E are generated using

$$E^{i+1} = E^i - u^i(R)\frac{E^i - E^{i-1}}{u^i(R) - u^{i-1}(R)}. \quad (14)$$

We have found that 7-10 iterations are required on average to achieve the precision presented in the tables.

The initial conditions at $z = 0$ must be chosen properly to produce either even or odd wavefunctions. Wavefunctions with even parity are generated by choosing $u(0) = c$ and $u'(0) = 0$, with c an arbitrary normalisation constant. Odd-parity wavefunctions require the choice of $u(0) = 0$ and $u'(0) = c$. The ground state has even parity and the excited states oscillate between even and odd parity.

The results were also computed for the special case of $\lambda = g = 0$ for which exact eigenvalues are readily obtained ($E_i = 2i - 1$). We found that our results were accurate to the 32-digit precision used in the calculations.

Table 1. Comparison of eigenvalues obtained by various methods: (*a*) present study, (*b*) Fack and Vanden Berghe (1985), (*c*) Mitra (1978), (*d*) Bessis and Bessis (1980), (*e*) Lai and Lin (1982), (*f*) Killingbeck (1979), (*g*) Handy (1985).

		$\lambda = 0.1,\ g = 0.1$
E_1	(*a*)	1.043 173 713 044 445 233 778 700 870 546 1
	(*b*)	1.043 173 71
	(*c*)	1.043 17
	(*d*)	1.043 173 71
	(*e*)	1.043 173 71
	(*f*)	1.043 174 08
	(*g*)	$1.043\ 173\ 71 < E_1 < 1.043\ 173\ 72$
E_2	(*a*)	3.120 081 864 016 152 708 645 886 536 523 5
	(*b*)	3.120 081 86
	(*c*)	3.120 08
	(*d*)	3.120 081 86
	(*e*)	3.120 081 86
	(*g*)	$3.120\ 081\ 864 < E_2 < 3.120\ 081\ 865$
E_3	(*a*)	5.181 094 785 884 700 927 110 409 072 888 3
	(*b*)	5.181 094 78
	(*c*)	5.181 09
	(*d*)	5.181 094 79
	(*e*)	5.181 094 79
	(*f*)	5.181 095 06
E_4	(*a*)	7.231 009 980 655 889 245 108 368 931 495 1
	(*b*)	7.231 009 95
	(*d*)	7.231 009 98
	(*e*)	7.231 009 98
E_5	(*a*)	9.272 816 970 035 252 254 582 438 478 906 5
	(*b*)	9.272 816 91
	(*f*)	9.272 818

Tables 1-6 present our results for seven sets of λ, g values, and compare them with calculations of other authors. In all of the computations N_r was set to 40, as we found that this value was better than required to obtain the precision desired. The value of N_s had to be varied in order to adjust the step size small enough to obtain this accuracy. For values of λ and $g \leqslant 10$, values of N_s in the range 80-100 were sufficient, whereas this had to be increased to 200-300 for those cases where $g = 100$. Even with this choice, the results for $g = 100$ are only accurate to 21-24 digits instead of the 32 obtained in the other cases. Higher precision requires larger N_s, more iterations and longer computation times.

As can be seen from tables 1-6, our results demonstrate that the calculations carried out by the other authors are in general quite good but there are some deficiences. In the cases where comparisons can be made, the results of Killingbeck (1979) are inaccurate in the last few digits. The results obtained by Fack and Vanden Berghe (1985) are accurate to nine places for the lowest eigenvalues, but tend to be less accurate for E_4 and E_5. Their results for the $\lambda = 100$ cases, however, are not as accurate as those obtained by others. The results obtained by Mitra (1978), Bessis and Bessis (1980) and Lai and Lin (1982) are generally good to the accuracy quoted, but most did not compute the higher eigenvalues. The upper and lower bounds computed by

Table 2. Eigenvalues (same format as in table 1).

		$\lambda = 0.1,\ g = 100.0$
E_1	(*a*)	1.000 841 102 403 452 905 18
	(*b*)	1.000 841 10
	(*c*)	1.000 84
	(*d*)	1.000 841 1
	(*f*)	1.000 841 43
E_2	(*a*)	3.000 983 177 778 238 663 773 08
	(*b*)	3.000 983 18
	(*c*)	3.000 98
	(*d*)	3.000 983 1
E_3	(*a*)	5.000 927 544 679 517 518 352
	(*b*)	5.000 927 54
	(*c*)	5.000 93
	(*d*)	5.000 925 7
	(*f*)	5.000 927 8
E_4	(*a*)	7.000 984 495 836 019 294 564 67
	(*b*)	7.000 984 47
	(*d*)	7.000 984 5
E_5	(*a*)	9.000 948 590 765 685 440 341
	(*b*)	9.000 948 53
	(*f*)	9.000 948

Table 3. Eigenvalues (same format as in table 1).

		$\lambda = 100.0,\ g = 0.1$
E_1	(*a*)	9.976 180 087 723 021 055 029 793 333 903 4
	(*b*)	9.976 178 31
	(*c*)	9.976 18
	(*d*)	9.976 180 09
	(*e*)	9.976 180 09
	(*f*)	9.976 180
	(*g*)	$9.976\ 180\ 07 < E_1 < 9.976\ 180\ 12$
E_2	(*a*)	29.781 191 110 776 574 481 828 222 255 353
	(*b*)	29.781 175 75
	(*c*)	29.781 19
	(*d*)	29.781 191 1
	(*e*)	29.781 191 11
	(*g*)	$29.781\ 191\ 10 < E_2 < 29.781\ 191\ 13$
E_3	(*a*)	49.292 690 504 626 860 802 043 097 677 054
	(*b*)	49.292 623 58
	(*c*)	49.292 69
	(*d*)	49.292 690 5
	(*e*)	49.292 690 50
	(*f*)	49.292 69
E_4	(*a*)	68.513 062 234 511 134 635 185 514 093 924
	(*b*)	68.512 861 08
	(*d*)	68.513 052 2
	(*e*)	68.513 062 23
E_5	(*a*)	87.444 711 409 977 161 062 121 962 028 609
	(*b*)	87.444 233 67
	(*f*)	87.444 7

Table 4. Eigenvalues (same format as in table 1).

		$\lambda = 100.0,\ g = 100.0$
E_1	(*a*)	1.836 335 833 448 218 317 117 92
	(*b*)	1.836 334 44
	(*c*)	1.836 4
	(*d*)	1.836 385 0
	(*f*)	1.836 337 3
E_2	(*a*)	3.983 098 339 487 812 876 056 641 094 2
	(*b*)	3.983 098 36
	(*c*)	3.983 1
	(*d*)	3.983 099 2
E_3	(*a*)	5.928 328 571 544 726 169 988 12
	(*b*)	5.928 327 90
	(*c*)	5.928
	(*d*)	5.928 352 5
	(*f*)	5.928 329 3
E_4	(*a*)	7.984 443 523 273 823 549 904 268 579 1
	(*b*)	7.984 443 54
	(*d*)	7.984 444 8
E_5	(*a*)	9.949 160 962 809 596 900 248 32
	(*b*)	9.949 160 38
	(*f*)	9.949 162

Table 5. Eigenvalues (same format as in table 1).

		$\lambda = 10.0,\ g = 10.0$
E_1	(*a*)	1.580 022 327 391 499 803 559 412 471 384 2
	(*b*)	1.580 022 33
	(*c*)	1.580 02
	(*d*)	1.580 024 9
E_2	(*a*)	3.879 036 830 882 568 129 891 720 413 272 4
	(*b*)	3.879 036 83
	(*c*)	3.879 03
	(*d*)	3.879 037 2
E_3	(*a*)	5.832 767 532 465 361 741 388 831 477 805 4
	(*b*)	5.832 767 52
	(*c*)	5.832 77
	(*d*)	5.832 769 2
E_4	(*a*)	7.903 154 159 824 102 829 908 846 549 867 6
	(*b*)	7.903 154 13
	(*d*)	7.903 154 9
E_5	(*a*)	9.882 298 728 779 887 266 853 513 125 186 7
	(*b*)	9.882 298 66

Table 6. Eigenvalues (same format as in table 1).

		$\lambda = 0.1,\ g = 2.0$
E_1	(*a*)	1.017 180 290 061 535 662 051 677 187 643 4
	(*e*)	1.017 281 60
	(*g*)	$1.017\,176 < E_1 < 1.017\,185$
E_2	(*a*)	3.032 765 793 421 440 006 669 974 400 493 4
	(*e*)	3.032 957 27
	(*g*)	$3.032\,758 < E_2 < 3.032\,772$
		$\lambda = 100.0,\ g = 2.0$
E_1	(*a*)	8.758 278 625 605 689 329 589 418 838 744 5
	(*e*)	8.758 278 63
	(*g*)	$8.757\,2 < E_1 < 8.759\,4$
E_2	(*a*)	23.743 325 864 919 321 032 558 358 876 985
	(*e*)	23.743 326 04
	(*g*)	$23.73 < E_2 < 23.75$

Table 7. Eigenvalues as a function of R.

	R	$\lambda = g = 1.0$
E_1	4	1.232 351 173 516 348 218 110 842 056 822 6
	6	1.232 350 723 406 058 865 196 218 560 628 4
	10	1.232 350 723 406 057 813 862 069 958 681 4
	15	1.232 350 723 406 057 813 862 069 958 681 4
	20	1.232 350 723 406 057 813 862 069 958 681 4
E_5	4	9.700 353 051 656 511 764 481 854 973 816 1
	6	9.684 042 017 103 850 820 123 068 959 191 4
	10	9.684 042 015 230 169 589 613 605 813 520 6
	15	9.684 042 015 230 169 589 613 605 813 520 6
	20	9.684 042 015 230 169 589 613 605 813 520 6
	R	$\lambda = g = 100.0$
E_1	4	1.836 336 592 285 584 867 892 06
	6	1.836 335 833 448 220 553 007 79
	10	1.836 335 833 448 218 317 117 92
	15	1.836 335 833 448 218 317 117 91
	20	1.836 335 833 448 218 317 117 91
E_5	4	9.967 764 880 800 496 450 452 86
	6	9.949 160 965 214 562 344 164 91
	10	9.949 160 962 809 596 900 248 32
	15	9.949 160 962 809 596 900 248 32
	20	9.949 160 962 809 596 900 248 32

Handy (1985) are correct, whereas there is significant error in the values found by Lai and Lin (1982) for $g = 2.0$.

We have also examined the question of how the value of R affects the eigenvalues. Table 7 presents the results for the cases $\lambda = 1.0$, $g = 1.0$ and $\lambda = 100.0$, $g = 100.0$, each computed for E_1 and E_5. It is readily apparent that the choice of $R = 10.0$ is optimal for the precision obtained in this study.

4. Conclusions

The analytic continuation procedure of Holubec and Stauffer (1985) offers a straightforward solution to the problem of obtaining high-accuracy wavefunctions and eigenvalues for Schrödinger's equation. Although the procdure is based on functions $P(z)$ and $Q(z)$ which are finite polynomials, in practice it works very well in any case where the functions (or the potential) can be expanded in a Taylor series, and analytic coefficients obtained. This was demonstrated in their paper by computing the phase shifts for the potential

$$V(r) = -(2+2/r)\exp(-2r). \tag{15}$$

The only real limit to the precision is the precision of the computer employed to carry out the calculations. The disadvantage of this technique lies in the requirement to construct the Taylor series (11) and (12) and the corresponding recurrence relations (13) for each specific potential under study. However, if high precision is required in the result, this is not an exorbitant cost.

It is obvious that this approach can be applied readily to a variety of potential forms. Work is currently in progress on the oscillator problem with a perturbation of the form $\lambda x^{2\alpha}$. Similar high-accuracy results are obtainable in this problem as well.

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