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1989 J. Phys. A: Math. Gen. 22 1303

(http://iopscience.iop.org/0305-4470/22/9/019)

J. Phys. A: Math. Gen. **22** (1989) 1303-1313. Printed in the UK

A unified treatment of Schrödinger's equation for anharmonic and double well potentials

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Received 19 September 1988

Abstract. We exploit some exactly soluble model potentials $V^{N}(\alpha, \beta) = V(A, B) + \lambda x^6$ in order to extrapolate (as $\lambda \to 0$) reliable eigenvalues of the one-dimensional Schrödinger equations with either anharmonic or symmetric double well potentials of the form $V(A, B) = \frac{1}{2}Ax^2 + Bx^4$ ($B > 0$). Our procedure, which corresponds to low-order Rayleigh-Schrödinger perturbation theory, is found to be competitive with both high-order Padé summation of conventional RSPT and large-scale variational calculations using harmonic oscillator basis functions.

1. Introduction

One standard procedure for calculating bound-state solutions of the non-relativistic Schrödinger equation

$$H\psi = E\psi \qquad \langle\psi|\psi\rangle = 1 \tag{1.1}$$

is to employ Rayleigh-Schrödinger (RS) perturbation theory (PT). Conventional applications of RSPT begin with the *formal* decomposition of a slightly generalised Hamiltonian $H(\lambda)$, usually written as

$$H(\lambda) = H_0 + \lambda H_1 . \tag{1.2}$$

Here, H_0 is a *soluble model* Hamiltonian and λH_1 is supposed small by comparison with H_0. The expansion parameter λ need not necessarily have physical significance; it serves mainly to monitor the terms of successively higher orders of the power series solutions of $H(\lambda)$:

$$\psi(\lambda) = \psi_0 + \lambda\psi_1 + \lambda^2\psi_2 + \ldots \tag{1.3}$$

and

$$E(\lambda) = E_0 + \lambda E_1 + \lambda^2 E_2 + \ldots . \tag{1.4}$$

A solution of $H(\lambda)$ is often required only for a few isolated values of λ (sometimes, only for the *single* value $\lambda = 1$) but in order to be meaningful, the expansions (1.3) and (1.4) for $\psi(\lambda)$ and $E(\lambda)$ are *assumed* to converge in some region of the complex λ-plane. To determine this region of convergence of $E(\lambda)$, it is generally necessary to compute the large-n dependence of the high-order coefficients $\{E_n\}$, itself a formidable task. Moreover, for the RSPT solution to be useful numerically, convergence of the energy expansion (1.4) for any particular value λ of interest should be reasonably *rapid* and be based on as few low-order coefficients as possible.

0305-4470/89/091303+11$02.50

Much of the recent work on RSPT has confirmed the suspicion that many energy series (1.4) are in fact *asymptotic*, but that nevertheless, useful numerical results can be extracted from the leading expansion coefficients $\{E_n\}$ by means of sophisticated summation techniques (see, for example, Bender and Orszag 1978). A generally *convenient* representation of the energy then takes the form of a *rational fraction*

$$E(\lambda) \sim [L/M] = \frac{P_0 + \lambda P_1 + \ldots + \lambda^L P_L}{1 + \lambda Q_1 + \ldots + \lambda^M Q_M} \tag{1.5}$$

which often yields acceptable accuracy for a wide range of λ values of physical interest and for L, M not too large.

Now the whole procedure of conventional RSPT may be viewed alternatively as follows. Instead of solving $H(\lambda_0)$ *exactly* for an *isolated* parameter value λ_0, we instead solve $H(\lambda)$ *approximately* for some *range of values* of λ, but only up to some predetermined power of λ; this solution is only *approximate* insofar as higher-order terms are not calculated. Nevertheless, an energy expression such as (1.5), based on only the first few orders of RSPT, is often remarkably accurate (Cohen and Feldmann 1981).

However, it may occasionally happen that it is possible to obtain an *exact* solution of $H(\lambda)$ for a discrete set of isolated values λ_i $(i = 1, \ldots, L+M+1)$ but *not* for some particular λ_0 of interest. An expression of the form of (1.5) may then be constructed and used to interpolate (or extrapolate) a value for $E(\lambda_0)$ from the set $\{E(\lambda_i)\}$. A procedure which is conceptually very similar to the present one was employed some years ago to calculate electric dipole polarisabilities of atoms within the Hartree–Fock approximation (Cohen and Roothaan 1965). However, to our knowledge, no previous application has employed *exact* solutions.

In the present work, we apply these ideas to a set of one-dimensional Schrödinger equations with potentials of the general form:

$$V(A, B) = \tfrac{1}{2}Ax^2 + Bx^4 \qquad (B > 0). \tag{1.6}$$

This set includes two subsets of some general interest, namely the quartic anharmonic oscillator $(A > 0)$ and the symmetric double well potential $(A < 0)$. The pure quartic oscillator $(A = 0)$ may be viewed as a natural bridging case between these subsets. Our procedure is as follows. First, we shall obtain the lower eigenvalue spectrum for the *model* potentials

$$V^N(\alpha, \beta) = \tfrac{1}{2}[\alpha^2 - (2N+3)\beta]x^2 + \alpha\beta x^4 + \tfrac{1}{2}\beta^2 x^6 \tag{1.7}$$

which admit of *exact* solutions for arbitrary α and β, provided that N is any *integer*. We then *choose* (N, α, β) for a *series* of integers N so that

$$V^N(\alpha, \beta) = V(A, B) + \lambda x^6 \qquad \lambda = \tfrac{1}{2}\beta^2. \tag{1.8}$$

Finally, we represent the corresponding $E^N(\alpha, \beta)$ by means of a rational fraction (1.5), and *extrapolate* from a series of small (but finite) values of λ to obtain the limit

$$E(A, B) = \lim_{\lambda \to 0} E^N(\alpha, \beta). \tag{1.9}$$

In some sense, our procedure is the *reverse* of standard RSPT, insofar as we seek results in the limit as λ becomes steadily *smaller*. We may therefore anticipate that this process will prove more reliable than the usual applications with *increasing* λ.

2. Solutions for the model Hamiltonian $H^N(\alpha, \beta)$

In order to obtain solutions of the Hamiltonian

$$H^N(\alpha, \beta) = -\frac{1}{2}\frac{d^2}{dx^2} + V^N(\alpha, \beta) \tag{2.1}$$

it is convenient to change the *scale* according to

$$x \to x/\alpha^{1/2} \qquad \beta/\alpha^2 \to \gamma \tag{2.2}$$

so that

$$H^N(\alpha, \beta) \to \alpha h^N(\gamma) \qquad h^N(\gamma) = -\frac{1}{2}\frac{d^2}{dx^2} + \tfrac{1}{2}[1-(2N+3)\gamma]x^2 + \gamma x^4 + \tfrac{1}{2}\gamma^2 x^6 \tag{2.3}$$

which implies that

$$E^N(\alpha, \beta) \to \alpha E^N(1, \gamma). \tag{2.4}$$

Standard analysis now shows that all eigenfunctions of $h^N(\gamma)$ have definite (even or odd) parity. The even-parity eigenfunctions may be written in the form

$$\psi_{2k}^N = \exp[-(\tfrac{1}{2}x^2 + \tfrac{1}{4}\gamma x^4)] \sum_{i=0}^{\infty} a_{2k,2i}^N \frac{(\gamma x^2)^i}{i!} \qquad (k = 0, 1, 2, \ldots) \tag{2.5}$$

and the odd-parity eigenfunctions

$$\psi_{2k+1}^N = \exp[-(\tfrac{1}{2}x^2 + \tfrac{1}{4}\gamma x^4)] x \sum_{i=0}^{\infty} a_{2k+1,2i+1}^N \frac{(\gamma x^2)^i}{i!} \qquad (k = 0, 1, 2, \ldots). \tag{2.6}$$

For simplicity in the following, we write a_{2i} for $a_{2k,2i}^N$, a_{2i+1} for $a_{2k+1,2i+1}^N$ and E for $E^N(1, \gamma)$. The appropriate recurrence relations for the coefficients $\{a_{2i}\}$, are then found to be

$$\mathrm{i}(N+2-2i)\gamma a_{2i-2} + [E-(2i+\tfrac{1}{2})]a_{2i} + (2i+1)a_{2i+2} = 0 \tag{2.7}$$

and for the coefficients $\{a_{2i+1}\}$:

$$\mathrm{i}(N+1-2i)\gamma a_{2i-1} + [E-(2i+\tfrac{3}{2})]a_{2i+1} + (2i+3)a_{2i+3} = 0. \tag{2.8}$$

In general, these equations lead to separate Hill determinants of *infinite* order, which must be truncated and solved for successively higher *finite* order k, $k+1$, $k+2, \ldots$, until numerical convergence of the eigenvalues is sufficient to allow reliable extrapolation to $k \to \infty$.

However, if N is any even integer ($N = 2M$, say) the Hill determinant derived from (2.7) splits into a *finite* $(M+1)$-dimensional determinant for the lowest $(M+1)$ even-parity solutions, together with an infinite-order determinant for the remainder. The finite determinant may then be solved *exactly* (albeit numerically) and the corresponding lowest $(M+1)$ even-parity eigenfunctions all have the form:

$$\psi_{2k}^{2M} = \exp[-(\tfrac{1}{2}x^2 + \tfrac{1}{4}\gamma x^4)] \sum_{i=0}^{M} a_{2k,2i}^{2M} \frac{(\gamma x^2)^i}{i!} \qquad (k = 0, 1, \ldots, M). \tag{2.9}$$

The remaining even-parity solutions, and all odd-parity solutions contain infinite series, and are given by (2.5) and (2.6).

Similarly, if N is an odd integer ($N=2M+1$, say) the Hill determinant derived from (2.8) splits into a finite $(M+1)$-dimensional determinant for the lowest $(M+1)$ odd-parity solutions, together with an infinite-order determinant for the remainder.

For example, in the case $N=2M=6$, and if we write for convenience $E=z+\frac{7}{2}$, the lowest four even-parity solutions satisfy

$$\begin{bmatrix} z-3 & 1 & 0 & 0 \\ 6\gamma & z-1 & 3 & 0 \\ 0 & 8\gamma & z+1 & 5 \\ 0 & 0 & 6\gamma & z+3 \end{bmatrix} \begin{bmatrix} a_0 \\ a_2 \\ a_4 \\ a_6 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}. \tag{2.10}$$

In summary, for any given integer value of N, the low-lying eigenvalues of $H^N(\alpha,\beta)$ can be written conveniently in one of the forms:

$$N=2M \qquad E_{2k}(\alpha,\beta)=\alpha[z_k(\gamma)+M+\tfrac{1}{2}] \qquad (k=0,\ldots M) \tag{2.11}$$

or

$$N=2M+1 \qquad E_{2k+1}(\alpha,\beta)=\alpha[z_k(\gamma)+M+\tfrac{3}{2}] \qquad (k=0,\ldots M) \tag{2.12}$$

where $z_k(\gamma)$ satisfies a polynomial equation of degree $M+1$. That all roots $z_k(\gamma)$ are necessarily real follows from the tridiagonal form of these Hill determinant equations. For convenience, we gather in the appendix the explicit equations for all $N\leqslant 9$.

3. Solutions for $H(A, B)$

To obtain eigenvalues for $H(A, B)$, we now equate the coefficients of x^2 and x^4 in $V^N(\alpha,\beta)$ and $V(A, B)$:

$$\alpha^2-(2N+3)\beta=A \tag{3.1}$$

$$\alpha\beta=B. \tag{3.2}$$

In order to describe bound states, we require a real solution with $\beta>0$. For $B>0$, it is easily verified that such a solution always exists. For any given pair of values of A and B, we thus obtain a set of parameters α, $\gamma=\beta/\alpha^2$ and $\lambda=\beta^2/2$ for each integral value of N considered. The energy calculated for successive (even or odd) values of N may then be fitted to (1.5), and finally extrapolated to $\lambda\to 0$.

For sufficiently large N, a solution of (3.1) and (3.2) is given asymptotically by

$$\alpha\sim(2N+3)^{1/3}B^{1/3} \qquad \gamma\sim(2N+3)^{-1} \qquad \lambda\sim B^{4/3}(2N+3)^{-2/3}/2 \tag{3.3}$$

independent of both the magnitude and the sign of A. Hence, the convergence of $E(\lambda)$ to E_0 is ultimately controlled mainly by the factor $(2N+3)^{-2/3}$, and even the effect of B should be negligible if N is sufficiently large. Thus, there appears to be no difference in principle between the cases $A>0$ (anharmonic oscillator), $A=0$ (pure quartic oscillator) and $A<0$ (double well potential), although the asymptotic results of (3.3) become *exact for all* $N\geqslant 0$ only in the limiting case when $A=0$. However, for different *given* values of A and B, we expect that the exact solutions $E^N(\alpha,\beta)$ of $H^N(\alpha,\beta)$ will reveal different rates of convergence towards $E(A, B)$ *for low* N.

Note that, quite generally, the energy $E(A, B)$ satisfies the scaling relation:

$$E(\eta^2A,\eta^3B)=\eta E(A, B) \tag{3.4}$$

and in particular (provided $A,\ B \neq 0$)

$$E(A, B) = |A|^{1/2} E(1, C^{-3/2}) = B^{1/3} E(C, 1) \tag{3.5}$$

where

$$C = |A| / B^{2/3}. \tag{3.6}$$

As we shall see, convergence is most rapid when C is *large*. Note that under the transformation $A \to \eta^2 A$, $B \to \eta^3 B$ of (3.4), C of (3.6) is *independent* of η, as is $\gamma = \beta/\alpha^2$ when α, β are determined from (3.1) and (3.2).

4. Some bounding properties for the eigenvalues

It is clear from the definition of $V^N(\alpha, \beta)$ in (1.7) that for *fixed* values of α and β and for all $M \geqslant N > 0$

$$V^M(\alpha, \beta) \leqslant V^N(\alpha, \beta). \tag{4.1}$$

Consequently, the ordered eigenvalues of $H^M(\alpha, \beta)$ and $H^N(\alpha, \beta)$ satisfy (see, for example, Löwdin 1965)

$$E_k^M(\alpha, \beta) \leqslant E_k^N(\alpha, \beta) \qquad (k = 0, 1, \ldots) \tag{4.2}$$

so that, for each k, the eigenvalue $E_k^N(\alpha, \beta)$ is bounded from above by $E_k^{N-1}(\alpha, \beta)$ and from below by $E_k^{N+1}(\alpha, \beta)$.

However, what we actually calculate are eigenvalues of $H^N(\alpha_N, \beta_N)$ for a series of successive (even or odd) integer values of N, with α_N, β_N chosen according to (3.1) and (3.2) for *fixed* values of A and B so that α_N, β_N are changing with N. Now

$$V^N(\alpha_N, \beta_N) = V(A, B) + \tfrac{1}{2}\beta_N^2 x^6 \tag{4.3}$$

and it is easily shown that, for $M \geqslant N$,

$$0 \leqslant \beta_M \leqslant \beta_N \tag{4.4}$$

so that the ordered eigenvalues of $H(A, B)$, $H^M(\alpha_M, \beta_M)$ and $H^N(\alpha_N, \beta_N)$ also satisfy

$$E_k(A, B) \leqslant E_k^M(\alpha_M, \beta_M) \leqslant E_k^N(\alpha_N, \beta_N) \qquad (k = 0, 1, \ldots). \tag{4.5}$$

Thus, for successive positive integer values of N, the eigenvalues of $H^N(\alpha_N, \beta_N)$ form steadily decreasing sequences which *converge from above* to the eigenvalues of $H(A, B)$. These results are also independent of the magnitude and sign of A.

In the particular case of double well potentials, it may be more convenient to write the potential

$$V(-A, B) = -\tfrac{1}{2}Ax^2 + Bx^4 \qquad (A, B > 0) \tag{4.6}$$

and note that there is a local maximum at $x = 0$ where $V_{\max} = 0$, and minima at $x = \pm\frac{1}{2}(A/B)^{1/2}$ where $V_{\min} = -\frac{1}{16}A^2/B$. A few of the lower levels of $H(-A, B)$ may then lie below zero energy, and we may obtain an upper bound to the *number* of such levels as follows.

For all real p, the potential $V(-A, B)$ is everywhere bounded below by the harmonic potential

$$V(p) = -\frac{1}{16}\frac{(A + p^2)^2}{B} + \tfrac{1}{2}p^2 x^2 \tag{4.7}$$

whose exact eigenvalues are given by

$$E_k(p) = (k+\tfrac{1}{2})p - \tfrac{1}{16}(A+p^2)^2/B \qquad (k=0,1,\ldots). \tag{4.8}$$

The number m of negative energy levels of $V(p)$ satisfies

$$m \leqslant \tfrac{1}{16}(A+p^2)^2/Bp + \tfrac{1}{2} \tag{4.9}$$

and m clearly provides an upper bound to the number of negative energy levels of $V(-A, B)$. However, the parameter p is still at our disposal, and if we minimise m as a function of p, we obtain the least upper bound

$$m \leqslant \frac{1}{B}\left(\frac{A}{3}\right)^{3/2} + \frac{1}{2} = \left(\frac{C}{3}\right)^{3/2} + \frac{1}{2} \tag{4.10}$$

where the quantity C is exactly as in (3.6).

5. Some representative results for small N

Traditionally, anharmonic oscillators with $A > 0$ and $A \gg B$ have been treated by RSPT starting with the harmonic oscillator model (coresponding to $B = 0$), but the energy series is asymptotic (Simon 1970), and fails to converge even for quite small B, particularly for excited states. Nevertheless, accurate results can be obtained from the RSPT series coefficients by means of Padé summation (see, for example, Simon 1970, Bender and Orszag 1978). Our procedure is more efficient, as we shall see.

As a first example, consider

$$V = \tfrac{1}{2}x^2 + \tfrac{1}{100}x^4 \tag{5.1}$$

(i.e. $A = 1$, $B = \frac{1}{100}$). Table 1 displays the exact results obtained for the lowest six states of $V^N(\alpha, \beta)$, calculated with $N \leqslant 10$ for even-parity states, and with $N \leqslant 11$ for

Table 1. Eigenvalues of $V^N(\alpha, \beta) = \frac{1}{2}x^2 + \frac{1}{100}x^4 + \lambda x^6$ ($C \simeq 21.54$).

N	λ †	E_0	E_1	E_2	E_3	E_4	E_5
0	4.8564	0.507 338	—	—	—	—	—
1	4.7673	—	1.536 180	—	—	—	—
2	4.6828	0.507 335	—	2.592 615	—	—	—
3	4.6026	—	1.536 162	—	3.675 241	—	—
4	4.5263	0.507 332	—	2.592 556	—	4.782 821	—
5	4.4536	—	1.536 146	—	3.675 108	—	5.914 244
6	4.3842	0.507 330	—	2.592 502	—	4.782 574	—
7	4.3179	—	1.536 130	—	3.674 986	—	5.913 845
8	4.2544	0.507 328	—	2.592 453	—	4.782 348	—
9	4.1935	—	1.536 117	—	3.674 874	—	5.913 478
10	4.1351	0.507 326	—	2.592 408	—	4.782 141	—
11	4.0790	—	1.536 104	—	3.674 772	—	5.913 141
$N \to \infty$‡							
[1/0]	0.0	0.507 256	1.535 649	2.590 851	3.671 114	4.774 962	5.901 130
[1/1]	0.0	0.507 256	1.535 649	2.590 845	3.671 083	4.774 874	5.901 120
Variational§		0.507 256	1.535 648	2.590 846	3.671 095	4.774 913	5.901 027

† In units of 10^{-5}.

‡ Fitting as in (1.5).

§ From Burrows and Core (1984) and Burrows *et al* (1989).

odd-parity states. For each value of N, we list the calculated values of λ as well as the derived energies. Also listed are the coefficients P_0 obtained by fitting the exact results at the *lowest* available values of N for each state to the rational fraction $[L/M]$ of (1.5). In this example, λ is very small even for $N=0$, and it is therefore not surprising that our extrapolations based on only two or three calculated values reproduce the variational values obtained with a fairly large basis of 25 harmonic oscillator functions (Burrows and Core 1984, Burrows *et al* 1988).

We list only *exact* values of the calculated energy levels, so that even eigenvalues are given only for even N and odd eigenvalues only for odd N. It would be possible to obtain *approximate* values at intermediate values of N in each case, but these would contribute nothing towards increasing the accuracy of the extrapolations as $N \to \infty$.

Next, we consider the example

$$V = \tfrac{1}{2}x^2 + \tfrac{1}{16}x^4 \tag{5.2}$$

which was expected to display rather poorer convergence since here $C \sim 6.35$ by comparison with $C \sim 21.54$ in the previous case. Results are gathered in table 2 for the lowest six states (three of each parity) together with the coefficient P_0 obtained from the [1/1] approximant fited at the three *lowest* N values available for each state. These approximations also reproduce the directly computed values for all higher N to five or six digits. Although the relevant λ values are now two orders of magnitude larger than those of table 1 our extrapolated values are still remarkably accurate.

A more stringent test is provided by the example

$$V = \tfrac{1}{8}x^2 + \tfrac{1}{8}x^4 \tag{5.3}$$

for which $C = 1$. Our results are presented in table 3, together with the coefficients P_0 of [1/1] and [2/2] approximants, which may be compared with both variational and Padé summed high-order RSPT values (Bender and Orszag 1978). Even here, our results are quite satisfactory, even though the λ values are now quite large for the smaller N

Table 2. Eigenvalues of $V^N(\alpha, \beta) = \frac{1}{2}x^2 + \frac{1}{16}x^4 + \lambda x^6$ ($C \simeq 6.35$).

N	λ†	E_0	E_1	E_2	E_3	E_4	E_5
0	1.664 907	0.541 552	—	—	—	—	—
1	1.529 963	—	1.694 790	—	—	—	—
2	1.422 184	0.541 287	—	2.974 386	—	—	—
3	1.333 401	—	1.693 545	—	4.357 839	—	—
4	1.258 555	0.541 107	—	2.971 295	—	5.830 681	—
5	1.194 312	—	1.692 659	—	4.352 229	—	7.382 622
6	1.138 366	0.540 975	—	2.969 010	—	5.822 126	—
7	1.089 064	—	1.691 987	—	4.347 954	—	7.370 873
8	1.045 184	0.540 872	—	2.967 231	—	5.815 445	—
9	1.005 798	—	1.691 453	—	4.344 554	—	7.361 506
10	0.970 187	0.540 789	—	2.965 794	—	5.810 035	—
11	0.937 786	—	1.691 016	—	4.341 765	—	7.353 806
$N \to \infty$‡							
[1/1]	0.0	0.539 706	1.684 899	2.946 776	4.302 189	5.737 402	7.242 983
Variational§		0.539 705	1.684 895	2.946 757	4.302 132	5.737 273	7.242 749

† In units of 10^{-3}.

‡ Fitting as in (1.5).

§ From Burrows *et al* (1989).

Table 3. Eigenvalues of $V^{\lambda}(\alpha, \beta) = \frac{1}{8}x^2 + \frac{1}{8}x^4 + \lambda x^6$ ($C = 1$).

N	λ†	E_0	E_1	E_2	E_3	E_4	E_5
0	11.182 358	0.417 925	—	—	—	—	—
1	8.618 720	—	1.428 121	—	—	—	—
2	7.176 474	0.412 569	—	2.717 549	—	—	—
3	6.227 849	—	1.412 940	—	4.187 162	—	—
4	5.546 471	0.410 277	—	2.690 939	—	5.799 971	—
5	5.028 373	—	1.405 008	—	4.149 381	—	7.533 528
6	4.618 360	0.408 940	—	2.675 227	—	5.751 938	—
7	4.284 110	—	1.399 969	—	4.125 150	—	7.476 162
8	4.005 305	0.408 043	—	2.664 607	—	5.719 231	—
9	3.768 465	—	1.396 423	—	4.107 981	—	7.435 287
10	3.564 256	0.407 391	—	2.656 841	—	5.695 185	—
11	3.385 991	—	1.393 762	—	4.095 033	—	7.404 332
$N \to \infty$‡							
[1/1]	0.0	0.401 944	1.369 206	2.590 329	3.972 558	5.484 068	7.104 994
[2/2]	0.0	0.401 886	1.368 949	2.589 649	3.971 193	—	—
Variational§		0.401 885	1.368 946	2.589 646	3.971 202	5.481 792	7.101 570

† In units of 10^{-3}.
‡ Fitting as in (1.5).
§ From Burrows *et al* (1989); see also Bender and Orszag (1978).

values employed. We observe that the comparison data quoted by Bender and Orszag (1978) requires Padé summation of at least 20 terms of the RSPT energy expansion for the ground state (cf Simon 1970) to achieve five figure accuracy, whereas our procedure requires no more than five successive N values to reproduce this result. It seems very likely that only a slightly more elaborate calculation (with higher N values, leading to higher-order finite determinants) can lead to results of much greater accuracy. We have not felt it worthwhile to undertake such a calculation in the present case.

The quartic oscillator problem

$$V = \tfrac{1}{2}x^4 \tag{5.4}$$

corresponds to $C = 0$, and might be expected to lead to even poorer convergence. However, as may be seen from table 4 (which includes some comparison with variational results of Banerjee *et al* (1978)), the loss of accuracy is quite modest, and it seems likely that, by solving for slightly larger N values, more reliable results may be obtained in this case also.

Finally, we consider the symmetric double well potentials with $A < 0$. The scaling relations (3.4) and (3.5) suggest that numerical convergence is still controlled by the *magnitude* of C, which is universally a positive quantity. Thus, we expect very similar rates of convergence for the corresponding potentials $V_0(\pm A, B)$ for N sufficiently large, although results for small N may be unrepresentative.

Table 5 contains our results for the case

$$V = -\tfrac{1}{2}x^2 + \tfrac{1}{16}x^4 \tag{5.5}$$

for which $C \sim 6.35$. This potential has minima at $x = \pm 2$, with wells of unit depth, and a maximum at the origin. Only the lowest even and odd bound states have negative-energy eigenvalues in accord with (4.10), but the convergence with increasing N is quite slow. However, even in this extreme case, extrapolation based on [1/1] and

Table 4. Eigenvalues of $V^{\wedge}(\alpha, \beta) = \frac{1}{2}x^4 + \lambda x^6$ ($C = 0$).

N	λ†	E_0	E_1	E_2	E_3	E_4	E_5
0	9.539 286	0.572 357	—	—	—	—	—
1	6.786 044	—	2.035 813	—	—	—	—
2	5.422 480	0.555 858	—	3.999 026	—	—	—
3	4.586 010	—	1.996 024	—	6.258 794	—	—
4	4.011 760	0.549 686	—	3.935 832	—	8.753 288	—
5	3.588 953	—	1.976 824	—	6.174 387	—	11.444 47
6	3.262 390	0.546 279	—	3.900 477	—	8.650 428	—
7	3.001 217	—	1.965 115	—	6.122 343	—	11.325 40
8	2.786 726	0.544 066	—	3.877 315	—	8.582 486	—
9	2.606 857	—	1.957 083	—	6.086 373	—	11.242 60
10	2.453 455	0.542 490	—	3.860 729	—	8.533 542	—
11	2.320 794	—	1.951 064	—	6.059 716	—	11.180 96
$N \to \infty$‡							
[1/1]	0.0	0.530 449	1.900 783	3.730 007	5.826 271	8.137 006	10.627 87
[2/2]	0.0	0.530 182	1.899 839	3.727 864	5.822 409	—	—
Variational§		0.530 181	1.899 837	3.727 849	5.822 373	8.130 913	10.619 19

† In units of 10^{-2}.
‡ Fitting as in (1.5).
§ From Banerjee *et al* (1978).

Table 5. Eigenvalues of $V^{\wedge}(\alpha, \beta) = -\frac{1}{2}x^2 + \frac{1}{16}x^4 + \lambda x^6$ ($C \simeq 6.35$).

N	λ†	E_0	E_1	E_2	E_3	E_4	E_5
0	59.276 890	0.090 760	—	—	—	—	—
1	23.467 592	—	0.432 735	—	—	—	—
2	13.396 387	−0.115 123	—	1.260 616	—	—	—
3	9.105 126	—	0.145 858	—	2.169 894	—	—
4	6.832 402	−0.200 652	—	0.991 161	—	3.219 447	—
5	5.455 951	—	0.022 400	—	1.882 683	—	4.377 223
6	4.543 444	−0.247 463	—	0.864 808	—	2.931 888	—
7	3.898 137	—	−0.045 681	—	1.728 986	—	4.091 074
8	3.419 263	−0.276 941	—	0.792 030	—	2.764 246	—
9	3.050 452	—	−0.088 817	—	1.633 214	—	3.912 522
10	2.757 933	−0.297 249	—	0.744 686	—	2.654 176	—
11	2.520 342	—	−0.118 675	—	1.567 605	—	3.790 036
$N \to \infty$‡							
[1/1]	0.0	−0.173 192	−0.244 146	0.532 946	1.218 268	2.098 154	3.082 314
[2/2]	0.0	−0.423 582	−0.308 737	0.487 921	1.156 216	—	—
Variational§		−0.427 588	−0.311 981	0.485 359	1.153 236	2.030 361	3.009 322

† In units of 10^{-3}.
‡ Fitting as in (1.5).
§ From Burrows *et al* (1989).

[2/2] approximants constructed from the *lowest* values of N yields quite promising results. These may be improved slightly, without going to the lengths of calculating solutions for higher N (which would allow construction of higher $[L/M]$ approximants) simply by employing instead the results at the *highest* N values available. For example, for the lowest (negative energy) state of the double well potential, the [1/1] approximant based on $N=6, 8, 10$ yields $-0.419\,649$ and the [2/2] approximant based on $N=2,\ldots,10$ yields $-0.426\,449$, indicating dramatically enhanced convergence towards the variational result ($-0.427\,588$).

6. Discussion

Our approach depends critically on the availability of a series of exactly soluble model systems from whose spectra we may extrapolate with confidence. As N increases, $H^N(\alpha, \beta)$ approaches $H(A, B)$ steadily *from above* so that we obtain upper bounds only, and there appears to be no possibility of obtaining lower bounds in the present case. In principle, the exact eigenfunctions contain steadily increasing numbers of terms, and ultimately involve *infinite* series in the limit as $N \to \infty$ (cf (2.2) and (2.3)). However, the coefficients of higher powers diminish very rapidly, so that for all practical purposes, the series may be truncated.

The fitting of our results according to (1.5) clearly ought to be carried out at higher values of N than we have used and should probably employ more coefficients $\{P_i, Q_i\}$ if high accuracy is sought. What is remarkable about our present results is the surprising accuracy of the simplest application possible. We reiterate that the use of Padé summation in the standard approach requires very many orders of RSPT to be calculated whereas our procedure is comparable with *low*-order RSPT, and involves very much less computation. Its success serves to emphasise the crucial importance of the proper choice of H_0 in perturbation problems.

Appendix

We list here the polynomial equations satisfied by $z = z^N(\gamma)$ for small N. For even N

$$N=0 \qquad z=0 \tag{A1}$$

$$2 \qquad z^2-(1+2\gamma)=0 \tag{A2}$$

$$4 \qquad z^3-4(1+4\gamma)z-16\gamma=0 \tag{A3}$$

$$6 \qquad z^4-10(1+6\gamma)z^2-96\gamma z+9(1+2\gamma)(1+10\gamma)=0 \tag{A4}$$

$$8 \qquad z^5-20(1+8\gamma)z^3-336\gamma z^2+64(1+16\gamma+46\gamma^2)z+768\gamma(1+8\gamma)=0. \tag{A5}$$

For odd N

$$N=1 \qquad z=0 \tag{A6}$$

$$3 \qquad z^2-(1+6\gamma)=0 \tag{A7}$$

$$5 \qquad z^3-4(1+8\gamma)z-16\gamma=0 \tag{A8}$$

$$7 \qquad z^4-10(1+10\gamma)z^2-96\gamma z+9(1+6\gamma)(1+14\gamma)=0 \tag{A9}$$

$$9 \qquad z^5-20(1+12\gamma)z^3-336\gamma z^2+64(1+24\gamma+126\gamma^2)z+768\gamma(1+12\gamma)=0 \tag{A10}$$

where $\gamma=\beta/\alpha^2$.

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