On the improvement of convergence of Hill determinants

1995 J. Phys. A: Math. Gen. 28 445

(http://iopscience.iop.org/0305-4470/28/2/019)

J. Phys. A: Math. Gen. 28 (1995) 445–457. Printed in the UK

On the improvement of convergence of Hill determinants

Alexander N Drozdov

Institute of High Temperatures of the Russian Academy of Sciences, 13/19 Izhorskaya Street, 127412 Moscow, Russia

Received 16 May 1994, in final form 21 September 1994

Abstract. We propose a simple approach to analytically determine a parameter of a convergence factor $\exp(-gx^2/4)$ in the Hill determinant method. It provides much more rapid convergence of the method than the other analytical approaches currently used for the g determination.

1. Introduction

Due to its simplicity and good behaviour, the Hill determinant method (HDM) is acknowledged as being one of the most efficient algorithms for the calculation of highly accurate eigenvalues of the Schrödinger equation for polynomial potentials

$$Hy(x) = Ey(x) \qquad \lim_{x\to\pm\infty} y(x) = 0 \tag{1a}$$

where H stands for the Hamiltonian

$$H = -\mathrm{d}_{xx}^2 + V(x) \qquad V(x) = \sum_{m=1}^{2M} v_m x^m \qquad v_{2M} > 0. \tag{1b}$$

The corresponding literature has been greatly enriched for the last two decades. A small sample of this work can be found in [1–23]. By convention, one can distinguish the variational [1–11] and the algebraic (Taylor-like) HDM [1, 2, 12–23], the type being determined by the basis functions chosen or (more correctly) by the way in which the eigenvalue problem is reduced to the appropriate matrix representation.

The variational approach consists of expanding $|y\rangle$ in terms of an arbitrary complete set of orthonormal basic vectors $\{|i\rangle\}$

$$|y\rangle = \sum_{i=0}^{\infty} C_i|i\rangle \tag{2}$$

and constructing the matrix representation of the Hamiltonian $H_{i,j} = \langle i|H|j\rangle$. Successive approximations to the eigenvalues of (1) $E_n^{(N)}$ can be then obtained at different levels of truncation by means of the Rayleigh–Ritz method, which consists of finding the roots of the secular determinant

$$\det(H_{i,j} - E\delta_{i,j}) = 0 \qquad i, j = 0, \ldots, N-1. \tag{3}$$

The advantage of the variational HDM is that it is always convergent, and ensures the traditional upper bound property, that is, as N increases, the roots of (3) tend to the exact

0305-4470/95/020445+13$19.50

eigenvalues from above $E_n^{(N)} \geqslant E_n$. Its main disadvantages are that diagonalization of large matrices is time consuming and may suffer from numerical instabilities and cumulation of round-off errors.

In a preceding paper I [11], we have described a rather simple variational procedure avoiding these difficulties. In order to make this article self-contained, we briefly sketch some of the findings of I. We have compared there three different basis sets. The most natural basis for the problem of interest appears to be in terms of the particle number operator $a^\dagger a$, determined through the introduction of creation and annihilation operators $a^\dagger$ and a

$$x = g^{-1/2}(a^\dagger + a) \qquad \mathrm{d}_x = g^{1/2}(a - a^\dagger)/2 \qquad [a, a^\dagger] = 1. \tag{4}$$

This choice is equivalent to using a set of scaled harmonic-oscillator eigenfunctions $|i) = |u_i(x))$, corresponding to the Hamiltonian

$$H_0 = -\mathrm{d}_{xx}^2 + g^2x^2/4 - g/2 \qquad H_0u_n(x) = gnu_n(x) \qquad n = 0, 1, \ldots \tag{5a}$$

$$u_n(x) = [(2\pi/g)^{1/2}2^n n!]^{-1/2} H_n[(g/2)^{1/2}x] \exp(-gx^2/4) \tag{5b}$$

where $H_n(x)$ are the usual Hermite polynomials and g is some parameter to be determined according to variational principles. When applied to (1), this leads to a $(2m + 1)$-term recurrence relation for the expansion coefficients C_i of the form

$$\sum_{j=i-2m}^{i+2m} (H_{i,j} - E\delta_{i,j})C_j = 0 \tag{6a}$$

m being determined by a particular choice of the potential coefficients $M \leqslant m \leqslant 2M$. An idea of Hautot and Magnus [1] (see also [6, 8]) was then used to determine the eigenvalues from the boundary condition

$$C_{N+i} = 0 \qquad 0 \leqslant i \leqslant m - 1 \tag{6b}$$

which is obviously equivalent to the Rayleigh–Ritz truncation of the secular determinant (3) at $N - 1$. The eigenvalue problem is thus reduced to calculating the roots of an $m \times m$ determinant, disregarding the number of basis functions taken into account. The recursive procedure so constructed allows us not only to avoid cumulation of round-off errors, but also minimizes storage requirements.

The efficiency of this kind of variational approach is known to be very sensitive to the value of the variational parameter, and the problem of importance is to properly determine it. An obvious way of doing this is to numerically choose that value of g, referred to henceforth as g_b, which minimizes the approximate eigenvalue of interest. Unfortunately, $E_n^{(N)}$ as a function of g has several local minima, the number of which is proportional to N. This makes searching for its global minimum we are interested in difficult; while the procedure itself becomes very arduous.

In any case, it is clear that the way of fixing g by the process of computation, although good, is both time consuming and inconvenient from the computational point of view, and a great deal of effort has been devoted in recent years to determine this parameter in a simple analytical way. At the present time, there are several more or less equivalent techniques for the g determination [1–5, 9, 11, 13, 23]. Most of these techniques rest on the simplest variational approach, which is to just use a single eigenstate of the basis Hamiltonian H_0

to get a best fit to the corresponding eigenstate of the true Hamiltonian H. The g value so determined appears to be independent of the number of basis functions taken into account. This is in contrast to the results of I which show that the g_b changes drastically as N increases. With the intention of obtaining N-dependence, we proposed to find out g by minimizing the trace of H

$$\partial_g\left(\sum_{n=0}^{N-1} H_{n,n}\right)(g = g_t) = 0. \tag{7}$$

One can note that an analogous method for fixing g has been successfully employed in obtaining the low-lying eigenvalues of the quartic anharmonic oscillator [5].

All the mentioned approaches were tested numerically on four particular systems, corresponding to one-well, double-well, triple-well symmetrical and asymmetrical oscillators. It was found that the g_t approach produces the same convergence rate as the g_b approach, which in turn is much higher than that obtained with the other analytical methods currently used for the g determination. Unfortunately, recurrence (6*a*) is rather difficult to determine and, for $m > 3$, is hardly usable.

Another less rigorous approach to the problem of interest is in terms of the algebraic HDM. The latter rests on a Taylor-like representation of the wavefunction written generally as

$$y(x) = \exp(\text{polynomial in } x)\sum_{i=0}^{\infty} C_i x^i. \tag{8}$$

This corresponds to using a non-orthogonal basis set of the type $\{x^i \exp(\ldots)\}$. When ansatz (8) is used in (1), the result is a recurrence relation for the C_i. We note the relative ease with which the eigenvalues can then be computed through a simple recursive scheme. We again emphasize that, due to its simplicity, the algebraic HDM is one of the most widespread algorithms for the calculation of eigenvalues [1, 2, 12–23]. On the other hand, it is less reliable when compared to the variational approach, which is reliable and efficient for all values of the potential coefficients and parameter g. Little is known about its mathematical grounds, i.e., how it works. There is still some controversy about its general validity [2, 17, 18, 20, 21]. Thus, for example, Chaudhuri [20] has treated the anharmonic oscillators of the type $ax^2 + bx^4 + cx^6$ and shown that, with a particular choice of the convergence factor $\exp(-\alpha x^4 + \beta x^2)$, the algebraic HDM may lead to incorrect eigenvalues. Hautot [2], in turn, has claimed that the use of this factor with variable β removes this inconsistency (see also [18, 21]).

Another interesting problem is to understand how the algebraic HDM converges. We intend to study this problem using the simple factor $\exp(-gx^2/4)$ and to show that the g_t approach also preserves its significance in such a case.

2. The algebraic HDM

For simplicity, we restrict ourselves to the symmetrical Hamiltonian

$$H = -\mathrm{d}_{xx}^2 + \sum_{m=1}^{M} v_{2m} x^{2m}. \tag{9}$$

Due to the symmetry of H, even and odd states can be treated separately. To be consistent with I, we rewrite (8) as

$$y(x) = \exp(-gx^2/4) \sum_{i=0}^{\infty} C_i x^{2i+p} \tag{10}$$

where $p = 0$ and 1 for the even and odd parity states, respectively. Substituting (10) into (1*a*) with (9), we arrive at

$$(2n+p+2)(2n+p+1)C_{n+1} + [E - g(2n+p+\tfrac{1}{2})]C_n + \tfrac{1}{4}g^2 C_{n-1} - \sum_{m=1}^{M} v_{2m} C_{n-m} = 0. \tag{11}$$

The calculation commences at $n = 0$, with $C_0 = 1$ and all other C coefficients zero for $0 > n \geqslant -M$. The eigenvalues are obtained from the roots

$$C_N = 0. \tag{12}$$

This can be achieved in any one of several ways already described in the literature (see, for example, [1, 2, 13, 14, 17, 21, 24]). Furthermore, due to Killingbeck's technique [21, 24], it is possible to find the expectation values, such as $\langle x^2 \rangle$, $\langle x^4 \rangle$, etc, without reconstructing the C_n sequence associated with an eigenvalue. It is also worthwhile noticing the minimal storage requirements inherent to the algebraic HDM.

In comparing this aproach with the variational HDM, we note the ease with which recurrence (11) is obtained for arbitrary M. We also note that, in contrast to recurrence (6*a*), the number of terms involved in (11) depends not on the M, but on the number of terms involved in the potential. We again emphasize that the calculation of the eivenvalues and the coefficients C_i of the eigenfunctions is simpler in the algebraic approach. For all these reasons, this approach must be preferred. Its one simple drawback is that it is more slowly convergent.

3. Analytical methods for the g determination

As we have already noted, the algebraic approach is less reliable than the variational approach. By this, we mean, first, that in each particular case, one needs to prove that the resulting wavefunction is square integrable in the algebraic approach and, second, that the roots of (12) through (11) are not convergent for any positive g. Moreover, in contrast to the Rayleigh–Ritz eigenvalues determined from (6) or (3), those of (12) through (11) are not bounds to the exact eigenvalues. That is, there is no simple criterion to fix g by the process of computation without resorting to external theoretical speculations.

As an example, one considers a method to fix g proposed by Hautot and Magnus [1, 2]. Before doing this, one notes that recurrence (11) is of order $M - 1$. Without the restriction $C_i = 0$ if $i < 0$, it has $(M - 1)$ independent solutions which are noted $C_i^{(m)}$. The method we discuss rests on the following two assumptions. First, it is assumed that these $(M - 1)$ solutions can always be ordered so that the k first dominate the others $(M - k - 1)$, i.e.

$$\lim_{i \to \infty} C_i^{(m')}/C_i^{(m)} = 0 \qquad 0 \leqslant m \leqslant k-1 < m' \leqslant M-2.$$

Let us denote r_i, the ratio of the largest subdominant solution to the smallest dominant solution. Then, another assumption is that the relative error due to truncating (11) at N

$$\varepsilon = (E_n^{(N)} - E_n)/E_n$$

is of order r_N, i.e.

$$|(E_n^{(N)} - E_n)/E_n| = |r_N|.$$

In order to obtain an optimum value of g, Hautot [2] proposed to solve the recurrence for various g by using the generalized Miller algorithm and then to select values which maximize the quotient

$$|\varepsilon|^{-1} \sim \frac{|\text{dominant solution}|}{|\text{subdominant solution}|}.$$

This ensures that one arrives at a true eigenvalue, however, the practical utility of such a method seems rather doubtful. Since an appropriate value of g has to be used for each eigenvalue, too large execution times would be necessary to converge results. Even though we use a single value of g for all the eigenvalues at once, the preparatory procedure need not be convenient for automatic computation.

The above observations have inspired the quest for methods to analytically determine g. The practical problem is that the condition for this parameter has to be simple enough to be exactly soluble, and yet general enough to provide as large a convergence rate as possible for any choice of the potential coefficients. Banerjee *et al* [13] were the first to propose an analytical expression for g. These authors studied the problem of generalized anharmonic oscillators $x^2 + v_{2M}x^{2M}$, and adjusted the value of the parameter $\alpha = g/4$ according to the state and value of the coupling constant considered:

$$g_e = 2 + 4n^{(M-1)/(M+1)}(v_{2M})^{1/(M+1)}. \tag{13}$$

This empirical formula avoids the above procedure, though the convergence produced with (13) (especially for the ground state) is far from optimal. In any case, as shown in *I*, it works equally well in both the variational and the algebraic HDM. It will now be our aim to show that the same is true for the variational criterion (7). That this is the case can be seen by the following heuristic argument.

The terms involved in (10) can always be rearranged so that they cast that expansion into the form

$$y(x) = \exp(-gx^2/4) \sum_{i=0}^{\infty} C_i H_{2i+p}[(g/2)^{1/2}x] \tag{14}$$

analogous to (2), and *vice versa*. Owing to this fact, one may expect that an optimal expression for g obtained in terms of one approach would be relevant for another, or, in other words, that a best choice of the basis set (read the g parameter) would be best irrespective of the method of determining the C_i coefficients.

Since the problem under study is parity invariant, we rewrite (7) as

$$\partial_g \left(\sum_{n=0}^{N-1} H_{2n+p,2n+p} \right)(g = g_t) = 0. \tag{15a}$$

When applied to (9), this condition leads to a $(M+1)$-order polynomial for g

$$X_2 g^{M+1} - \sum_{m=1}^{M} 4m v_{2m} X_{2m} g^{M-m} = 0 \tag{15b}$$

$$X_{2m} = \sum_{n=0}^{N-1} X_{2m}(2n+p) \tag{15c}$$

where we use the shorthand

$$\langle n|x^{2m}|n\rangle = X_{2m}(n)/g^m \tag{15d}$$

for the coefficients $X_{2m}(n)$, which can easily be found if one makes use of the well known relationship

$$x|\mathrm{i}\rangle = g^{-1/2}[(\mathrm{i}+1)^{1/2}|\mathrm{i}+1\rangle + \mathrm{i}^{1/2}|\mathrm{i}-1\rangle].$$

Some of these are given by

$$\begin{aligned} &X_2(n) = 1 + 2n \qquad X_4(n) = 3 + 6n + 6n^2 \\ &X_6(n) = 15 + 40n + 30n^2 + 20n^3 \\ &X_8(n) = 105 + 280n + 350n^2 + 140n^3 + 70n^4 \\ &X_{10}(n) = 945 + 2898n + 3150n^2 + 2520n^3 + 630n^4 + 252n^5. \end{aligned} \tag{16a}$$

Upon substituting (16*a*) into (15*c*), one obtains explicitly the first few coefficients

$$\begin{aligned} X_2 &= 2N^2 - N + 2pN \\ X_4 &= 8N^3 - 6N^2 + N + 12pN^2 \\ X_6 &= 40N^4 - 40N^3 + 20N^2 - 5N + p(80N^3 + 10N) \\ X_8 &= 224N^5 - 280N^4 + 280N^3 - 140N^2 + 21N + p(560N^4 + 280N^2) \\ X_{10} &= 1344N^6 - 2016N^5 + 3360N^4 - 2520N^3 + 966N^2 - 189N \\ &\quad + p(4032N^5 + 5040N^3 + 378N). \end{aligned} \tag{16b}$$

Equation (15*b*) can be then solved for g for a particular choice of the potential coefficients by using any root-finding procedure. It is obvious, however, that the utility of the present approach seems rather doubtful for $M > 5$, because as m increases the coefficients X_{2m} become rather difficult to determine. Thankfully, in practical calculations, it is not necessary to solve (15*b*) exactly. It is largely sufficient to approximately calculate its solution. To achieve this, we first note that, with increasing N, X_{2M} becomes much larger than the other X's in (15*b*), thus providing us with an approximate solution of the form

$$g_t = (4M v_{2M} X_{2M}/X_2)^{1/(M+1)}. \tag{17}$$

Interestingly, it only depends on the main coefficient v_{2M}. This is in agreement with the heuristic assumption of Hautot and Magnus [1] that all characteristics depend on the highest power in the potential.

Proceeding further, it is a matter of exercise to prove that in the leading order in n

$$X_{2m}(n) = x_{2m}n^m + \mathrm{O}(n^{m-1}) \qquad x_{2m} = \sum_{i=0}^{m}\left[\frac{m!}{i!(m-i)!}\right]^2. \tag{18}$$

Substituting (18) into (15*c*), we arrive at

$$X_{2m} = 2^m x_{2m} N^{m+1}/(m+1) + \mathrm{O}(N^m)$$

leaving us finally with

$$g_t = 2[M v_{2M} x_{2M} N^{M-1}/(M+1)]^{1/(M+1)}. \tag{19}$$

The utility of the present approach was tested numerically, by applying it to three particular systems. Results are given in the next section. We note that in all cases considered, starting with $N \sim 20$, the eigenvalues determined with g_t, obtained numerically from (15*b*), are found to be practically indistinguishable from those determined with (19).

For completeness, we also tested the other currently used expressions for g, including that of Banerjee *et al* (13). For this reason, we briefly discuss them below. Hautot and Magnus [1] solved (11) for C_i in the limit $i \to \infty$ and obtained, in the way described above, an expression for g which reads, in our notation, as ($\omega_{\mathrm{opt}} = g_r/4$)

$$g_r = -2\cot gS \tan\frac{M+1}{2}S\left(1 - \cot gS\tan\frac{M+1}{2}S\right)^{(1-M)/(M+1)} \times (2N + M/2 + 1)^{(M-1)/(M+1)} \tag{20a}$$

where S is determined from

$$\cos\frac{M+1}{2}S = -(\cos S)^{(M+1)/2} \qquad \frac{\pi}{M+1} < S < \frac{2\pi}{M+1}. \tag{20b}$$

Although the above expression was obtained for the ground state of the potential $V = x^{2M}$, the authors of [1] claim that it is also perfectly suited to the numerical resolution of the $x^2 + v_{2M}x^{2M}$ problem. It is seen, however, that it does not depend on the coupling constant (cf (19)). The authors of [1] did not find it important to take v_{2M} into account, but one can readily conceive situations where it must be so.

There also exist several, more or less, general techniques to determine g according to variational principles. The simplest variational calculation is to choose $u_0(x)$ as the trial eigenfunction and to determine g by minimizing $H_{0,0}$:

$$\partial_g H_{0,0}(g = g_0) = 0. \tag{21a}$$

This yields the condition

$$g^{M+1} - \sum_{m=1}^{M} 4m(2m-1)!!v_{2m}g^{M-m} = 0. \tag{21b}$$

Particular cases of the above polynomial, for $M = 2$ and 3, were obtained in the literature in many seemingly different ways [3,4,9]. With the scaling factor so determined, the variational HDM appears to be well suited to the numerical resolution of the Schrödinger equation for one-well potentials [3,4,9,11].

The same, however, is not true for double-well potentials. In such a case, the efficacy of the method deteriorates rapidly as either the potential barrier or the quantum number increases [3,11]. One of the reasons for this seems to be the fact that minimization of $H_{0,0}$ lacks a sound theoretical basis in the case of excited states. In particular, in the odd case, it would seem more reasonable to choose u_1 as the trial eigenfunction, rather than u_0, from which follows

$$3g^{M+1} - \sum_{m=1}^{M} 4m(2m+1)!!v_{2m}g^{M-m} = 0. \tag{22}$$

Unfortunately, the use of two conditions (21) and (22), instead of one (21), inessentially improves convergence properties.

To change the situation drastically, one can use an appropriate scaling factor for each eigenvalue. Thus, for example, should one fit g by minimizing $H_{n,n}$, it immediately gives the condition

$$X_2(n)g^{M+1} - \sum_{m=1}^{M} 4mv_{2m}X_{2m}(n)g^{M-m} = 0. \tag{23}$$

In the following, the g values so found will be identified by using the appropriate subscript n with g, i.e. g_0, g_1, g_2 etc.

Another way to fit g is to minimize the deviation of the basis Hamiltonian H_0 from the true Hamiltonian

$$\partial_g \langle n|(H - H_0)^2|n\rangle (g = g_d) = 0. \tag{24a}$$

Then, the new condition is

$$\begin{aligned}[1 - X_2(n) + \tfrac{1}{4}X_4(n)]g^{2M+2} &- \sum_{m=2}^{M}(m-1)v_{2m}[X_{2m}(n) - \tfrac{1}{2}X_{2m+2}(n)]g^{2M+1-m} \\ &- \sum_{m=2}^{M} mX_{2m}(n)\left[\sum_{i=1}^{m-1} v_{2i}v_{2(m-i)}\right]g^{2M-m} \\ &- \sum_{m=M+1}^{2M} mX_{2m}(n)\left[\sum_{i=1}^{M} v_{2i}v_{2(m-i)}\right]g^{2M-m} = 0. \end{aligned} \tag{24b}$$

As shown in *I*, both (23) and (24) produce much better convergence than condition (21). It is seen, however, that the g values so found are dependent of n. As a result, before calculating an eigenvalue, we have first to determine, at least approximately, the number of eigenvalues $n(E)$ less than the trial energy E chosen to start calculations in terms of (6) or (11). This can be achieved either analytically, through asymptotic approximations to $n(E)$ for $E \to \infty$ [25], or by the process of computation. Moreover, if the eigencolumns obtained are to be used for other calculations, it is best to use a fixed g to describe the basis; this ensures that the eigencolumns for different energy levels are theoretically orthogonal.

To resolve the above problem, one can fix g by simultaneously imposing the following two conditions [3]:

$$\partial_g H_{n,n} = 0 \qquad \partial_n H_{n,n} = 0 \tag{25a}$$

which lead to

$$X_2(n)g^{M+1} - \sum_{m=1}^{M} 4m v_{2m} X_{2m}(n) g^{M-m} = 0$$

$$g^{M+1} + \sum_{m=1}^{M} 2v_{2m} X'_{2m}(n) g^{M-m} = 0 \tag{25b}$$

where a prime denotes differentiation with respect to n. In order to distinguish the g determined by (25) from the other g values it will be referred to as g_s. The disadvantage of (25) is that, for particular choices of the potential coefficients, it may have either several or no real and positive roots for g.

4. Numerical applications

To compare the above mentioned criteria for evaluating g, we choose the simplest example which proves to be easily tractable by each criterion. It is given by the Hamiltonian

$$H = -\mathrm{d}_{xx}^2 + v_2 x^2 + v_4 x^4. \tag{26}$$

It is noteworthy that, when applied to (26), recurrence (11) is well behaved. Owing to this fact, no factorization is required. In numerical computations, we have used double-precision arithmetic by truncating the results to 15 decimal digit accuracy.

In order to see the relative efficacy of the above methods for the g determination in giving precise eigenvalues, we carried out computations of the six lowest even-parity eigenvalues of (26). For the purpose of comparing computational results with those of I, we used the same values of (v_2, v_4), namely $(1, 1)$, $(1, 10)$, $(1, 100)$, $(0, 1)$, $(-1, 1)$, $(-1, 0.025)$ and $(-1, 0.01)$. Since the conclusions drawn in all the cases are essentially the same, the results for only $n = 0, 2$ and for $(1, 100)$, $(0, 1)$, $(-1, 0.025)$ are projected in tables 1, 2 and 3 which show both the convergence rate of successive approximations as a function of the truncation order and the comparison of the results for different g approaches. The tables contain the relative error ε obtained for $N = 20$, 40, 60, 80 and 100. In deriving these results, we have made use of the 'exact' eigenvalues obtained in I, by the variational HDM, by systematically increasing the dimension N, and the maximum uncertainty in these eigenvalues is ± 1 in the last figure.

To be consistent with the condition under which (13) was obtained, we first consider the quartic anharmonic oscillator defined by (26) with $v_2 = 1$. Table 1 shows that, in such a case, all the methods, excepting the g_s approach, work (more or less) well, however, the present approach produces much better convergence than the others. However, the g_s approach fails to produce any real and positive roots for g, when $v_2 \geqslant 0$.

The same is true for the pure quartic oscillator $V = x^4$ (see table 2) which was considered by us in order to test the arguments of Hautot and Magnus [1]. These authors claim that at each value of ε there is an optimal value g_r, such that, for calculating the

Table 1. The fractional error ε of successive approximations for the two lowest even-parity eigenvalues of the potential $x^2 + 100x^4$, obtained with different g approaches as a function of the truncation order. The correct eigenvalues $E_0 = 4.999\,417\,545\,137\,59$ and $E_2 = 34.873\,984\,261\,994\,8$ were used as a basis for the calculations. (Exponential notation–k means that the number preceding is to be multiplied by 10^{-k}).

	N				
g	20	40	60	80	100
	$n=0$				
g_t	5.6–09	0	0	0	0
g_e	−4.6–01	6.8–02	4.7–02	−4.2–02	2.9–02
g_r	3.3–03	1.5–06	−1.8–10	−8.5–13	0
g'_r	5.6–09	0	0	0	0
g_0	−8.4–05	−7.0–08	−2.2–10	−8.7–13	0
g_d	−4.0–05	−9.2–09	−3.4–11	−2.6–13	0
	$n=2$				
g_t	8.8–08	0	0	0	0
g_e	1.9–06	7.8–12	0	0	0
g_r	9.8–02	8.7–06	−3.4–08	−4.3–11	−2.6–14
g'_r	8.8–08	0	0	0	0
g_0	−1.1–03	−1.1–06	−6.6–09	−4.4–11	−8.3–14
g_2	1.0–05	−9.5–09	−8.1–13	0	0
g_d	6.5–05	−1.9–08	−1.0–11	−1.0–14	0

Table 2. The same as in table 1, but for the pure quartic oscillator x^4 with $E_0 = 1.060\,362\,090\,484\,18$ and $E_2 = 7.455\,697\,937\,986\,74$.

	N				
g	20	40	60	80	100
	$n=0$				
g_t	6.2–09	0	0	0	0
g_e	1.7–03	1.4–05	−1.6–07	−3.8–09	2.1–10
g_r	6.2–09	0	0	0	0
g_0	−9.8–05	−9.0–08	−3.0–10	−1.2–12	0
g_d	−4.5–05	−1.2–08	−4.5–11	−3.5–13	0
	$n=2$				
g_t	9.3–08	0	0	0	0
g_e	2.1–07	−2.1–14	0	0	0
g_r	9.3–08	0	0	0	0
g_0	−1.3–03	−1.4–06	−8.7–09	−6.0–11	−8.1–14
g_2	1.1–05	−1.1–08	−1.0–12	0	0
g_d	7.3–05	−2.2–08	−1.3–11	−1.2–14	0

eigenvalue E_n with the given precision, a minimal dimension N_r is required. From figure 1 it is seen, however, that there is no optimal value of g, but rather an optimal range. From numerical computations, we have found that, as N increases, this range becomes wider and shifts to larger g values. Moreover, its location was found to be rather sensitive to the choice of the potential coefficients. This is inconsistent with the statement of Hautot and Magnus

Table 3. The same as in table 1, but for the double-well oscillator $-x^2 + 0.025x^4$, with $E_0 = -8.611\,880\,719\,334\,11$ and $E_2 = -5.949\,734\,589\,556\,63$.

	N				
g	20	40	60	80	100
			$n = 0$		
g_t	3.1–03	6.6–08	3.7–14	0	0
g_e	−1.2–02	−6.5–06	2.9–09	1.3–12	1.0–09
g_r	−7.6–01	−4.7–01	−2.7–01	−1.4–01	−6.8–02
g_r'	3.2–03	−1.1–08	1.4–13	0	0
g_0	8.3–01	1.6+00	2.7+00	2.8+00	3.1+00
g_d	7.4–04	8.3–06	−1.8–08	−1.8–11	−1.7–11
g_s	−1.0–02	−8.0–06	2.7–09	2.7–12	1.0–08
			$n = 2$		
g_t	−1.3–02	2.7–06	−1.1–12	0	0
g_e	−3.9–01	−9.6–06	−1.2–12	0	0
g_r	−1.1+00	−8.3–01	−5.8–01	−3.7–01	−2.2–01
g_r'	−1.3–02	1.4–06	3.1–12	0	0
g_2	3.3–01	1.2+00	2.4+00	2.4+00	2.9+00
g_d	−2.7–01	−1.7–04	1.5–07	6.6–11	1.0–08
g_s	−2.2–01	−2.5–04	1.9–07	1.4–10	1.0–08

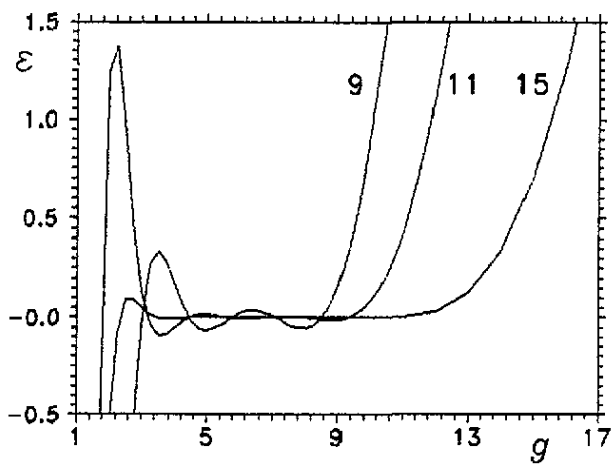

Figure 1. The dependence of the relative error ε (in %) of the ground-state energy obtained by the algebraic HDM on g and $N = 9, 11, 15$ for $V(x) = x^4$.

[1] that it is possible to deal with the generalized anharmonic oscillators $x^2 + v_{2M}x^{2M}$ by adopting the values of g_r which are deduced for the pure x^{2M} oscillator. We consider this statement to be confusing, because the g_r approach, perfectly suited for the pure quartic oscillator, was found to work much worse when v_{2M} differs significantly from unity (cf tables 1, 2 and 3). For the sake of comparison, the authors of [1] proposed us to correct their formula, multiplying (20) by $(v_{2M})^{1/(M+1)}$,

$$g_r' = (v_{2M})^{1/(M+1)} g_r. \tag{27}$$

Tables 1 and 3 shows that the new g_r provides much better results than (20). It is worthwhile noticing also the similarity of this corrected formula to (19).

As a third numerical example, we consider the quartic double-well potential given by (26) with $v_2 = -1$. In such a case, the accuracy of the HDM appears to be very sensitive to the choice of the parameter g, because the higher the potential barrier $\Delta V = v_2^2/(4v_4)$, the narrower the range of optimal g's. It is found, in particular, that the g_r (respectively, g_n) approach provides g values which are too large (respectively, too small). That is the reason why the convergence properties of these approaches deteriorate very rapidly as v_4 decreases and, for $v_4 = 0.025$ ($\Delta V = 10$), they fail to produce convergent results. The rest of the approaches work, more or less, well, however, we again emphasize that the g_t and g_r' approaches produce much more rapid convergence than any others.

The superiority of the present method for the determination of g over the other analytical methods, based on equations (13) and (21)–(25), is understandable because these are all apparently independent of N. In contrast, criterion (15a) depends on N explicitly, and is found to provide us, at each value of N, with a value of g which lies just in the middle of the optimal range.

Further calculations were performed to check the utility of the present method, as applied to the three-term potentials $v_2x^2 + v_4x^4 + v_6x^6$. First, the method was applied to the special double-well potential $-2x^2 - 2x^4 + x^6$, which Chaudhuri [20] and Killingbeck [21] used in their works. We quickly found the two lowest even-parity energies -1 and 3.629 826 493 984 12. The latter value improves Killingbeck's value 3.629 826 5; higher eigenvalues are also easily calculated. Second, we treated the triple-well potential $10x^2 - 50x^4 + 25x^6$ which we used in *I*. The correct eigenvalues were obtained.

One can note, in addition, that the present method for the g determination is thought to be well suited for potential models that are not parity invariant. That this is the case is shown in *I* in terms of the variational HDM. Now we wish to generalize the equation for g to the case of an arbitrary Hamiltonian of the form (1b). To treat this case, it is sufficient to replace $X_{2m}(2n + p)$ in (15c) by $X_{2m}(n)$, which immediately yields

$$X_{2m} = x_{2m}N^{m+1}/(m + 1) + O(N^m)$$

and, therefore,

$$g_t = [4Mv_{2M}x_{2M}N^{M-1}/(M + 1)]^{1/(M+1)}. \tag{28}$$

We note the relative ease with which both (19) and (28) have been obtained.

5. Conclusion

In this paper, we have studied the convergence properties of the algebraic HDM with the simple convergence factor $\exp(-gx^2/4)$. It is obvious that, generally, the best choice of g is a function of $n, N, v_2, \ldots, v_{2M}$. In most cases, however, the methods currently used for the g determination provide us with g independent of N. This is in disagreement with both analytical [1, 2] and numerical [5, 11] calculations, which show that g_b is very sensitive to N and v_{2M}, being practically independent of the other parameters.

On the similarity of (10) to (14), we have employed a standard variational technique and determined N dependence by minimizing the trace of the matrix representation of the Hamiltonian for a given N. The only assumption we have made is that the best choice

of g is independent of the method to be used to determine the expansion coefficients C_i. Parameter g is thus matched in a very easy way because the necessary calculations are extremely simple. It is interesting to note that, within a constant factor, our result exactly coincides with that of Hautot and Magnus (27), obtained in a quite different way. In the application to three particular systems, both the approaches g_t and g'_r have produced much more rapid convergence of the eigenvalues than the other analytical approaches currently used for the g determination.

In addition, we note that the present material is not exhaustive with respect to methodology. Work in applying an analogous approach to determining the parametric dependence of the HDM with an arbitrary convergence factor is in progress.

Acknowledgments

This research is supported by a grant MT2 000 from the International Science Foundation. I would like to thank the authors of [1] for useful comments on the manuscript.

References

[1] Hautot A and Magnus A 1979 *J. Comp. Appl. Math.* **5** 3
[2] Hautot A 1986 *Phys. Rev.* D **33** 437
[3] Balsa R, Plo M, Esteve J G and Pacheco A F 1983 *Phys. Rev.* D **28** 1945
[4] Hsue C S and Chern J L 1984 *Phys. Rev.* D **29** 643
[5] Quick R M and Miller H G 1985 *Phys. Rev.* D **31** 2682
[6] Znojil M, Sandler K and Tater M 1985 *J. Phys. A: Math. Gen.* **18** 2541
[7] Blackmore R and Shizgal B 1985 *Phys. Rev.* A **31** 1855
[8] Fernández F M, Ogilvie J F and Tipping R H 1986 *J. Chem. Phys.* **85** 5850
[9] Chaudhuri R N and Mondal M 1989 *Phys. Rev.* A **40** 6080
[10] Killingbeck J P and Jolicard G 1992 *Phys. Lett.* **166A** 159
[11] Drozdov A N 1994 *J. Comput. Phys.* (submitted)
[12] Biswas S N, Datta K, Saxena R P, Srivastava P K and Varma V S 1971 *Phys. Rev.* D **4** 3617; 1973 *J. Math. Phys.* **14** 1190
[13] Banerjee K, Bhatnagar S P, Choudhry V and Kanwal S S 1978 *Proc. R. Soc.* A **360** 575
[14] Banerjee K 1978 *Proc. R. Soc.* A **364** 265
[15] Singh V, Biswas S N and Datta K 1978 *Phys. Rev.* D **18** 1901
[16] Masson D 1983 *J. Math. Phys.* **24** 2074
[17] Hautot A and Nicolas M 1983 *J. Phys. A: Math. Gen.* **16** 2953
[18] Znojil M 1982 *Phys. Rev.* D **26** 3750; 1986 *Phys. Rev.* D **34** 1224
[19] Chaudhuri R N and Mukherjee B 1984 *J. Phys. A: Math. Gen.* **17** 3327
[20] Chaudhuri R N 1985 *Phys. Rev.* D **31** 2687
[21] Killingbeck J 1985 *J. Phys. A: Math. Gen.* **18** L1025
[22] Tater M 1987 *J. Phys. A: Math. Gen.* **20** 2483
[23] Fernández F M 1991 *Phys. Rev.* A **44** 3336
[24] Killingbeck J 1985 *J. Phys. A: Math. Gen.* **18** 245
[25] Newell G F 1980 *J. Math. Phys.* **21** 2193