

## Calculation of eigenvalues through recurrence relations

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# Calculation of eigenvalues through recurrence relations

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A simple, fast, and accurate method is developed to calculate eigenvalues when the secular equation can be written as a  $(2m + 1)$ -term recurrence relation. Several physically interesting examples are discussed to show that the present algorithm compares favorably with the most efficient ones.

## I. INTRODUCTION

At present, there exist several more or less general techniques to obtain highly accurate solutions to the stationary Schrödinger equation for simple quantum-mechanical models. Among them we mention the Rayleigh–Ritz method,<sup>1–4</sup> perturbation theory,<sup>5–7</sup> the iterative approach,<sup>8,9</sup> the Hill determinant,<sup>10–12</sup> and the gradient method.<sup>13</sup> The main disadvantage of the Rayleigh–Ritz method<sup>1–4</sup> is that diagonalization of large matrices is time consuming and may be subject to cumulation of round-off errors. In this sense, the iterative approach<sup>8,9</sup> is preferable provided it is convergent. Convergence problems also arise in the case of perturbation theory where large-order calculations are very laborious and very accurate perturbation coefficients are required.<sup>5–7</sup>

The method based on the Hill determinant (HDM) is simple and has yielded accurate results.<sup>10–12</sup> However, there is still some controversy about its general validity,<sup>12,14–16</sup> and it has been argued that one should be cautious in applying it to a certain type of doubly anharmonic oscillator.<sup>16</sup> Besides, since an appropriate scaling factor has to be used for each eigenvalue,<sup>11</sup> this procedure becomes very arduous.

In view of the above, it is clear that it would be useful to have an algorithm as simple as the HDM but free of its drawbacks. We show in this paper that such a technique can be derived from the results obtained by Znojil *et al.*<sup>17,18</sup> The method is developed in Sec. II and some useful particular cases are explicitly discussed. Our procedure is compared with the HDM and the technique developed by Denham *et al.*<sup>19</sup> in Secs. III and IV, respectively. The anharmonic oscillator and the linear confining potential model are used as test examples in the former and latter cases, respectively. Further comments and conclusions are found in Sec. V.

## II. THE METHOD

The time-independent Schrödinger equation can always be written

$$U|\psi\rangle = 0, \quad (1a)$$

where  $U$  is defined in terms of two Hermitian operators  $A$  and  $B$  and the eigenvalue  $E$  as

$$U = A - EB. \quad (1b)$$

In particular,  $A = H$  and  $B = I$ , the Hamiltonian and identity operators, respectively.

If  $|\psi\rangle$  is expanded in terms of an arbitrary basis set  $\{|j\rangle\}$ ,

$$|\psi\rangle = \sum_{j=0}^{\infty} C_j |j\rangle, \quad (2)$$

then Eq. (1) becomes

$$\sum_{j=0}^{\infty} U_{i,j} C_j = 0, \quad i = 0, 1, \dots, \quad (3)$$

where  $U_{i,j} = \langle i|U|j\rangle$ .

Successive approaches to the eigenvalues of Eq. (1) can be obtained by means of the Rayleigh–Ritz method that consists of finding the roots of the secular determinant

$$D_N = \det U^{(N)} = 0, \quad (4)$$

where  $U_{i,j}^{(N)} = U_{i,j}$ ,  $i, j = 0, 1, \dots, N-1$ . As  $N$  increases, the roots of Eq. (4) tend to the exact eigenvalues from above. For very large matrices, however, this procedure may suffer from numerical instabilities and cumulation of round-off errors.

When  $U_{i,j} = 0$  for all  $|i-j| > m$ , Eq. (3) can be rewritten as a  $(2m+1)$ -term recurrence relation:

$$C_{n+m} = -U_{n,n+m}^{-1} \sum_{i=-m}^{m-1} U_{n,n+i} C_{n+i}, \quad n = 0, 1, \dots, \quad (5)$$

where it must be understood that  $C_j = 0$  if  $j < 0$ . Since the coefficient  $C_m$  is given by

$$C_m = \sum_{i=0}^{m-1} a_{m,i} C_i, \quad (6)$$

where  $a_{m,i} = -U_{0,i}/U_{0,m}$ , and Eq. (5) is linear, we conclude that all coefficients  $C_n$  can be expressed as linear combinations of the first  $m$  ones:

$$C_n = \sum_{i=0}^{m-1} a_{n,i} C_i. \quad (7)$$

It follows immediately that

$$a_{n,i} = \delta_{n,i} \quad \text{if } 0 \leq n < m, \quad (8)$$

and that the coefficients  $a_{j,i}$  have to obey the recurrence relation (5): i.e.,

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$$a_{n+m,i} = -U_{n,n+m} \sum_{k=-m}^{m-1} U_{n,n+k} a_{n+k,i}, \quad (9)$$

$$0 \leq i < m-1, \quad n \geq 0.$$

Therefore, all of them can be calculated exactly as functions of  $E$ .

As discussed before, the Rayleigh–Ritz method consists of truncating the secular equation at (say)  $U_{N-1,N-1}$  [cf. Eq. (4)], and it is therefore equivalent to the boundary condition

$$C_{N+j} = 0, \quad 1 \leq j \leq m, \quad (10)$$

that leads to the following set of homogeneous linear equations:

$$\sum_{i=0}^{m-1} a_{N+j,i} C_i = 0, \quad 1 \leq j \leq m. \quad (11)$$

Clearly, the only  $E$  values leading to nontrivial solutions are the roots of

$$\det M = 0, \quad (12)$$

where  $M_{i,j} = a_{N+j,i}$ ,  $1 \leq j \leq m$ ,  $0 \leq i < m$ . In this way, the eigenvalue problem reduces to calculating the roots of an  $m \times m$  determinant disregarding the number of basis vectors taken into account in the representation of  $|\psi\rangle$  [Eq. (2)]. In other words, we can carry out very accurate calculations avoiding the use of large matrices.

It can be easily shown from Eqs. (8) and (9) that the coefficients  $a_{m,i}$  are given by

$$a_{n+m,i} = (-1)^{n+1} (U_{0,m} U_{1,m} \cdots U_{n,n+m})^{-1} \det Q_{n+1}^{(i)}, \quad (13a)$$

where

$$Q_{n+1}^{(i)} = \begin{pmatrix} U_{0,i} & U_{0,m} & 0 & 0 \cdots \\ U_{1,i} & U_{1,m} & U_{1,m+1} & 0 \cdots \\ \cdots & \cdots & \cdots & \cdots \\ U_{n,i} & U_{n,m} & U_{n,m+1} & \cdots & U_{n,m+n-1} \end{pmatrix}. \quad (13b)$$

Although this result, which was obtained previously by Znojil<sup>17</sup> in a different way, is not necessary for our present purposes, we show it here for the sake of completeness.

It is worthwhile to notice the way the wave function is approached. On introducing Eq. (7) into the expression for the Rayleigh–Ritz wave function

$$|\psi^{(N)}\rangle = \sum_{n=0}^{N-1} C_n |n\rangle \quad (14)$$

and interchanging the sums we obtain

$$|\psi^{(N)}\rangle = \sum_{i=0}^{m-1} C_i |i^{(N)}\rangle, \quad (15a)$$

where

$$|i^{(N)}\rangle = \sum_{n=0}^{N-1} a_{n,i} |n\rangle. \quad (15b)$$

In other words, this procedure, called the zero-coefficient method (ZCM), allows the wave function to be expanded as a linear combination of  $m$  nonorthogonal functions. Both these functions and the expansion coefficients are improved

as  $N$  increases, tending to the exact solutions of the Schrödinger equation because the Rayleigh–Ritz method is convergent.

In order to show that the present algorithm is simple and easy to use, let us consider two particular cases. When  $m = 1$ , we have a three-term recurrence relation that can be written more simply as

$$F_i C_{i-1} + G_i C_i + F_{i+1} C_{i+1} = 0, \quad i = 0, 1, \dots, \quad (16)$$

where  $F_0 = 0$ ,  $F_i = U_{i,i-1}$  ( $i > 0$ ), and  $G_i = U_{i,i}$  ( $i \geq 0$ ). In this case, all the coefficients  $C_i$  are proportional to  $C_0$  (that can be arbitrarily chosen equal to unity), and the condition  $C_N = 0$  suffices to calculate the Rayleigh–Ritz eigenvalues. In fact, a straightforward algebraic manipulation shows that

$$C_n = (-1)^n (F_1 F_2 \cdots F_n)^{-1} D_n. \quad (17)$$

Obviously, the condition  $C_N = 0$  is equivalent to the Rayleigh–Ritz one  $D_N = 0$ . Upon substituting, Eq. (17) into Eq. (16), we obtain a well known determinant recurrence relation<sup>20</sup>:

$$D_{n+1} = B_n D_n - A_n^2 D_{n-1}. \quad (18)$$

Let us now write the five-term recurrence relation explicitly because it is used in the following sections. When  $m = 2$ , we have

$$C_{j+2} = -U_{j,j+2}^{-1} (U_{j,j+1} C_{j+1} + U_{j,j} C_j + U_{j,j-1} C_{j-1} + U_{j,j-2} C_{j-2}), \quad j = 0, 1, \dots, \quad (19)$$

If  $C_0$  is set equal to unity all the remaining coefficients can be written

$$C_j = a_j + b_j C_1, \quad (20)$$

where  $a_j$  and  $b_j$  obey Eq. (19). Since  $a_0 = b_1 = 1$  and  $a_1 = b_0 = 0$ , we can calculate all the coefficients  $a_j(E)$  and  $b_j(E)$ . The Rayleigh–Ritz eigenvalues are finally obtained from the roots of [cf. Eq. (12)]

$$a_{N+1} b_{N+2} - a_{N+2} b_{N+1} = 0, \quad (21)$$

that comes from  $C_{N+1} = C_{N+2} = 0$ .

When applying the HDM to the generalized anharmonic oscillator ( $V = \omega^2 x^2 + \mu x^3 + \lambda x^4$ ), two unknowns arise, namely the energy  $E$  and the coefficient  $C_1$  ( $C_0$  can arbitrarily be chosen equal to unity). Therefore, the roots of two successive determinants are required to determine both  $E$  and  $C_1$ . This can be achieved quite simply through the procedure developed above.

The relation between the coefficients  $C_j$  and the secular determinants  $D_n$  is not as simple in this case as in the previous one. From the general result (13), we obtain

$$a_j = (-1)^{j-1} (U_{0,2} U_{1,3} \cdots U_{j-2,j})^{-1} D_{j-1}^{(1)}, \quad (22a)$$

$$b_j = (-1)^{j-1} (U_{0,2} U_{1,3} \cdots U_{j-2,j})^{-1} D_{j-1}^{(0)}, \quad (22b)$$

where  $D_j^{(i)} = \det Q_j^{(i)}$ . Upon substituting Eq. (22) into Eq. (20) and using the condition  $C_{N+1} = 0$ , we obtain

$$C_1 = -D_N^{(1)} / D_N^{(0)}, \quad (23a)$$

$$C_j = (-1)^{j-1} [U_{0,2} U_{1,3} \cdots U_{j-2,j} D_N^{(0)}]^{-1} \times [D_{j-1}^{(1)} D_N^{(0)} - D_{j-1}^{(0)} D_N^{(1)}]. \quad (23b)$$

The coefficient  $C_{N+2}$  can be proved to be proportional to  $D_N$ .

The ZCM is more suitable than the HDM for calculating highly excited states because in the former technique it is not necessary to obtain all the coefficients  $C_n$  (read  $a_{n,i}$ ) from  $C_0$  upwards. In fact, for large enough eigenvalues the expansion coefficients  $C_j$  are found to have the largest value when (say)  $j \approx n$  and then decrease as  $|n - j|$  increases. One can, therefore, choose a sufficiently large value of  $k$  and set

$$C_j = 0 \quad \text{if } |j - n| > k. \quad (24)$$

In this way, we have [cf. Eq. (5)]

$$C_{n+m-k} = -U_{n-k,n+m-k}^{-1} \sum_{i=0}^{m-1} U_{n-k,n-k+i} C_{n-k+i}. \quad (25)$$

In other words, all the coefficients  $C_j$  ( $|j - n| \leq k$ ) can be written as linear combinations of  $C_{n-k}, C_{n-k+1}, \dots, C_{n-k+m-1}$ . It is convenient to define

$$u_j = C_{n-k+j}, \quad 0 \leq j \leq 2k \quad (26)$$

and

$$T_{i,j} = U_{n-k+i,n-k+j}, \quad 0 \leq i, j \leq 2k, \quad (27)$$

in which case we can write

$$u_{j+m} = -T_{j,j+m}^{-1} \sum_{i=-m}^{m-1} T_{j,j+i} u_{j+i} \quad (28)$$

and apply the procedure developed before. If the state  $|n+k\rangle$  is the largest one required to obtain a given accuracy, then one needs  $n+k+1$  states when using the complete recurrence relation and only  $2k+1$  ( $n \gg k$  is assumed) in this last case.

### III. COMPARISON WITH THE METHOD OF THE HILL DETERMINANT

To compare the ZCM and the HDM, we choose an example which proves to be easily tractable by both procedures, namely the anharmonic oscillator

$$H = p^2 + x^2 + \lambda x^4, \quad p = -id/dx. \quad (29)$$

If the wave function is written

$$\psi(x) = \exp(-\alpha x^2/2) \sum_{j=0}^{\infty} c_j x^{2j+v}, \quad (30)$$

where  $v = 0$  or  $1$  for the even or odd states, respectively, the expansion coefficients  $c_j$  are found to obey

$$c_{j+1} = t_j^{-1} (q_j c_j + r_j c_{j-1} + s_j c_{j-2}), \quad j = 0, 1, \dots, \quad (31a)$$

where  $r_0 = s_0 = s_1 = 0$  and

$$t_j = (2j + v + 1)(2j + v + 2), \quad (31b)$$

$$q_j = \alpha(4j + 2v + 1) - E, \quad (31c)$$

$$r_j = 1 - \alpha^2, \quad (31d)$$

$$s_j = \lambda. \quad (31e)$$

Clearly, all the expansion coefficients can be obtained from this recurrence relation as functions of the energy  $E$  by choosing the initial condition  $c_0 = 1$ .

It follows immediately from Eq. (31) that<sup>12</sup>

$$c_j = (-1)^j (t_0 t_1 \dots t_{j-1})^{-1} D_j, \quad j > 0. \quad (32)$$

Substitution of Eq. (32) into Eq. (31a) leads to a well known determinant recurrence relation.<sup>10-12</sup>

When  $\alpha = 1$ , Eq. (31) becomes a simple three-term recurrence relation. However, this choice is not suitable for dealing with very large values of  $\lambda$  and  $n$ .<sup>11</sup> In order to facilitate numerical calculation, it is advisable to factorize the asymptotic form of the determinants (or expansion coefficients) in the recurrence relation<sup>10</sup>; too fast an increase (decrease) of the determinants (expansion coefficients) is thus avoided.

The secular equation for the anharmonic oscillator using a scaled harmonic-oscillator basis set can be easily obtained as follows: the change of variables  $x \rightarrow \alpha^{-1/2} x$  transforms Eq. (29) into

$$H = \alpha H_0 + (\alpha^{-1} - \alpha)x^2 + \lambda \alpha^{-2} x^4, \quad (33)$$

where  $H_0 = p^2 + x^2$ . Since the eigenvectors  $|n\rangle$  of  $H_0$  ( $H_0|n\rangle = (2n+1)|n\rangle$ ,  $n = 0, 1, \dots$ ) satisfy

$$x|n\rangle = 2^{-1/2} [n^{1/2}|n-1\rangle + (n+1)^{1/2}|n+1\rangle], \quad (34)$$

the calculation of all the matrix elements  $H_{i,j} = \langle i|H|j\rangle$  is straightforward. Some of them are shown below, and the remaining ones follow from the matrix symmetry  $H_{i,j} = H_{j,i}$ :

$$H_{n,n-4} = \lambda(4\alpha^2)^{-1} [n(n-1)(n-2)(n-3)]^{1/2}, \quad (35a)$$

$$H_{n,n-2} = 2^{-1} [\alpha^{-1} - \alpha + \lambda\alpha^{-2}(2n-1)] [n(n-1)]^{1/2}, \quad (35b)$$

$$H_{n,n} = 2^{-1}(\alpha^{-1} + \alpha)(2n+1) + \lambda(4\alpha^2)^{-1}(6n^2 + 6n + 3). \quad (35c)$$

The recurrence relation for the expansion coefficients is found to be

$$C_{n+4} = -H_{n,n+4}^{-1} [H_{n,n+2} C_{n+2} + (H_{n,n} - E)C_n + H_{n,n-2} C_{n-2} + H_{n,n-4} C_{n-4}]. \quad (36)$$

The initial conditions  $C_0 = 1$  ( $n = 0, 2, \dots$ ) or  $C_1 = 1$  ( $n = 1, 3, \dots$ ) lead to the even- or odd-parity solutions, respectively. This five-term recurrence relation can be treated as discussed in Sec. II. Owing to the fact that it is well behaved, no factorization is required.

The rate of convergence of the procedures outlined above depends on the value of the scaling parameter. There are many ways of choosing it<sup>1-4,6,7,9,11,12</sup> but we do not discuss them here since our aim is to compare the ZCM and the HDM. To do this, we select the value  $\alpha = 1$  that would be appropriate for the ground state of the anharmonic oscillator according to the empirical formula proposed by Banerjee *et al.*<sup>11</sup> The value of  $\alpha$  remains unchanged when computing the first excited even eigenvalue, thus proving that the HDM is more sensitive than the ZCM to the use of a nonoptimum value of the scaling parameter. Owing to this fact, calculation is simpler when the latter method is applied.

As shown in Table I, the ZCM converges much more quickly than the HDM, particularly for the first excited even state, in confirmation of what was stated above. In addition to this, the ZCM is more reliable since the Rayleigh-Ritz

TABLE I. Energy eigenvalues for the ground and first even excited states of  $H = p^2 + x^2 + x^4$ .  $N$  is the number of terms taken into account in the wave function expansion ( $\alpha = 1$ ).

$N$	$n$	ZCM	HDM
6	0	1.394 907	1.256 238
	2	8.937 495	6.872 112
8	0	1.392 566	1.433 555
	2	8.660 375	18.418 945
10	0	1.392 355	1.392 369
	2	8.656 312	6.844 716
12	0	1.392 352	1.384 125
	2	8.655 058	9.120 729
14	0	1.392 352	1.398 557
	2	8.655 050	22.273 821
16	0	1.392 352	1.389 725
	2	8.655 050	8.179 592
42	0	1.392 351	1.392 351
	2	8.654 388	8.654 388
52	0	1.392 352	1.392 352
	2	8.655 045	8.655 045
62	0	1.392 352	1.392 352
	2	8.655 058	8.655 058
72	0	1.392 352	1.392 352
	2	8.655 051	8.655 051
74	0	1.392 352	1.392 352
	2	8.655 050	8.655 050

eigenvalues are known to be convergent provided a complete set of vectors is used in the expansion of the wave function. We therefore conclude that the HDM, which is one of the most widespread algorithms for calculation of highly accurate eigenvalues,<sup>10-12</sup> may be advantageously replaced by the ZCM.

For the general  $2m$  anharmonic oscillator potential

$$V = \sum_{j=2}^{2m} v_j x^j, \quad v_{2m} > 0 \quad (37)$$

we obtain a  $(2m + 1)$ -term recurrence relation when using the basis set discussed before. Therefore, the general procedure proposed in Sec. II applies to this problem in a straightforward manner.

#### IV. COMPARISON WITH THE NORM METHOD

The purpose of this section is twofold. First, we show that the method developed by Denham *et al.*,<sup>19</sup> which is called the norm method (NM), can be applied to confining potential models. Second, we compare it with the ZCM.

The NM is based on the well known fact that a solution of Eq. (1) is not normalizable unless  $E$  equals an eigenvalue. Therefore, it stands to reason that the minima of the finite sum

$$\sigma_N(E) = \sum_{n=0}^N |C_n|^2 \quad (38)$$

converge towards the actual eigenvalues as  $N$  increases.<sup>19</sup> This assumption has been successfully checked for a number of one-dimensional problems finding rapid convergence in all cases.<sup>19</sup>

To apply the NM to the confining potential models

$$H = \frac{1}{2} p^2 - (1/r) + \lambda r^\nu, \quad \nu = 1, 2, \dots, p = -i\nabla, \quad (39)$$

we need an appropriate recurrence relation for the expansion coefficients  $C_i$ . Such a relation can easily be found by writing  $p$  and  $r$  in terms of the three  $SO(2,1)$  generators realized as<sup>7,9</sup>

$$k_0 = \frac{1}{2} (\alpha r p^2 + r/\alpha), \quad k_1 = \frac{1}{2} (\alpha r p^2 - r/\alpha), \quad k_2 = \mathbf{r} \cdot \mathbf{p} - i. \quad (40)$$

Thus, the time-independent Schrödinger equation for Eq. (39) can be written as in Eq. (1) with

$$A = rH = \frac{1}{2\alpha} (k_0 + k_1) - 1 + \lambda \alpha^{\nu+1} (k_0 - k_1)^{\nu+1}, \quad (41a)$$

$$B = r = \alpha (k_0 - k_1). \quad (41b)$$

The matrix elements of  $U$  in the basis set of eigenvectors of  $k_0$  follow immediately from

$$k_0 |n, l\rangle = n |n, l\rangle, \quad (42a)$$

$$k_1 |n, l\rangle = k_n^l |n+1, l\rangle + k_{n-1}^l |n-1, l\rangle, \quad (42b)$$

where  $l$  is the angular momentum quantum number and

$$k_n^l = \frac{1}{2} [(n-l)(n+l+1)]^{1/2}, \quad n > l. \quad (42c)$$

It is then clear that the secular equation for the general case is a  $(2\nu + 3)$ -term recurrence relation to which the procedure developed in Sec. II applies.

For the sake of simplicity, we consider explicitly only the case  $\nu = 1$  that leads to the recurrence relation (19) with (the remaining matrix elements follow from the matrix symmetry  $U_{i,j} = U_{j,i}$ )

$$U_{n,n-2} = \lambda \alpha^2 k_{n-1}^l k_{n-2}^l, \quad (43a)$$

$$U_{n,n-1} = \left[ \frac{1}{2\alpha} - \lambda \alpha^2 (2n-1) \right] k_{n-1}^l + \alpha E k_{n-1}^l, \quad (43b)$$

$$U_{n,n} = \lambda \alpha^2 [(k_n^l)^2 + (k_{n-1}^l)^2 + n^2] + \frac{1}{2\alpha} n - 1 - \alpha E n. \quad (43c)$$

Since Denham *et al.*<sup>19</sup> showed how to deal with five-term recurrence relations [generalization to  $(2m + 1)$ -term ones is straightforward] in detail, we do not need to duplicate their results here.

Table II shows that both methods converge very quickly to the actual eigenvalues.<sup>9</sup> However, the ZCM is preferable because of its greater simplicity and more rapid convergence. Besides, when calculating only eigenvalues by means of the ZCM, it is not necessary to store all the coefficients  $C_i$  (as in the case of the NM and the iterative method<sup>9</sup>) because only the last five ones are required in each step. Although the iterative method can be programmed very easily and leads to highly accurate results,<sup>9</sup> we find the ZCM more convenient because it does not exhibit convergence problems.

In order to calculate a large number of accurate eigenvalues, it is advisable to select proper  $\alpha$  values.<sup>1-4,6,7,9,11,12</sup> The choice  $\alpha = 1$  is appropriate enough for our present purpose of comparison of different methods.

Finally, we point out that the utility of these simple approaches is immediately realized by taking into account the large amount of computational work required to carry out a

TABLE II. Lowest eigenvalues of  $H = p^2 - (1/r) + r$  for  $l = 0$  using the scaling factor  $\alpha = 1$ .  $N$  is the number of basis functions taken into account in the wave function expansion.

$N$	$n$	ZCM	NM
12	1	0.556 794	0.556 996
	2	2.406 402	2.433 340
	3	3.715 399	3.789 631
17	1	0.556 764	0.556 765
	2	2.405 079	2.406 227
	3	3.693 682	3.701 288
22	1	0.556 764	0.556 764
	2	2.405 054	2.405 095
	3	3.692 906	3.693 334
27	1	0.556 764	0.556 764
	2	2.405 054	2.405 054
	3	3.692 880	3.692 894
32	1	0.556 764	0.556 764
	2	2.405 053	2.405 053
	3	3.692 879	3.692 880

straightforward Rayleigh–Ritz calculation for the models considered in this section.<sup>21</sup>

## V. CONCLUSIONS

Due to its simplicity and good behavior, the method proposed in this paper appears to be preferable to all the other techniques currently used in obtaining accurate solutions to the time-independent Schrödinger equation.<sup>1–13</sup> It is particularly suitable for use with small microcomputers and even programmable pocket calculators because it does not

require complicated programs or large machine memory. Furthermore, the ZCM can be used to calculate expectation values through Killingbeck's procedure.<sup>12,22</sup>

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<sup>1</sup>S. I. Chan and D. Stelman, *J. Mol. Spectrosc.* **10**, 278 (1963).

<sup>2</sup>C. E. Reid, *J. Mol. Spectrosc.* **36**, 183 (1970).

<sup>3</sup>R. Balsa, M. Plo, J. G. Esteve, and A. F. Pacheco, *Phys. Rev. D* **28**, 1945 (1983).

<sup>4</sup>R. M. Quick and H. G. Miller, *Phys. Rev. D* **31**, 2682 (1985).

<sup>5</sup>See *Int. J. Quantum Chem.* **21**, (No. 1) (1982), and references therein.

<sup>6</sup>G. A. Arteca, F. M. Fernandez, and E. A. Castro, *J. Math. Phys.* **25**, 3492 (1984).

<sup>7</sup>F. M. Fernandez, A. M. Meson, and E. A. Castro, *Phys. Lett. A* **111**, 104 (1985).

<sup>8</sup>B. L. Burrows and P. W. Core, *J. Phys. A* **17**, 559 (1984).

<sup>9</sup>F. M. Fernandez, A. M. Meson, and E. A. Castro, *J. Phys. A* **18**, 1389 (1985).

<sup>10</sup>S. N. Biswas, K. Datta, R. P. Saxena, P. K. Srivastava, and V. S. Varma, *Phys. Rev. D* **4**, 3617 (1971); *J. Math. Phys.* **14**, 1190 (1973).

<sup>11</sup>K. Banerjee, S. P. Bhatnagar, V. Choudhry, and S. S. Kanwal, *Proc. R. Soc. London Ser. A* **360**, 575 (1978); K. Banerjee, *ibid.* **364**, 265 (1978).

<sup>12</sup>J. Killingbeck, *J. Phys. A* **18**, L1025 (1985).

<sup>13</sup>G. Schiffrer and D. Stanzial, *Nuovo Cimento B* **90**, 74 (1985).

<sup>14</sup>G. P. Flessas and G. S. Anagnostatos, *J. Phys. A* **15**, L437 (1982).

<sup>15</sup>A. Hautot and M. Nicolas, *J. Phys. A* **16**, 2953 (1983).

<sup>16</sup>R. N. Chaudhuri, *Phys. Rev. D* **31**, 2687 (1985).

<sup>17</sup>M. Znojil, *J. Phys. A* **16**, 293 (1983); **17**, 1603 (1984).

<sup>18</sup>M. Znojil, K. Sandler, and M. Tater, *J. Phys. A* **18**, 2541 (1985).

<sup>19</sup>S. A. Denham, B. C. Harms, and S. T. Jones, *Nucl. Phys. B* **188**, 155 (1981); *Am. J. Phys.* **50**, 374 (1982).

<sup>20</sup>F. M. Fernandez and E. A. Castro, *Phys. Lett. A* **107**, 215 (1985).

<sup>21</sup>C. C. Gerry, *Phys. Lett. A* **115**, 9 (1986).

<sup>22</sup>J. Killingbeck, *J. Phys. A* **18**, 245 (1985).