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A simple iterative solution of the Schrödinger equation in matrix representation form

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Abstract. A simple procedure for solving the Schrödinger equation is presented. It is based upon an iterative solution of the secular equation. A large enough convergence rate is obtained by using a basis set of properly scaled functions. The effect of the scaling parameter on the convergence rate is studied in order to improve the calculation. The method is applied to simple, though non-trivial, quantum mechanical models such as the quartic, sextic and octic anharmonic oscillators, a double well potential, and the linear confining potential. Highly accurate eigenvalues for all values of the coupling parameter are obtained.

1. Introduction

Burrows and Core (1984) have recently applied a technique for solving nonlinear operator equations iteratively to quantum mechanical calculations. To this end the Schrödinger equation is written as

$$T\Psi = f(\Psi), \tag{1}$$

where Ψ belongs to the domain of a self-adjoint operator T and T^{-1} exists. In general $f(\Psi)$ may be nonlinear.

On solving (1) the related sequence of equations

$$T\psi^{(s+1)} = f(\psi^{(s)}), \tag{2}$$

is tried, where

$$\psi^{(s)} = e_0 + \sum_{i=1}^{N(s)} a_i^{(s)} e_i, \tag{3}$$

and

$$\langle e_i | Te_j \rangle = \alpha_i \delta_{ij}, \qquad (\alpha_i > 0). \tag{4}$$

The sequence of functions $\psi^{(s)}$ is supposed to converge towards Ψ as $s \to \infty$ (see Burrows and Core (1984) and references therein for a more detailed discussion).

Burrows and Core (1984) rearranged the Schrödinger equation in different ways and studied the effect of different choices for $f(\psi)$ and $N(s)$ on the convergence rate. However, they have not considered the influence of the basis set of functions which is of great practical importance.

In the present paper a modified version of the iterative technique proposed by Burrows and Core (1984) is applied to some quantum mechanical problems of physical

interest. A basis set of properly scaled functions is used and the effect of the scaling parameter on the convergence rate is studied. The method is developed in § 2. In § 3 it is applied to the anharmonic oscillators and to a double well potential model. The linear confining potential is discussed in § 4. In all the cases we go further than Burrows and Core (1984) did and study excited states in addition to the ground state.

2. The method

Our goal is to solve the eigenvalue equation

$$A|\Psi_n\rangle = E_n B|\Psi_n\rangle, \tag{5}$$

where A and B are two self-adjoint operators. To this end we expand the eigenvector $|\Psi_n\rangle$ in a basis set of orthonormal vectors $|i\rangle$

$$|\Psi_n\rangle = \sum_{i=0}^{\infty} c_{in}|i\rangle. \tag{6}$$

The coefficients c_{in} are solutions of the secular equation

$$\sum_i A_{ji}c_{in} = E_n \sum_i B_{ji}c_{in}, \qquad j = 0, 1, \ldots, \tag{7}$$

where

$$A_{ij} = \langle i|A|j\rangle, \qquad B_{ij} = \langle i|B|j\rangle. \tag{8}$$

Notice that (5) becomes a nonlinear equation like (1) by setting $E_n = \langle n|A|\Psi_n\rangle/\langle n|B|\Psi_n\rangle$. This choice proves to be convenient when $|n\rangle$ is an acceptable approximation to $|\Psi_n\rangle$. In the following sections we show how to obtain an appropriate basis set of vectors for some problems of physical interest.

If c_{nn} is arbitrarily set equal to unity we can rewrite (7) as

$$E_n = \left(B_{nn} + \sum_{i\neq n} B_{ni}c_{in}\right)^{-1}\left(A_{nn} + \sum_{i\neq n} A_{ni}c_{in}\right), \tag{9}$$

when $j = n$ and

$$c_{jn} = (A_{jj} - E_n B_{jj})^{-1} \sum_{i\neq j} (E_n B_{ji} - A_{ji})c_{in} \tag{10}$$

when $j \neq n$. Equations (9) and (10) are easily solved by iteration provided that $E_n \neq A_{jj}/B_{jj}$ for all $j \neq n$ during the process. Notice that (7) is also the secular equation for $H|\Psi_n\rangle = E_n|\Psi_n\rangle$ when $|\Psi_n\rangle$ is expanded in a non-orthogonal basis set of vectors $|i\rangle$. In this case $A_{ij} = \langle i|H|j\rangle$ and $B_{ij} = \langle i|j\rangle$.

The success of the method may strongly depend on the starting point. A sensible choice appears to be

$$c_{in}^{(0)} = \delta_{in}, \qquad E_n^{(0)} = A_{nn}/B_{nn}, \tag{11}$$

which is based upon the assumption that $|n\rangle$ is a close enough approach to $|\Psi_n\rangle$. Instead of using the coefficients $c_{in}^{(s)}$ obtained in the sth step to calculate $c_{jn}^{(s+1)}$, as suggested by (2) and (3), it is easier, from a computational viewpoint, to operate

according to the Gauss-Seidel iterative scheme:

$$E_n^{(s)} = \left(B_{nn} + \sum_{i \neq n} B_{ni} c_{in}^{(s)} \right)^{-1} \left(A_{nn} + \sum_{i \neq n} A_{ni} c_{in}^{(s)} \right), \tag{12a}$$

$$c_{jn}^{(s+1)} = (A_{jj} - E_n^{(s)} B_{jj})^{-1} \left(\sum_{i<j} (E_n^{(s)} B_{ji} - A_{ji}) c_{in}^{(s+1)} + \sum_{i>j} (E_n^{(s)} B_{ji} - A_{ji}) c_{in}^{(s)} \right), \tag{12b}$$

which proves to converge more quickly (Kuo 1965). The main advantage of doing the Rayleigh-Ritz calculation iteratively is that roundoff errors only occur at the final iteration whereas the usual eigenvalue techniques can be subject to a cumulation of errors.

Though (9) and (10) are also the starting point of the Brillouin-Wigner perturbation formula (Morse and Feshbach 1953) the present approach differs from that in the way the iterative process is performed.

When $A_{ij} = 0$ for $|i-j| > I$ and $B_{ij} = 0$ for $|i-j| > J$ we can write the right-hand side of (12) explicitly and treat A_{ij} and B_{ij} as mere numbers instead of as elements of matrices. In such a case much less memory space is required since only the vector $(c_{1n}, c_{2n}, \ldots)$ is to be stored up. On the other hand, in the usual eigenvalue techniques it is mandatory to store up the matrices A_{ij} and B_{ij}. Besides, the iterative procedure can also be used to produce analytical expressions for both the eigenvalues and eigenfunctions. Notice that the number of non-vanishing coefficients increases by a fixed amount in each iteration step. In general our sth approximation to the wavefunction $|\Psi_n\rangle$ will be

$$|\Psi_n^{(s)}\rangle = |n\rangle + \sum_{i=0}^{M} c_{in}^{(s)} |i\rangle, \tag{13}$$

where M and the maximum s $(= N)$ value are determined so that results do not change when they are increased. If the secular equation (7) is a three-term recursion relationship $(I = J = 1)$, the present procedure is similar, though not exactly equivalent step by step, to the continued fraction calculation.

The iterative technique requires a good deal less computational work than the Rayleigh-Schrödinger perturbation theory does and it will be shown later on that the former converges where the latter does not.

In this paper we do not determine rigorously the general conditions under which the iterative method is convergent. However, we will show that it actually converges at least for the low-lying eigenvalues of a number of quantum mechanical models. In addition to this, the effect of the chosen basis set of vectors $|i\rangle$ on the convergence is studied.

3. Anharmonic oscillators and double well potentials

The first example we study in this paper is the Schrödinger equation for the one-dimensional Hamiltonian operator

$$H_{2k}(\omega^2, \lambda) = p^2 + \omega^2 x^2 + \lambda x^{2k}, \qquad p = -\mathrm{i}\, \mathrm{d}/\mathrm{d}x, \qquad k = 2, 3, \ldots, \tag{14}$$

which represents a $2k$-anharmonic oscillator when $\omega^2 > 0$ and a double well potential when $\omega^2 < 0$. There has been great interest in these models partly due to their applications in quantum mechanics and field theory but mainly because of the singularities

of the eigenvalues of the $2k$-anharmonic oscillators in the complex λ plane which account for the divergence of the perturbation series in powers of λ (Bender and Wu 1969, Simon 1970).

In studying the aforementioned models it is convenient to write the Hamiltonian operator (14) in second quantised form through the introduction of creation and annihilation operators a^+ and a,

$$x=(g/2)^{1/2}(a+a^+), \qquad p=\mathrm{i}(2g)^{-1/2}(a^+-a), \qquad [a^+,a]=1. \tag{15}$$

The real, positive parameter g enables one to improve convergence as will be shown later on.

Our basis set of vectors $|i\rangle$ will be composed of the complete set of eigenvectors of the particle number operator a^+a. This choice is equivalent to using a set of scaled harmonic oscillator eigenfunctions which has proved to be very useful in obtaining analytic expressions for the eigenvalues of the Hamiltonian operator (14) (McWeeny and Coulson 1948, Banerjee 1978, Dias de Deus 1982, Fernández and Castro 1983a). When g is determined according to variational principles,

$$(\partial H_{nn}/\partial g)(g=g_v)=0, \tag{16}$$

the scaled trial functions obey the virial theorem (Fock 1930, Löwdin 1959). Besides, the basis set of scaled functions built this way has also proved to be suitable for Rayleigh-Ritz calculations (Lu and Nigam 1969, Reid 1970, Balsa *et al* 1983) and for other non-perturbative approaches (Banerjee 1978, Banerjee *et al* 1978). The major attraction of the variational condition (16) is that $H_{nn}(g)$ is given a dependence on n (quantum number) and λ that closely resembles the exact one (McWeeny and Coulson 1948, Banerjee 1978, Dias de Deus 1982, Fernández and Castro 1982a).

If H is split into a zeroth-order operator H_0 containing all the terms that commute with a^+a and a perturbation $V=H-H_0$, we are led to a recently developed and quite promising variational perturbative scheme (Feranchuk and Komarov 1982, Gerry and Silverman 1983, Yamazaki 1984). If $g=g_v$ a very few perturbation terms yield quite accurate results. However, it has been recently shown that the use of g_v is not convenient when large-order perturbation calculations are required because it leads to divergent power series (Fernández *et al* 1984). A numerical investigation has revealed that there is an interval of g values for each λ and n leading to convergent series and that g_v usually lies outside it (Fernández *et al* 1984). This fact will be exploited in the present paper to make the iterative procedure converge quickly enough.

In order to obtain the matrix elements H_{ij} we first put the Hamiltonian operator (14) in second quantised form and then make use of the well known relationships

$$a|i\rangle=i^{1/2}|i-1\rangle, \qquad a^+|i\rangle=(i+1)^{1/2}|i+1\rangle. \tag{17}$$

On doing it we are led to a particular case of (7) where $A_{ij}=H_{ij}$ and $B_{ij}=\delta_{ij}$. Notice that $H_{ij}=0$ if $|i-j|>2k$. Since the calculation of the matrix elements is straightforward, it is not necessary to give them explicitly in each case.

In order to illustrate the effect of g on the convergence rate we have calculated $\log|E_0^{(s)}-E_0^{(s+1)}|$ for the ground state of the quartic oscillator $H_4(0,1)$. The best g value (g_b) in this and in the other examples has been obtained approximately by numerical search. The convergence rate decreases noticeably as $|g-g_b|$ increases as shown in figure 1. This situation occurs in all the examples studied and reveals the great practical importance of finding a suitable basis set of functions. In most cases it is not necessary to calculate g_b accurately because the convergence rate of the iterative

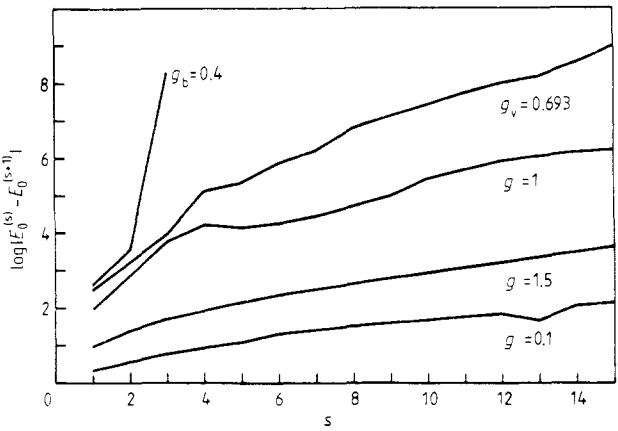

Figure 1. Convergence rate of the sequence $E_0^{(s)}$ for $H_4(0, 1)$ for different values of the scaling parameter g.

method is large enough provided $|g - g_b| < \varepsilon$ where ε depends on the problem. It is found that ε decreases largely as λ, k or n increases. Calculations show that the present procedure converges more quickly and for a larger range of g values than the perturbation method of Feranchuk and Komarov (1982) does (Fernández *et al* 1984). For example, in the case of the quartic oscillator (figure 1) the present technique converges for $g = g_v$ and even for the basis set of unscaled functions ($g = 1$).

The lowest eigenvalues of $H_{2k}(1, \lambda)$ and $H_{2k}(0, 1)$ ($k = 2, 3,$ and 4) are shown in tables 1-6 together with g_b and the number of iterations (N) required to make the last figure stable. (The number of basis vectors M is also large enough to assure stability of the results.) Present results agree with those obtained previously by Banerjee (1978) and Banerjee *et al* (1978).

The convergence rate decreases markedly when λ, n or k increases. Calculation for very large λ values (say $\lambda > 100$) is facilitated by taking into account that the

Table 1. Eigenvalues of $H_4(1, \lambda)$.

λ	n	E_n	g_b	N	E_n (Banerjee 1978)
10^{-4}	0	1.000 074 986 880 200	1.00	2	1.000 074 986 880 20
	1	3.000 374 896 936 121	1.00	2	3.000 374 896 936 12
	2	5.000 974 615 938 386	1.00	3	5.000 974 615 938 39
	3	7.001 874 016 667 660	1.00	3	7.001 874 016 667 66
1	0	1.392 351 641 530 292	0.35	11	1.392 351 641 530 29
	1	4.648 812 704 212 078	0.35	11	4.648 812 704 212 08
	2	8.655 049 957 759 310	0.35	12	8.655 049 957 759 31
	3	13.156 803 898 049 88	0.35	12	13.156 803 898 049 9
10^4	0	22.861 608 870 272 47	0.02	17	22.861 608 870 272 5
	1	81.903 316 953 284 47	0.02	18	81.903 316 953 284 5
	2	160.685 912 611 711 5	0.02	18	160.685 912 611 712
	3	250.950 743 891 712 4	0.02	19	250.950 743 891 713

Table 2. Eigenvalues of $H_6(1, \lambda)$.

λ	n	E_n	g_b	N	E_n (Banerjee 1978)
10^{-4}	0	1.000 187 228 153 681	1.00	3	1.000 187 228 153 68
	1	3.001 308 843 629 600	1.00	4	3.001 308 843 629 60
	2	5.004 664 711 299 977	1.00	5	5.004 664 711 299 98
	3	7.011 720 523 720 425	1.00	5	7.011 720 523 720 43
1	0	1.435 624 619 003 392	0.20	28	1.435 624 619 003 39
	1	5.033 395 937 720 267	0.20	27	5.033 395 937 720 27
	2	9.966 621 999 718 110	0.20	31	9.966 621 999 718 11
	3	15.989 440 787 825 73	0.22	49	15.989 440 787 825 7
10^4	0	11.478 798 042 264 54	0.20	31	11.478 798 042 264 5
	1	43.457 784 742 680 45	0.20	27	43.457 784 742 680 4
	2	90.821 278 911 708 85	0.20	31	90.821 278 911 708 8
	3	149.457 970 316 336 1	0.23	74	149.457 970 316 336

Table 3. Eigenvalues of $H_8(1, \lambda)$.

λ	n	E_n	g_b	N	E_n (Banerjee 1978)
10^{-4}	0	1.000 646 369 874 074	0.85	10	1.000 646 369 874 07
	1	3.005 726 955 351 208	0.76	12	3.005 726 955 351 21
	2	5.025 394 969 087 810	0.70	14	5.025 394 969 087 81
	3	7.076 668 972 602 773	0.70	19	7.076 668 972 602 77
1	0	1.491 019 895 662 205	0.120	59	1.491 019 895 662 21
	1	5.368 778 061 748 129	0.102	72	5.368 778 061 748 13
	2	10.993 737 335 502 95	0.102	83	10.993 737 335 503 0
10^4	0	7.778 272 214 311 099	0.120	68	7.778 272 214 311 10
	1	30.106 900 557 858 13	0.130	58	30.106 900 557 858 1
	2	64.760 471 754 927 17	0.120	59	64.760 471 754 927 2

Table 4. Eigenvalues of $H_4(0, 1)$.

n	E_n	g_b	N	E_n (Banerjee *et al* 1978)
0	1.060 362 090 484 183	0.40	13	1.060 362 090 484 18
1	3.799 673 029 801 394	0.40	15	3.799 673 029 801 39
2	7.455 697 937 986 738	0.40	14	7.455 697 937 986 74
3	11.644 745 511 378 16	0.40	17	11.644 745 511 378 2

Table 5. Eigenvalues of $H_6(0, 1)$.

n	E_n	g_b	N
0	1.144 802 453 797 053	0.20	29
1	4.338 598 711 513 981	0.20	27
2	9.073 084 560 921 433	0.20	35
3	14.935 169 634 910 74	0.22	95

Table 6. Eigenvalues of $H_8(0, 1)$.

n	E_n	g_b	N
0	1.225 820 113 800 492	0.12	54
1	4.755 874 413 960 76	0.13	55
2	10.244 946 977 236 86	0.13	50

eigenvalues of $H_{2k}(1, \lambda)$ obey (Simon 1970)

$$E_n(1, \lambda) = \lambda^{1/(k+1)} E_n(\lambda^{-2/(k+1)}, 1). \tag{18}$$

The strategy is solving the secular equation for $H_{2k}(\lambda^{-2/(k+1)}, 1)$ to obtain the eigenvalues of $H_{2k}(1, \lambda)$. The improvement is due to the fact that the convergence rate for $H_{2k}(0, 1)$ is large enough as shown in tables 4-6.

Convergence depends most critically on k and n. For example, the sequences $E_n^{(s)}$ and $\psi_n^{(s)}$ diverge when $k = 4$ and $n > 2$ unless λ is small enough. Though there are several numerical techniques to improve convergence of iterative methods (Collatz 1966, Ortega and Rheinboldt 1970, Dahlquist and Björk 1974) we do not discuss them here because we are interested in keeping our procedure as simple as possible. Besides, the lowest states of the quantum mechanical models studied here are very important for many physical purposes and the iterative method applies successfully to them.

The next example we consider is the double well potential model posed by the Hamiltonian operator $H_4(-Z^2, 1) = p^2 - Z^2x^2 + x^4$. The two lowest eigenvalues are shown in table 7 for several Z values. The convergence rate decreases markedly and g_b increases slowly as Z increases. The iterative procedure is divergent for $Z^2 > 10$. Fortunately $Z^2 = 10$ is large enough for many physical purposes. Convergence when $5 < Z^2 \leqslant 10$ is assured by solving the secular equation for $H_4(-1, Z^{-3})$. The eigenvalues of $H_4(-Z^2, 1)$ are then obtained as $E_n(-Z^2, 1) = ZE_n(-1, Z^{-3})$. Our results agree with

Table 7. Eigenvalues of $H_4(-Z^2, 1) = p^2 - Z^2x^2 + x^4$.

Z^2	n	E_n	g_b	N	E_n(Balsa *et al* 1983)
0.5	0	0.870 017 518 371 6121	0.4	15	0.870 017 518 372
	1	3.333 779 329 887 006	0.4	19	3.333 779 329 89
1	0	0.657 653 005 180 7150	0.4	16	0.657 653 005 191
	1	2.834 536 202 119 304	0.4	15	2.834 536 202 12
2	0	0.137 785 848 188 2225	0.4	19	0.137 785 848 189
	1	1.713 027 897 767 676	0.4	15	1.713 027 897 77
4	0	−1.710 350 450 132 640	0.4	32	−1.710 350 450 13
	1	−1.247 922 492 066 215	0.4	25	−1.247 922 492 07
5	0	−3.410 142 761 239 830	0.4	44	−3.410 142 761 24
	1	−3.250 675 362 289 236	0.4	38	−3.250 675 362 29
7	0	−8.671 105 208 704 203	0.5	208	−8.671 105 208 70
	1	−8.662 452 224 881 444	0.5	199	−8.662 452 224 88
10	0	−20.633 576 702 947 80	0.5	324	−20.633 576 702 9
	1	−20.633 546 884 404 92	0.5	300	−20.633 546 884 4

those obtained by Balsa *et al* (1983) who carried out a Rayleigh-Ritz calculation with a properly scaled basis set of eigenfunctions of the harmonic oscillator. The latter technique is preferable when results for $Z^2 > 10$ are required.

4. Linear confining model

The Hamiltonian operator $H(Z, \lambda) = \frac{1}{2}p^2 - Z/r + \lambda r$ has received considerable attention as a suitable model in particle physics (see, for example, Quigg and Rosner 1979, Eichten *et al* 1978). The Schrödinger equation is most conveniently written as

$$(\tfrac{1}{2}rp^2 - Z + \lambda r^2)|\Psi_n\rangle = E_n r|\Psi_n\rangle, \tag{19}$$

which is a particular case of (5) where $A = \frac{1}{2}rp^2 - Z + \lambda r^2$ and $B = r$.

On obtaining an appropriate secular equation for this model it is convenient to write the operators A and B in terms of the three generators K_0, $K_\pm = K_1 \pm iK_2$ of the SO(2, 1) Lie algebra which obey the following commutation relations:

$$[K_0, K_\pm] = \pm K_\pm, \qquad [K_-, K_+] = 2K_0. \tag{20}$$

The Casimir invariant is found to be

$$Q = K_0^2 - \tfrac{1}{2}(K_+K_- + K_-K_+). \tag{21}$$

We shall utilise the eigenvectors $|n, k\rangle$ of K_0 as our basis set:

$$K_0|n, k\rangle = (n + k)|n, k\rangle, \qquad n = 0,1\ 2, \ldots, k > 0. \tag{22}$$

The Lie algebra is realised as

$$K_0 = \tfrac{1}{2}(g^{-1}rp^2 + gr), \qquad K_1 = \tfrac{1}{2}(g^{-1}rp^2 - gr), \tag{23a, b}$$

$$K_2 = \boldsymbol{r}\cdot\boldsymbol{p} - i, \tag{23c}$$

in order to obtain a scaled basis set of states. Properly scaled basis set of functions proved to be very useful in many approximate calculations on central field quantum mechanical models (Lu and Nigam 1969, Gromes and Stamatescu 1979, Dias de Deus *et al* 1981, Fernández and Castro 1983b, Gerry and Silverman 1984) and in the present paper the scaling parameter g will be determined in order to obtain a large enough convergence rate. The way we introduce the scaling parameter g into the Schrödinger equation is simpler than, though entirely equivalent to, that of Gerry and Silverman (1983) who resorted to a unitary transformation of the operator $r(H - E)$.

In this case $k = l + 1$, where $l = 0, 1, \ldots, n - 1$ is the angular momentum quantum number and $n = 1, 2, \ldots$ is the principal quantum number. The matrix elements for the operators A and B are easily obtained from (see Gerry and Silverman (1983) and references therein)

$$K_0|n, l\rangle = n|n, l\rangle, \tag{24a}$$

$$K_1|n, l\rangle = \tfrac{1}{2}[(n-l)(n+l+1)]^{1/2}|n+1, l\rangle + \tfrac{1}{2}[(n+l)(n-l-1)]^{1/2}|n-1, l\rangle. \tag{24b}$$

Clearly $A_{ij} = \langle i, l|A|j, l\rangle = 0$ if $|i-j| > 2$ and $B_{ij} = \langle i, l|B|j, l\rangle = 0$ if $|i-j| > 1$.

The lowest six eigenvalues of $H(0, 1)$ are shown in table 8. When $l = 0$ they are simply related to the zeros a_n ($n = 1, 2, \ldots$) of the regular Airy function: $E_{n0} = -a_n/2^{1/3}$ (Abramowitz and Stegun 1970). Our results compare favourably with those obtained by numerical integration of the Schrödinger equation (Eichten *et al* 1978).

Table 8. Eigenvalues of $H(0, 1) = \frac{1}{2}p^2 + r$.

(n, l)	E_{nl}(present)	g_b	N	E_{nl}
(1, 0)	1.855 757 081 489 239	0.852	35	1.855 757 08[a]
(2, 0)	3.244 607 624 003 159	0.889	212	3.244 607 62[a]
(2, 1)	2.667 829 482 852 616	0.612	52	2.667 9[b]
(3, 0)	4.381 671 239 286 131	0.922	447	4.381 671 24[a]
(3, 1)	3.876 791 997 803 478	0.731	171	3.876 8[b]
(3, 2)	3.371 784 491 979 285	0.677	82	3.371 8[b]

[a] Abramowitz and Stegun (1970).
[b] Eichten *et al* (1978).

A difficulty arises when applying the method to $H(1, \lambda)$. Only those states with $n = l+1$ are obtained for each l value disregarding the value set for n. However, this undesirable behaviour of the sequences $E_{nl}^{(s)}$ is easily removed by solving the secular equation iteratively for $H(\lambda^{-1/3}, 1)$ and then obtaining the eigenvalues of $H(1, \lambda)$ as $E_{nl}(1, \lambda) = \lambda^{2/3} E_{nl}(\lambda^{-1/3}, 1)$. This strategy is used only when $n > l+1$ and the convergence rate of the sequences $E_{nl}^{(s)}(\lambda^{-1/3}, 1)$ and $E_{nl}^{(s)}(0, 1)$ are quite similar as shown in

Table 9. Eigenvalues of $H(1, \lambda) = \frac{1}{2}p^2 - 1/r + \lambda r$.

λ	(n, l)	E_{nl} (present)	g_b	N	E_{nl}
500	(1, 0)	108.365 810 438 635 8	0.07	41	108.365 80[a]
	(2, 0)	198.514 307 138 606 0	0.72	139	
	(2, 1)	162.895 637 328 560 8	0.06	43	
	(3, 0)	271.273 083 062 621 6	0.92	441	
	(3, 1)	240.089 707 956 872 6	0.72	148	
	(3, 2)	208.513 378 897 178 9	0.06	38	
62.5	(1, 0)	24.856 298 746 885 86	0.13	41	24.856 30[a]
	(2, 0)	48.127 003 723 054 18	0.73	141	
	(2, 1)	39.409 253 950 052 92	0.11	52	
	(3, 0)	66.613 899 513 284 91	0.92	449	
	(3, 1)	58.977 740 052 241 80	0.72	159	
	(3, 2)	51.144 563 618 567 93	0.12	33	
0.976 562 50	(1, 0)	0.556 763 812 860 182 9	0.40	33	0.556 767[a]
	(2, 0)	2.405 052 980 059 900	0.72	125	
	(2, 1)	1.937 413 616 076 400	0.49	32	
	(3, 0)	3.692 879 407 153 785	0.92	432	
	(3, 1)	3.278 753 867 982 728	0.72	144	
	(3, 2)	2.814 025 139 978 173	0.47	29	
0.05	(1, 0)	−0.428 119 973 006 343 9	0.91	10	−0.428 120[b]
	(2, 0)	0.111 019 874 415 110 6	0.72	123	
	(2, 1)	0.068 731 817 681 159 94	0.99	12	
	(3, 0)	0.349 963 355 109 784 6	0.92	433	
	(3, 1)	0.310 633 263 431 254 0	0.72	142	
	(3, 2)	0.255 536 883 056 485 7	0.987	26	

[a] Eichten *et al* (1978).
[b] Austin (1981).

tables 8 and 9. Our results are very accurate in the whole range of λ values and compare favourably with those obtained by Eichten *et al* (1978) and Austin (1981) (also see Killingbeck 1981).

5. Conclusions

The iterative procedure presented in this paper is very simple and yields highly accurate eigenvalues with very little computation. When it is convergent, it seems to be preferable to any other technique. The eigenfunctions obtained this way must be as accurate as those coming from Rayleigh-Ritz calculations. The method applies succesfully also to many dimensional quantum mechanical systems such as coupled anharmonic oscillators as will be shown in a forthcoming paper.

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