A method of successive approximations for the generalized anharmonic problem

G. Bozzolo
Analex Corporation, 21775 Brookpark Rd., Fairview Park, OH 44126, U.S.A.

C. Esebbag, J. Núñez, A. Plastino
Departamento de Física, Universidad Nacional de La Plata, C.C. 67, 1900 La Plata, Argentina

J. Rovine
Physics Department, Oberlin College, Oberlin OH 44074, U.S.A.

(Recibido el 27 de julio de 1988; aceptado el 12 de mayo de 1989)

Abstract. An extremely simple method for dealing with the generalized anharmonic oscillator problem by recourse to a series of successive approximations to the exact results is presented and illustrated with reference to the x^4 and x^6 cases.

PACS: 03.65.Ca; 11.90.+t; 33.10.Cs

1. Introduction

In this work we propose a method of successive approximations to the exact eigenvalues E_J of the Hamiltonian

$$H = -\frac{d^2}{dx^2} + V(x), \tag{1.1}$$

with $V(x)$ representing a broad class of even functions of the coordinate ($V(x) \in C^\infty$) which admits a series expansion

$$V(x) = \sum_{j=0}^{\infty} \frac{V^{(j)}(0)}{j!} x^j. \tag{1.2}$$

The knowledge of the eigenvalues of Hamiltonians of the type (1.1) is of great relevance in many branches of physics and chemistry [1–16], and efforts towards finding them are currently being carried out by numerous investigators.

2. Formalism

2.1 The exact solution

We introduce, first of all, the creation and destruction operators

$$a^\dagger = \frac{x - ip}{\sqrt{2}}, \qquad a = \frac{x + ip}{\sqrt{2}} \tag{2.1}$$

so that

$$[a, a^\dagger] = 1, \tag{2.2}$$

and rewrite Eq. (1.1) in the fashion (remembering that V is even)

$$H = \frac{1}{2}\left(2a^\dagger a + 1 - a^{\dagger 2} - a^2\right) + \sum_{j=0}^{\infty} \frac{V^{(2j)}(0)(a + a^\dagger)^{2j}}{(2j)!2^j}. \tag{2.3}$$

The operators $(a + a^\dagger)^{2j}$ appearing in Eq. (2.3) can be expanded in an "ordered" form so that H is, finally,

$$H = \frac{1}{2}\left(2a^\dagger a + 1 - a^{\dagger 2} - a^2\right) + \sum_{rs} \sum_{j=\frac{r+s}{2}} \frac{V^{(2j)}(0)}{(2j)!2^j} A_{rs}^{(j)} a^{\dagger r} a^s \tag{2.4}$$

where

$$A_{2r-s,s}^{(j)} = \binom{2r}{s}\binom{j}{r}\frac{(2j-1)!!}{(2r-1)!!}. \tag{2.5}$$

The central idea is that of relating the eigenstates $|J\rangle$ of H to the corresponding ones $|j\rangle$ of the harmonic oscillator Hamiltonian by means of a unitary transformation, effected by the operator T:

$$|J\rangle = T|j\rangle \tag{2.6}$$

where

$$T = \prod_{k=1}^{\infty} \exp(iF_k) = \prod_{k=1}^{\infty} \exp(-h_k B_k), \tag{2.7}$$

$$F_k = ih_k(a^{\dagger 2k} - a^{2k}) = ih_k B_k, \tag{2.8}$$

and the h_k are variational parameters to be adjusted so as to minimize

$$E_j = \langle j|T^\dagger HT|j\rangle. \tag{2.9}$$

A minimization of (2.7) with respect to the (infinite) set of parameters h_k would yield (or closely approximate) the exact ground state of the Hamiltonian (1.1) (and for reasons of symmetry, also the first excited state). As this is (of course) not feasible, we propose now a (hopefully) suitable algorithm that enables one to "progress" towards the exact eigenvalues E_j of H by recourse to a series of successive approximations.

2.2 Algorithm for obtaining successive approximations

The objective of this section is to provide simple expressions for the ground state and first excited state energies in term of the variational parameters h. In the process of achieving this goal, a systematic way of defining successive approximations to the exact results [cf. Eq. (2.9)] will become apparent.

Instead of dealing with the operator T as defined by Eq. (2.7), it seems convenient to introduce a new series of operators, which will eventually replace $T^\dagger HT$ by a more manageable expression.

Such hierarchy of operators is given by

$$H_0 = H \tag{2.10}$$

$$H_1(h_1) = \exp(h_1 B_1) H_0 \exp(-h_1 B_1) \tag{2.11}$$

$$H_2(h_1, h_2) = \exp(h_2 B_2) H_1(h_1) \exp(-h_2 B_2) \tag{2.12}$$

$$\vdots$$

$$H_N(h_1, h_2, \ldots, h_N) = \exp(h_N B_N) H_{N-1}(h_1, \ldots, h_{N-1}) \exp(-h_N B_N) \tag{2.13}$$

and for the sake of a more concise notation, we define the vector $\vec{h}$ of components $h_1, h_2, \ldots, h_N$.

Note that when $N \to \infty$, the transformed Hamiltonian $H(\vec{h})$ is equivalent to $T^\dagger HT$.

The advantage of rewriting $T^\dagger HT$ this way lies in the fact that the operators H_N allow for a simpler expansion in terms of the creation and destruction operators a and $a^\dagger$, thus facilitating the computation of expectation values.

By a suitable reordering of the second quantization operators involved, we can always recast Eq. (2.13) as

$$H_N(h_N) = \sum_r \sum_s H_{rs}^{(N)} a^{\dagger r} a^s. \tag{2.14}$$

In doing this, we are replacing $T^{\dagger}HT$ by a convenient "power series", in which the expansion coefficients, $H_{rs}^{(N)}$, will have the explicit dependence on the variational parameters h_j, needed to carry out the minimization outlined in the previous section.

Our goal is now that of devising a recurrence algorithm in order to obtain the coefficients $H_{rs}^{(N)}$. This can be conveniently achieved if we introduce an additional set of operators, given by

$$C^{(1,0)} = H_0 \tag{2.15}$$

$$C^{(2,0)} = H_1(h_1) \tag{2.16}$$

$$\vdots$$

$$C^{(N,0)} = H_{N-1}(\vec{h}_{N-1}) \tag{2.17}$$

and

$$C^{(m,n+1)} = \left[B_m, C^{(m,n)}\right] \tag{2.18}$$

so as to be in a position to write

$$H_2(h_2) = \sum_i \frac{h_2^i}{i!} C^{(2,i)} \tag{2.19}$$

and in a similar fashion

$$C^{(N,n+1)} = \left[B_N, C^{(N,n)}\right], \tag{2.20}$$

$$H_N(h_N) = \sum_r \sum_s \frac{h_N^i}{i!} C^{(N,i)}. \tag{2.21}$$

The motivation in introducing the operators $C^{(N,m)}$ becomes clear once we notice that the transformed Hamiltonian $H_N(\vec{h}_N)$ can be written as in Eq. (2.21), thus "separating" the highest-order variational parameter dependence in the form of a power series. Further simplification arises when one "expands" the operators $C^{(N,m)}$ in terms of the elementary operators $a^{\dagger r}a^s$, as it was done before with $H_N(\vec{h}_N)$ [cf. Eq. (2.14)]. If we assume that $C^{(N,m)}$ can be written as

$$C^{(N,n)} = \sum_r \sum_s c_{rs}^{(N,n)} a^{\dagger r} a^s, \tag{2.22}$$

where the coefficients $c_{rs}^{(N,n)}$ are given by

$$c_{rs}^{(N,n+1)} = -(2N)! \sum_{p=1}^{2N} \frac{f(C^{(N,n)})}{(2N-p)!p!} \tag{2.23}$$

where

$$f(C^{(N,n)}) = \frac{(s+p)!}{s!} c_{r+p-2N,s+p}^{(N,n)} + \frac{(r+p)!}{r!} c_{r+p,s+p-2N}^{(N,n)}. \tag{2.24}$$

These last expressions are obtained after a straightforward application of (2.20) to (2.22), yielding a recurrence relation between the expansion coefficients $c_{rs}^{(N,n)}$.

After replacing (2.22) in (2.21), and comparing with (2.14), we finally obtain the following identity for the coefficients $H_{rs}^{(N)}$:

$$H_{rs}^{(N)} = \sum_n \frac{h_N^n}{n!} c_{rs}^{(N,n)} \tag{2.25}$$

so that the transformed Hamiltonian is given by

$$H_N(h_N) = \sum_r \sum_s \frac{h_N^n}{n!} c_{rs}^{(N,n)} a^{\dagger r} a^s. \tag{2.26}$$

This expression can be understood as some sort of series expansion of the operator $T^\dagger HT$ in powers of the variational coefficients h_j, which is most important when dealing with the computation of expectation values. Remembering that in the case of the eigenstates of the harmonic oscillator states $|j\rangle$,

$$\langle j|a^{\dagger r} a^s|j\rangle = \frac{j!}{(j-r)!}, \tag{2.27}$$

we finally arrive at

$$E_j^{(N)}(h_N) = \sum_n \frac{h_N^n}{n!} \sum_{r=0}^{j} r! \binom{j}{r} c_{rr}^{(N,n)}(\vec{h}_{N-1}). \tag{2.28}$$

In particular, for $j = 0$ (ground state) and $j = 1$ (first excited state), one finds

$$E_0^{(N)} = \sum_n \frac{h_N}{n!} c_{00}^{(N,n)} \tag{2.29}$$

and

$$E_1^{(N)} = \sum_n \frac{h_N^n}{n!}(c_{00}^{(N,n)} + 2c_{11}^{(N,n)}). \tag{2.30}$$

It is important to notice that only in these cases the energies (2.28) are upper bounds for the corresponding exact results.

In (2.28) we still face an N-parameter minimization procedure. It is at this point where the procedure outlined in this section appears to be particularly useful in the search for alternate, approximate algorithms to deal with the multiple minimization problem. A convenient scheme of successive approximations suggests itself if we realize that a "step-by-step" algorithm can be defined by first evaluating

$$e_j^{(1)} = \langle j|H_1(h_1)|j\rangle \tag{2.31}$$

and minimizing with respect to the only variational parameter involved: h_1. Once this parameter is fixed, say h_1^*, one goes on to

$$e_j^{(2)}(h_1, h_2) = \langle j|H_2(h_1, h_2)|j\rangle \tag{2.32}$$

and use h_1^* for the value of h_1, thus retaining the simplicity of a one-parameter minimization, with respect to h_2. The process continues with e_3, etc., until convergence is achieved. Because of the way in which the operators H_N were defined [cf. Eq. (2.28)], each successive step is as computationally simple as the previous one.

3. Application to the anharmonic oscillator

As an illustration of the formalism introduced in the previous section, we consider the following Hamiltonians:

$$H_4 = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 + \lambda x^4 \tag{3.1}$$

and

$$H_6 = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 + \lambda x^6, \tag{3.2}$$

which in appropriate units can be recast as

$$H_n = -\frac{d^2}{dx^2} + x^2 + \lambda x^m; \qquad m = 4, 6. \tag{3.3}$$

Energies corresponding to the ground state (g.s.) and to the first excited state of H_4 are tabulated in Table 1 for several values of λ. For each λ-value, six figures are

	N	0.1	0.2	0.4	0.6	0.8	1.0	2.0	4.0	8.0	20.	50.	100.
	1	1.0662	1.1206	1.2098	1.2833	1.3468	1.4033	1.6250	1.9288	2.3333	3.0625	4.0785	5.0952
E_0	2	1.0653	1.1184	1.2052	1.2766	1.3385	1.3935	1.6098	1.9070	2.3034	3.0190	4.0172	5.0167
	3	1.0653	1.1183	1.2048	1.2759	1.3375	1.3924	1.6076	1.9033	2.2980	3.0110	4.0060	5.0050
E_0 (exact)		1.0653	1.1183	1.2048	1.2758	1.3375	1.3923	1.6075	1.9031	2.2975	3.0099	4.0040	4.9992

	1	3.3103	3.5468	3.9161	4.2100	4.4592	4.6782	5.5199	6.6479	8.1274	10.764	14.441	18.047
E_1	2	3.3069	3.5393	3.9020	4.1907	4.4358	4.6512	5.4799	6.5922	8.0524	10.657	14.262	17.856
	3	3.3069	3.5390	3.9012	4.1895	4.4342	4.6493	5.4763	6.5865	8.0442	10.648	14.250	17.840
E_1 (exact)		3.3069	3.5390	3.9011	4.1893	4.4338	4.6488	5.4758	6.5857	8.0431	10.643	14.242	17.830

TABLE 1. Energies for the ground state (E_0) and first excited state (E_1) for the potential $V(x) = x^2 + x^4$. Successive approximations to the exact results of Ref. [17] obtained with the present approach are labeled $N = 1$ (for F_1), $N = 2$ (for $F_1 + F_2$) and $N = 3$ (for $F_1 + F_2 + F_3$).

	N	0.1	0.2	0.4	0.6	0.8	1.0	2.0	4.0	8.0	20.	50.	100.
	1	1.1199	1.1928	1.2949	1.3704	1.4317	1.4841	1.6756	1.9162	2.2136	2.7100	3.3488	3.9470
E_0	2	1.1103	1.1768	1.2709	1.3410	1.3982	1.4471	1.6271	1.8543	2.1363	2.6085	3.2177	3.7889
	3	1.1090	1.1738	1.2653	1.3332	1.3886	1.4360	1.6105	1.8310	2.1054	2.5656	3.1601	3.7185
E_0 (exact)		1.1090	1.1738	1.2651	1.3329	1.3882	1.4356	1.6099	1.8304	2.1046	2.5646	3.1590	3.7169

	1	3.6384	3.9664	4.4022	4.7140	4.9633	5.1738	5.9313	6.8651	8.0042	9.8851	12.228	14.525
E_1	2	3.6007	3.9100	4.3235	4.6205	4.8586	5.0598	5.7859	6.6835	7.7806	9.5953	11.915	14.079
	3	3.6007	3.9097	4.3228	4.6194	4.8570	5.0578	5.7823	6.6778	7.7724	9.5944	11.903	14.062

TABLE 2. Energies for the ground state (E_0) and first excited state (E_1) for the potential $V(x) = x^2 + x^4$. Successive approximations to the exact results of Ref. [17] obtained with the present approach are labeled $N = 1$ (for F_1), $N = 2$ (for $F_1 + F_2$) and $N = 3$ (for $F_1 + F_2 + F_3$).

given, which correspond, respectively, to $e_j^{(1)}(h_1), \ldots, e_j^{(5)}(h_5)$ $(j = 0, 1)$ and to the exact results of Biswas *et al.* [7]. Similar results are displayed in Table 2 for H_6.

Figure 1 shows the wave functions for the ground state and first excited state of H_4. The corresponding harmonic oscillator wave functions are also shown for comparison. Fig. 2 shows similar results for H_6.

The convergence of the wave functions is displayed in Table 3, where the overlap between wave functions computed at successive orders of approximation is shown.

Convergence is seen to be quite rapidly achieved in all cases studied, although there are some practical limitations to the method that might not warrant the same behavior in other situations; in order to obtain a reasonable precision in the results, particular care should be taken when dealing with higher powers of the coordinate x or with large coupling constants.

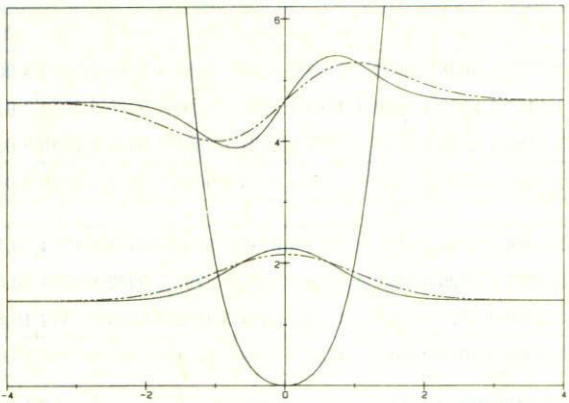

FIGURE 1. Ground state and first excited state wave functions (solid lines) for the potential well $V(x) = x^2 + x^4$. The potential well and the corresponding harmonic oscillator wave functions (dashed lines) are also displayed.

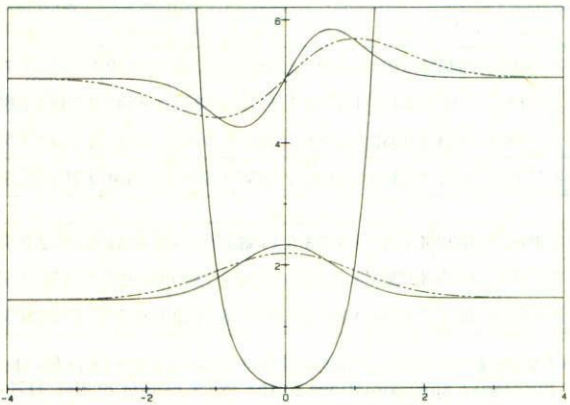

FIGURE 2. Ground state and first excited state wave functions (solid lines) for the potential well $V(x) = x^2 + x^6$. The potential well and the corresponding wave functions (dashed lines) are also displayed.

$V(x)$	$N=1$ $N=2$	$N=2$ $N=3$	$N=3$ $N=4$
$x^2 + x^4$ (g.s.)	0.9807	0.9960	0.9999
$x^2 + x^4$ (f.e.s.)	0.9623	0.9888	0.9999
$x^2 + x^6$ (g.s.)	0.9800	0.9912	0.9988
$x^2 + x^6$ (f.e.s.)	0.9601	0.9876	0.9982

TABLE 3. Overlap between two successive approximations to the wave function. N denotes the N-th order approximation to the eigenstates of the anharmonic oscillator. g.s. denotes the ground state and f.e.s. the first excited state.

4. Conclusions

An extremely simple algorithm for finding the exact eigenvalues corresponding to Hamiltonians of the general form (1.1) has been introduced. It is a non-perturbative method of successive approximations that converges quite rapidly, as illustrated by the examples shown in Section 3. Our approach yields good upper bounds to the ground state and first excited state of (3.3).

Acknowledgements

This work was partially supported by the Engineering Directorate, NASA Lewis Research Center, Cleveland, OH 44135, U.S.A. Partial support is also acknowledged to USDOE Contract # DE-ACO2-85ER40199.

References

1. K. Banerjee, S.P. Bhatnagar, V. Choudhury and S.S. Konwal, *Proc. R. Soc.* **A360** (1978) 375.
2. C. Bender and T.T. Wu, *Phys. Rev.* **184** (1969) 1231.
3. C. Bender and T.T. Wu, *Phys. Rev.* **D7** (1973) 1620.
4. J.P. Boyd, *J. Math. Phys.* **18** (1978) 1445.
5. G. Bozzolo, A. Plastino, *Phys. Rev.* **D24** (1981) 3113.
6. S.I. Chan, D. Stelman and L.E. Thompson, *J. Chem. Phys.* **41** (1984) 2828.
7. Y.T. Fung, Y.W. Chan and W.Y. Wan, *J. Phys. A.: Math. Gen.* **11** (1978) 829.
8. G.H. Gillespie, *Lett. Nuovo Cim.* **16** (1976) 86.
9. S. Graffi, V. Grecchi and B. Simon, *Phys. Lett.* **32B** (1970) 631.
10. S. Graffi, V. Grecchi and E. Turchetti, *Nuovo Cim.* **9B** (1971) 313.
11. S. Graffi and V. Grecchi, *Phys. Rev.* **D8** (1973) 3487.
12. F.R. Halpern, *J. Math. Phys.***14** (1973) 219.
13. F.T. Hioe, D. MacMillan and E.W. Montroll, *J. Math. Phys.* **17** (1976) 1320.
14. A.M. Jaffe, *Commun. Math. Phys.* **1** (1965) 127.
15. J.M. Kinkaid and E.G.D. Cohen, *Phys. Rep.* **22C** (1975) 57.
16. P. Lu, S.S. Wald and B.L. Young, *Phys. Rev.* **D7** (1973) 1701.
17. S.N. Biswas, M. Datta, R.P. Saxena, P.K. Srivastava and V.S. Varma, *Phys. Rev.* **D12** (1971) 3617; *ibid., J. Math. Phys.* **14** (1973) 1190.

Resumen. Se presenta un método extremadamente simple para tratar el problema del oscilador anarmónico generalizado, basado en una serie de aproximaciones sucesivas a los resultados exactos, y se ilustra con una aplicación a los casos x^4 y x^6.