Two-step approach to one-dimensional anharmonic oscillators

Chen-Shiung Hsue and J. L. Chern
Institute of Physics, National Tsing Hua University, Hsinchu Taiwan 300, Republic of China
(Received 5 July 1983)

We propose a two-step approach to one-dimensional anharmonic oscillators. A generalized coherent-state ansatz is introduced for the first step. A theorem of Wick's ordering and a Bogoliubov transformation are used to simplify the derivation. This is shown to be equivalent to the Hartree approximation. In the second step, standard diagonalization is used for the transformed Hamiltonian. The method yields a clear physical picture and is capable of producing accurately all the low-lying energy levels in a single diagonalization. Asymptotic expansions for the energy levels are easily obtained. The connection with a pure quartic oscillator is pointed out and as a by-product no calculation is necessary in that model. We also include cubic couplings and apply the method successfully for the two-well oscillator.

I. INTRODUCTION

In the last few decades, intensive activities were carried out on the one-dimensional anharmonic oscillators.[1-3] They are of interest because of their importance in molecular vibrations as well as their role in the modeling of nonlinear quantum field theory.[4] In particular, Bender and Wu[2] obtained the disconcerting result that the perturbation series diverged for all values of the coupling parameter for a quartic anharmonic oscillator, no matter how small the coupling was.

In this paper, we present a two-step approach to investigate this system. This approach has a clear physical picture and is capable of producing eigenvalues with high accuracy. As a preparation we discuss a theorem of Wick's ordering in Sec. II, which will help to make the derivation in a simple way. We give a simple derivation for this beautiful trick. In Sec. III, for the first step we assume a "generalized coherent state" of the form

$$|\phi\rangle=\exp\left[\frac{t}{2}a^{\dagger 2}\right]|0\rangle ,$$

where the parameter t is determined by the variation principle. A Bogoliubov transformation is essential in simplifying the calculation. This step is shown to be equivalent to the Hartree approximation. In Sec. IV for the second step we use the standard method to diagonalize the transformed Hamiltonian, with confidence that all the catastrophy effects have been taken care of by the coherent-state ansatz in the first step. The convergence is indeed fast for all values of the quartic coupling. This is given in Sec. V. The asymptotic behavior of the eigenvalues and its connection with a pure quartic oscillator is given in Sec. VI. As a by-product, there is no need to calculate the pure quartic oscillator at all. In Sec. VII a straightforward extension of the model to the case where a cubic coupling is included in addition to quartic anharmonicity is given. As a special case we apply our method to a double-well oscillator. Even the tiny splittings due to tunneling are accurately obtained. The discussion and conclusions are given in the final section.

II. THEOREM ABOUT WICK'S REORDERING

Before we plunge into the problem of the anharmonic oscillators, we will discuss a theorem about Wick's reordering. We start from the Cambell-Baker-Hausdorff formula. In the particular case when the commutator of two operators $[A,B]$ is a c number, we have

$$e^{A+B}=e^{A}e^{B}e^{-[A,B]/2} . \tag{1}$$

Introducing

$$A=\alpha a^{\dagger} \tag{2}$$

and

$$B=\alpha a , \tag{3}$$

where $a^{\dagger}$ and a are any pair of creation and annihilation operators and whose commutator

$$[A,B]=-\alpha^2 \tag{4}$$

is indeed a c number, we have

$$\begin{aligned} e^{\alpha(a+a^{\dagger})}&=e^{\alpha a^{\dagger}}e^{\alpha a}e^{\alpha^2/2} \\ &=e^{\alpha^2/2}:e^{\alpha(a+a^{\dagger})}: . \end{aligned} \tag{5}$$

Here the : : sign means normal ordering with respect to the pair of creation operator $a^{\dagger}$ and annihilation operator a. The usefulness of Eq. (5) in field theory was emphasized recently by Coleman.[5] Expanding Eq. (5) in powers of α, and comparing the coefficients of α^n, we arrive at the following set of relations:

$$(a^{\dagger}+a)^2=:(a^{\dagger}+a)^2:+1 , \tag{6a}$$

$$(a^{\dagger}+a)^3=:(a^{\dagger}+a)^3:+3(a^{\dagger}+a) , \tag{6b}$$

$$(a^{\dagger}+a)^4=:(a^{\dagger}+a)^4:+6:(a^{\dagger}+a)^2:+3 , \tag{6c}$$

and similar formulas for higher orders. These formulas will help simplify all the derivations in the following. Its

generalization to more degrees of freedom and to field theory is straightforward. In fact, this formula is equivalent to Coleman's theorem[5] in field theory.

III. FIRST STEP: COHERENT-STATE ANSATZ AND HARTREE APPROXIMATION

We start with the Hamiltonian

$$H=\tfrac{1}{2}p^2+\tfrac{1}{2}x^2+\lambda x^4 . \tag{7}$$

Equation (7) can be put in a second-quantized form by introducing the creation and annihilation operators $a^\dagger$ and a,

$$a^\dagger=\frac{x-ip}{\sqrt{2}} , \tag{8a}$$

$$a=\frac{x+ip}{\sqrt{2}} , \tag{8b}$$

which yield

$$H=a^\dagger a+\frac{1}{2}+\frac{\lambda}{4}(a+a^\dagger)^4 . \tag{9}$$

We now make an ansatz for a trial state to be a generalized coherent state of the form

$$|\phi\rangle=e^{(t/2)a^{\dagger 2}}|0\rangle . \tag{10}$$

Using the commutator relation, it is straightforward to show that $|\phi\rangle$ satisfies the relation

$$a|\phi\rangle=ta^\dagger|\phi\rangle . \tag{11}$$

Hence, it is natural to introduce a Bogoliubov transformation:

$$b=\frac{a-ta^\dagger}{(1-t^2)^{1/2}} , \tag{12a}$$

$$b^\dagger=\frac{a^\dagger-ta}{(1-t^2)^{1/2}} . \tag{12b}$$

The new pair of creation and annihilation operators $b^\dagger$ and b retain the same commutator relation as the original pair of operators a and $a^\dagger$:

$$[b,b^\dagger]=1 . \tag{13}$$

Furthermore, b is the annihilation operator for the trial wave function

$$b|\phi\rangle=0 . \tag{14}$$

Thus, b and $b^\dagger$ are the annihilation and creation operators for the new "vacuum" state $|\phi\rangle$. The parameter t is chosen by the variational principle so that the energy acquires its minimum value:

$$E(t)=\frac{\langle\phi|H|\phi\rangle}{\langle\phi|\phi\rangle} , \tag{15}$$

$$\frac{dE(t)}{dt}=0 . \tag{16}$$

Using Eqs. (6a), (6b), and (6c), the Hamiltonian (7) may be written as

$$H=E_0+\left[\frac{t}{1-t^2}+\frac{3\lambda}{2}\left[\frac{1+t}{1-t}\right]^2\right](b^2+b^{\dagger 2}) + \left[\frac{1+t^2}{1-t^2}+3\lambda\left[\frac{1+t}{1-t}\right]^2\right]b^\dagger b + \frac{\lambda}{4}\left[\frac{1+t}{1-t}\right]^2 :(b+b^\dagger)^4: \tag{17}$$

with

$$E_0=\frac{1}{2}+\frac{t^2}{1-t^2}+\frac{3\lambda}{4}\left[\frac{1+t}{1-t}\right]^2 . \tag{18}$$

Introducing the variable

$$\omega=\frac{1-t}{1+t} , \tag{19}$$

we have the expression for E_0,

$$E_0=\frac{1+\omega^2}{4\omega}+\frac{3\lambda}{4\omega^2} . \tag{20}$$

The variation principle now yields

$$\frac{dE_0}{d\omega}=0 \tag{21}$$

or

$$\omega-\omega^3+6\lambda=0 . \tag{22}$$

It is important to notice that Eq. (22) also guarantees that the coefficients of b^2 and $b^{\dagger 2}$ in H are zero. This is clearly the condition for the new creation and annihilation operators b and $b^\dagger$ to correspond to the normal modes, and is the general requirement for the Hartree approximation. The Hamiltonian (17) now takes the form

$$H=E_0+\omega b^\dagger b+\frac{\lambda}{4\omega^2}:(b+b^\dagger)^4: \tag{23}$$

with

$$E_0=\frac{1+3\omega^2}{8\omega} . \tag{24}$$

Formula (24) yields the ground-state energy with errors less than 2% for all values of the coupling strength.

V. SECOND STEP : PERTURBATION EXPANSION

We believe that, with the coherent state $|\phi\rangle$ taking care of all the coherent effects, no additional catastrophy will be encountered from now on. In fact we have employed the standard coupled-cluster method[6] which is of the form

$$|\psi\rangle=e^s|\phi\rangle \tag{25}$$

to solve the problem.

A two-term approximation

$$s=\frac{s_2}{2}a^{\dagger 2}+\frac{s_4}{4!}a^{\dagger 4} \tag{26}$$

already yields less than 0.3% error for all values of the coupling constant λ. Here we use an even more straight-

TABLE I. Energy levels of the single anharmonic oscillator with a quartic anharmonicity.

λ	Size of determinant	E_0	E_1	E_2	E_3	E_4
0.1	5×5	0.559 185	1.772 6	3.142 4	4.836	6.72
	9×9	0.559 1470	1.769 507	3.138 70	4.632 6	6.226
	19×19	0.559 14633	1.769 5026	3.138 624	4.628 883	6.220 30
	Exact	0.559 14633	1.769 5026	3.138 624	4.628 883	6.220 30
0.5	5×5	0.696 62	2.334 9	4.337	7.37	10.9
	9×9	0.696 188	2.324 57	4.329 1	6.591 4	9.040 7
	19×19	0.696 1758	2.324 406	4.327 525	6.578 41	9.028 809
	Exact	0.696 1758	2.324 406	4.327 525	6.578 40	9.028 779
1.0	5×5	0.804 607	2.753 07	5.193 9	9.122	13.69
	9×9	0.803 795	2.738 28	5.182 4	7.960 5	10.982 3
	19×19	0.803 77066	2.737 892	5.179 292	7.942 43	10.963 64
	Exact	0.803 77066	2.737 892	5.179 292	7.942 40	10.963 58
10.0	5×5	1.508 16	5.361 35	10.390	19.3	29.8
	9×9	1.505 07	5.323 47	10.359	16.12	22.47
	19×19	1.504 972	5.321 609	10.347 06	16.090 3	22.408 9
	Exact	1.504 972	5.321 608	10.347 06	16.090 1	22.408 8
100.0	5×5	3.139 183	11.277	22.01	41.5	64.5
	9×9	3.131 631	11.192	21.94	34.28	47.87
	19×19	3.131 3843	11.187 255	21.906 91	34.182 8	47.706 6
	Exact	3.131 3842	11.187 254	21.906 90	34.182 5	47.707 2
1000.0	5×5	6.711 5	24.167	47.24	89.4	139
	9×9	6.694 8	23.983	47.08	73.6	102.8
	19×19	6.694 221	23.972 21	47.017 36	73.419 79	102.517
	Exact	6.694 221	23.972 21	47.017 34	73.419 11	102.516

forward approach. In the Hamiltonian (23), we interpret ω to be the frequency for the true physical exciton normal modes. We therefore use the set of vectors

$$|n\rangle=\frac{b^{\dagger n}}{\sqrt{n!}}|\phi\rangle \tag{27}$$

as a basis. The matrix elements for H are then trivial. The only nonzero matrix elements are

$$\langle n|H|n\rangle=n\omega+\frac{6\lambda}{4\omega^2}N(n-1)\,, \tag{28a}$$

$$\langle n-2|H|n\rangle=\langle n|H|n-2\rangle=\frac{\lambda}{\omega^2}[n(n-1)]^{1/2}(n-2)\,, \tag{28b}$$

$$\langle n-4|H|n\rangle=\langle n|H|n-4\rangle=\frac{\lambda}{4\omega^2}[n(n-1)(n-2)(n-3)]^{1/2}\,. \tag{28c}$$

Truncating the basis by limiting $n\leq N$, we may then use the standard diagonalization scheme such as the Jacobi method to obtain all the eigenvalues and the eigenvectors. The resultant eigenvalues are stable with the increase of N for all values of the coupling strength λ. The eigenvalues converge very fast throughout the whole range of λ. Table I gives the results for $N=5$, 9, 19.

VI. ASYMPTOTIC EXPANSION AND THE CONNECTION WITH PURE QUARTIC OSCILLATOR

From Eq. (22), the asymptotic value of the root ω for asymptotic value of λ is

$$\omega(6\lambda)^{1/3}\,. \tag{29}$$

Combining with Eqs. (23) and (24), we have the asymptotic behavior of the root E_n for $\lambda\gg1$ as

$$E_n=\epsilon_n(\lambda)^{1/3}\,, \tag{30}$$

where the coefficients ϵ_n are given by

$$\epsilon_n=\tfrac{3}{8}(6)^{1/3}+\lambda_n\,, \tag{31}$$

and λ_n are the roots of a single operator

$$K=b^{\dagger}b+\tfrac{1}{24}:(b+b^{\dagger})^4:\,. \tag{32}$$

Table II gives the first 20 values of the coefficients. These coefficients will yield all the levels in the pure quartic oscillator since the latter is the limiting case of $\epsilon\to0$ of the

TABLE II. Coefficients ϵ_n for $n=0,1,\ldots,20$ of the asymptotic expansion of the quartic anharmonic oscillator.

n	ϵ_n
0	0.667 986 259
1	2.393 644 02
2	4.696 795 39
3	7.335 730 00
4	10.244 308 5
5	13.379 336 6
6	16.711 889 6
7	20.220 849 5
8	23.889 993 6
9	27.706 393 4
10	31.659 456 5
11	35.740 315 3
12	39.941 416 8
13	44.256 235 4
14	48.679 065 9
15	53.204 869 8
16	57.829 158 4
17	62.547 902 8
18	67.357 462 8
19	72.254 530 3
20	77.236 082 7

following Hamiltonian:

$$H=\tfrac{1}{2}p^2+\tfrac{1}{2}\epsilon x^2+\lambda x^4 . \tag{33}$$

A scaled transformation gives an equivalent form:

$$H=\epsilon\left[\tfrac{1}{2}p^2+\tfrac{1}{2}x^2+\frac{\lambda}{\epsilon^3}x^4\right] . \tag{34}$$

Taking the limit $\epsilon\to 0$, we obtain from (30) the following value of the eigenvalues for the pure quartic oscillator:

$$E_n=\epsilon_n(\lambda)^{1/3} . \tag{35}$$

VII. INCLUSION OF CUBIC COUPLING AND ITS APPLICATION TO DOUBLE-WELL OSCILLATOR

We can extend our treatment for the following Hamiltonian:

$$H=\tfrac{1}{2}p^2+\tfrac{1}{2}x^2+\lambda x^4+gx^3 . \tag{36}$$

From (6b), the inclusion of the cubic term does not alter the discussion in the first step or the Hartree approximation. The only difference lies in the second stage. The Hamiltonian (23) should be changed to

$$H=E_0+\omega b^\dagger b+\frac{\lambda}{4\omega^2}:(b+b^\dagger)^4:$$
$$+\frac{g}{(\sqrt{2\omega})^3}[:(b+b^\dagger)^3:+3(b+b^\dagger)] . \tag{37}$$

For g of the order of λ, the convergence is again uniformly fast. Typical results are given in Table III.

As a severe test of our method, we apply it to the two-well oscillator model which has the Hamiltonian

TABLE III. Typical results of the anharmonic oscillator with cubic and quartic anharmonicity.[a]

G3	G4	Size of determinant	E_0	E_1	E_2	E_3	E_4
0.1	0.1	9×9	0.553 518	1.745 51	3.095 7	4.570	6.148
		19×19	0.553 516 18	1.745 509 3	3.095 397 2	4.567 642	6.142 150
		Exact value	same	same	same	same	6.142 148
1.0	1.0	9×9	0.720 5	2.501 5	4.848	7.53	10.5
		19×19	0.720 463 07	2.501 359 6	4.838 677 84	7.508 78	10.445 7
		Exact value	0.720 463 05	2.501 359 5	4.838 677 8	7.508 76	10.4455
10.0	10.0	9×9	0.826 5	3.934	8.52	13.90	19.9
		19×19	0.825 351 4	3.930 657	8.487 95	13.798 8	19.727
		Exact value	0.825 351 1	3.930 655	8.487 93	13.798 6	19.726
100.	100.	9×9	−3.74	4.21	12.3	23.3	35.8
		19×19	−3.774 20	4.152 83	11.994 3	22.313	34.025
		Exact value	−3.774 23	4.152 76	11.993 9	22.311	34.014
1000	1000	10×10	−81.2	−37.4	−2.5	15.0	39.0
		19×19	−82.278	−40.29	−6.79	11.20	29.76
		Exact	−82.291	−40.37	−6.95	11.06	29.34

[a]All the exact values quoted can be obtained by diagonalization with a size of 30×30.

TABLE IV. Energy levels of the double-well oscillator.

λ^{ϵ}	ϵ_0 ϵ_1	ϵ_2 ϵ_3	ϵ_4 ϵ_5
0.04	1.371 122 236	3.901 359 952	5.838 911 090
	1.371 308 461	3.918 263 338	6.183 906 204
0.05	1.358 422 104	3.746 917 081	5.369 059 360
	1.360 133 598	3.848 838 300	6.177 383 139
0.06	1.343 027 202	3.542 342 544	5.181 424 577
	1.350 326 968	3.819 606 255	6.315 544 236
0.07	1.323 274 074	3.342 216 720	5.187 369 934
	1.343 365 616	3.833 129 938	6.532 394 860
0.08	1.298 249 887	3.184 662 443	5.288 919 012
	1.340 294 971	3.881 190 140	6.787 428 110
0.09	1.268 237 584	3.075 954 576	5.435 992 044
	1.341 520 024	3.954 001 892	7.059 115 212
1.10	1.234 507 163	3.009 488 545	5.605 133 797
	1.346 940 869	4.043 546 040	7.336 113 819
0.12	1.162 626 585	2.967 723 297	5.968 432 268
	1.368 699 619	4.251 215 607	7.884 603 611
0.14	1.093 828 994	3.000 806 735	6.336 018 860
	1.401 614 901	4.475 767 277	8.411 046 927

$$H=\tfrac{1}{2}p^2+\frac{\lambda}{2}\left[x^2-\frac{1}{2\lambda}\right]^2 . \tag{38}$$

A translational shift

$$x\rightarrow x-\frac{1}{\sqrt{2\lambda}} \tag{39}$$

changes the Hamiltonian into the form of an anharmonic oscillator centered at one of the wells with cubic and quartic anharmonic coupling:

$$H=\tfrac{1}{2}p^2+\frac{\lambda}{2}x^4-\sqrt{2\lambda}x^3+x^2 , \tag{40}$$

which may further be reduced to the standard form (36) by a scale change:

$$H=2\left[\tfrac{1}{2}p^2+\tfrac{1}{2}x^2+\frac{\lambda}{16}x^4-\frac{\sqrt{\lambda}}{4}x^3\right] . \tag{41}$$

Table IV gives the typical result of the first six lowest energy levels for some of the couplings. The fast convergence is strong support for this model. These values are in agreement with the results of Banerjee[7] whenever they have entries.

III. DISCUSSION AND CONCLUSION

We consider the success of these results to be a strong justification for the simple physical interpretation of our two-step approach. For the Bogoliubov transformation (12) to be unitary, it is essential that $t<1$. For small λ, there are three roots in Eq. (22), but only one solution satisfies $t<1$. This solution is a continuous function of λ for the whole range of λ. We obtain all the lowest eigenvalues by a single diagonalization. This is in contrast with the approach of Banerjee.[8] Furthermore, contrary to what has been believed, numerical test runs indicate that the Brillouin-Wigner perturbation expansion on the transformed Hamiltonian (23) converges for $\lambda\leq 1$. The convergence of the Brillouin-Wigner series for larger λ is still an open question.[9]

It is interesting to note that this model can even be extended to the case for a negative but small value of λ. Strictly speaking, no bound states are present in this case. But, for small λ and for energy levels far below the dissociation limit we may neglect tunneling and consider them as bound states. Application of our two-step method has also yielded stunning success.[10]

The extensions to the case with higher order of anharmonicity or with higher dimension are straightforward. Successful test runs in two-dimensional coupled oscillators have been performed. They agree with the results in Ref. 3. We have also extended our method to one-dimensional ϕ^4 field theory. They will all be reported in future publications.

ACKNOWLEDGMENTS

Many of the ideas originated from our collaboration with Professor H. Kümmel in the application of this model to one-dimensional ϕ^4 field theory. Part of that work was done while one of the authors (C.S.H.) spent a two month visit in Bochum in fall, 1981. He would like to thank Professor H. Kümmel for hospitality and for stimulating discussions. We would also like to thank our colleagues in National Tsing Hua University for stimulating discussions. The work of C.S.H. was supported by the National Science Council of the Republic of China.

[1]The application of the perturbation method in the anharmonic oscillator was treated by Ta-You Wu, *Vibrational Spectra and Structure of Polyatomic Molecules* (National University of Peking, Peking, 1939).

[2]C. M. Bender and T. T. Wu, Phys. Rev. 184, 1231 (1969).

[3]For a review and references, see F. T. Hioe, D. MacMillen, and E. W. Montroll, Phys. Rep. 43C, 303 (1978).

[4]S. J. Chang, Phys. Rev. D 12, 1071 (1975).

[5]S. Coleman, Phys. Rev. D 11, 2088 (1975).

[6]J. L. Chern, C.-S. Hsue, and H. Kümmel (unpublished).

[7]K. Banerjee and S. P. Bhatnagar, Phys. Rev. D 18, 4767 (1978). We believe that the entries in $\lambda=0.07$ contain a misprint.

[8]K. Banerjee *et al.*, Proc. R. Soc. London A260, 575 (1978).

[9]For all values of $\lambda\gg 1$, the first nine orders of the Brillouin-Wigner perturbation series oscillates and converges to the exact value, but the amplitude of oscillation does not seem to die down for the next two orders of perturbation for $\lambda\gg 1$.

[10]Chen-Shiung Hsue (unpublished).