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New two-step approach to one-dimensional anharmonic oscillators

C. Esebbag, J. Núñez, and A. Plastino
Physics Department, National University, C.C. 67, La Plata 1900, Argentina

G. Bozzolo
Department of Physics, Iowa State University, Ames, Iowa 50011
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The two-step approach of Hsue and Chern is reinterpreted in physical terms that allow for a powerful reformulation of their original treatment for one-dimensional anharmonic oscillators.

I. INTRODUCTION

Interest in the one-dimensional anharmonic oscillator has been both sustained and intense in the last few years, due mainly to its relevance for the study of molecular vibrations and to its role in the modeling of nonlinear quantum field theories. A small (and by no means representative) sample is that of Refs. 1–12.

Recently, a very elegant and powerful approach was introduced by Hsue and Chern,[13] who present a two-step approach in order to investigate Hamiltonians of the form

$$\hat{H}=\hat{p}^2/2+\hat{x}^2/2+\sum_{i=3}^{m}\lambda_i x^i=\hat{T}+\hat{V}(x)\ . \tag{1}$$

Their approach has a clear physical meaning and is capable of producing eigenvalues with high accuracy. The idea is to introduce, after recasting (1) into second-quantization shape [we restrict ourselves, for simplicity, to $i=4$ and 3 in (1)]

$$a^\dagger=(\hat{x}-i\hat{p})/\sqrt{2},\quad a=(\hat{x}+i\hat{p})/\sqrt{2}, \tag{2}$$

$$\hat{H}=a^\dagger a+\tfrac{1}{2}+\lambda_3(a^\dagger+a)^3+\lambda_4(a^\dagger+a)^4\ , \tag{3}$$

a generalized coherent-state ansatz for the first step, of the form

$$|\phi\rangle=\exp(ta^{\dagger 2}/2)|0\rangle\ , \tag{4}$$

where the parameter t is determined by the variational principle.

Then, after (i) reordering by recourse to Wick's theorem and (ii) a Bogliubov transformation,

$$b=\frac{a-ta^\dagger}{(1-t^2)^{1/2}}\ , \tag{5a}$$

$$b^\dagger=\frac{a^\dagger-ta}{(1-t^2)^{1/2}}\ , \tag{5b}$$

$$[b,b^\dagger]=1\ , \tag{5c}$$

$$b|\phi\rangle=0\ , \tag{5d}$$

the Hamiltonian (in terms of the b's)[13]

$$\hat{H}=E_0+\omega b^\dagger b+\frac{\lambda_3}{(\sqrt{2}\omega)^3}[:(b+b^\dagger)^3:+3(b+b^\dagger)]+\frac{\lambda_4}{4\omega^2}:(b+b^\dagger)^4:\ , \tag{6a}$$

$$\omega=(1-t)/(1+t) \tag{6b}$$

is diagonalized in the basis

$$|n\rangle=(n!)^{-1/2}b^{\dagger n}|\phi\rangle\ , \tag{7}$$

a process that accurately yields all low-lying energy levels.

The purpose of the present effort is to provide one with yet a different physical interpretation of Hsue and Chern's beautiful scheme, so as to be in a position to reformulate it and obtain a still more powerful method.

To this end we shall first show that the treatment of Ref. 13 is tantamount to diagonalizing H in a *scaled* oscillator basis. The parameter t is then seen to be just *a scaling factor* and its determination by recourse to the variational principle (minimizing thus the ground-state energy E_0) *automatically* predetermines a basis whose "width" is just the one adjusted to the particular one-body potential $V(x)=\lambda_3x^3+\lambda_4x^4+x^2/2$. Of all possible oscillator bases, one selects then the most appropriate one for the problem at hand.

II. COHERENT ANSATZ AND SCALING FACTOR

In order to achieve our goal it is convenient to work in the coordinate representation, where the ground state of the harmonic oscillator $|0\rangle$ reads

$$\phi_0(x)=\langle x|0\rangle=\pi^{-1/4}e^{-x^2/2}\ . \tag{8}$$

We define a new coordinate representation in terms of the operators in (5),

$$b=(\hat{Q}+i\hat{P})/\sqrt{2},\quad b^\dagger=(\hat{Q}-i\hat{P})/\sqrt{2}\ ,$$
$$[\hat{Q},\hat{P}]=i,\quad \langle Q|0\rangle=\pi^{-1/4}e^{-Q^2/2}=\phi_0(Q)\ , \tag{9}$$

so that

$$Q=[(1-t)/(1+t)]^{1/2}x=\sqrt{u}x \quad (10)$$

and

$$\langle x|\phi\rangle=\langle x|e^{ta^{\dagger 2}/2}|0\rangle=(u/\pi)^{1/4}e^{-ux^2/2} . \quad (11)$$

Thus the coherent ansatz (4) is clearly seen to be a scaled wave function, where the scaling factor is just $u^{1/2}$. The creation operator $b^\dagger$ generates then a complete scaled basis. It is of interest to point out that the operator defining the transformation (4) is intimately related to

$$\hat{S}=e^{-h(a^{\dagger 2}-a^2)} , \quad (12)$$

exhaustively studied in Refs. 11 and 12. $\hat{S}$ is the most general scaling operator and one can easily find that it scales any wave function in the $\hat{x}$ representation with the scaling factor $\alpha=\exp(-4h)$.

III. MODIFIED HSUE AND CHERN APPROACH

The potential term $\hat{V}(x)$ in (1) does not, in general, possess any special symmetry with respect to the origin. The corresponding "wells" may be located far from it. Expanding the wave functions in an "origin-centered" basis may not always be, then, the best procedure. Consequently, in addition to adjusting the "width" of the basis wave functions by means of a scaling factor, a "shifting" should surely improve things, so as to place them in a better location along the coordinate axis. This is achieved by writing the coordinate $\hat{Q}$ as

$$\hat{Q}=\sqrt{\mu}(x+\gamma/\sqrt{\mu}) , \quad (13)$$

and recasting things appropriately. This entails working with a coherent-state ansatz of the form

$$|\phi\rangle=\exp(\alpha a^\dagger+\tfrac{1}{2}\beta a^{\dagger 2})|0\rangle , \quad (14)$$

where α and β are determined by recourse to the variational principle. The Bogoliubov transformation now reads

$$B=\frac{1}{(1-\beta^2)^{1/2}}(a-\beta a^\dagger-\alpha)=b-\gamma ,$$
$$\gamma=\frac{\alpha}{(1-\beta^2)^{1/2}} , \quad (15)$$
$$B|\phi\rangle=0 ,$$

and the Hamiltonian is then to be recast in terms of the B operators. As the relation between the "old" $b^\dagger$'s and the "new" $B^\dagger$'s is a very simple one, we can easily write down things in terms of the $B^\dagger$'s and get

$$\hat{H}=E_0+h_1B^\dagger B+h_2(B^\dagger+B)+h_3(B^{\dagger 2}+B^2)+h_4{:}(B^\dagger+B)^3{:}+h_5{:}(B^\dagger+B)^4{:} , \quad (16)$$

with

$$E_0=\frac{1+\omega^2}{4\omega}+\frac{3\omega_4}{4\omega^2}-\frac{6\lambda_3\gamma}{2\omega\sqrt{2\omega}}+\left(\frac{1}{\omega}+\frac{6\lambda_4}{\omega^2}\right)\gamma^2-\frac{8\lambda_3\gamma^3}{2\omega\sqrt{2\omega}}+\frac{4\lambda_4\gamma^4}{\omega^2} , \quad (17)$$

$$h_1=\frac{1+\omega^2}{2\omega}+\frac{3\lambda_4}{\omega^2}-\frac{12\lambda_3\gamma}{2\omega\sqrt{2\omega}}+\frac{12\lambda_4\gamma^2}{\omega^2} , \quad (18)$$

$$h_2=\frac{3\lambda_3}{2\omega\sqrt{2\omega}}-\left(\frac{1}{\omega}+\frac{6\lambda_4}{\omega^2}\right)\gamma+\frac{12\lambda_3\gamma^2}{2\omega\sqrt{2\omega}}-\frac{8\lambda_4\gamma^3}{\omega^2} , \quad (19)$$

$$h_3=\frac{(1-\omega^2)}{4\omega}+\frac{3\lambda_4}{2\omega^2}-\frac{6\lambda_3\gamma}{2\omega\sqrt{2\omega}}+\frac{6\lambda_4\gamma^2}{\omega^2} , \quad (20)$$

$$h_4=\frac{\lambda_3}{2\omega\sqrt{2\omega}}-\frac{2\lambda_4\gamma}{\omega^2} , \quad (21)$$

$$h_5=\frac{3\lambda_4}{4\omega^2} . \quad (22)$$

TABLE I. Energy values obtained with the present approach for the $\lambda_1x^3+\lambda_2x^4$ anharmonic oscillator (ground state and four excited states). The order of the corresponding diagonalization is shown in column 3.

λ_1	λ_2	Order	E_0	E_1	E_2	E_3	E_4
0.5	0.1	9	−0.255 323 790	0.464 359 331	1.248 679 381	2.346 432 789	3.782 327 465
		15	−0.255 477 028	0.452 258 771	1.196 278 554	2.192 411 618	3.332 150 666
		20	−0.255 477 259	0.452 236 430	1.196 137 185	2.191 475 677	3.328 453 666
1.0	0.1	9	−76.417 239 033	−72.061 007 200	−67.760 421 050	−63.516 438 265	−59.323 649 646
		15	−76.417 239 044	−72.061 007 491	−67.760 454 918	−63.517 420 335	−59.333 898 861
		20	−76.417 239 044	−72.061 007 491	−67.760 454 922	−63.517 420 570	−59.333 906 601
5.0	1.0	9	−55.396 844 924	−48.302 887 939	−41.424 499 570	−34.762 664 987	−28.212 111 872
		15	−55.396 845 517	−48.302 899 053	−41.425 155 011	−34.782 041 802	−28.394 994 972
		20	−55.396 845 173	−48.302 899 063	−41.425 156 169	−34.782 102 830	−28.396 845 618
10.0	1.0	9	−1019.245 576 728	−1004.329 821 529	−989.587 154 720	−974.828 845 635	−960.117 875 863
		15	−1019.245 576 729	−1004.329 821 537	−989.587 156 261	−974.828 950 735	−960.118 582 259
		20	−1019.245 576 729	−1004.329 821 537	−989.587 156 261	−974.828 950 736	−960.118 582 276
50.0	10.0	9	−640.364 516 561	−616.897 582 446	−593.620 807 341	−570.536 630 331	−547.638 583 374
		15	−640.364 516 576	−616.897 582 762	−593.620 851 062	−570.538 220 935	−574.653 798 678
		20	−640.364 516 576	−616.897 582 762	−593.620 851 064	−570.538 221 040	−574.653 802 277
100.	10.0	9	−10495.068 783 74	−10447.712 304 85	−10400.401 977 50	−10353.137 886 74	−10305.920 114 44
		15	−10495.068 783 74	−10447.712 304 85	−10400.401 977 64	−10353.137 912 52	−10305.920 220 55
		20	−10495.068 783 74	−10447.712 304 85	−10400.401 977 64	−10353.137 912 52	−10305.920 220 55

TABLE II. Results obtained with the method of Hsue and Chern for the $\lambda_1 x^3 + \lambda_2 x^4$ anharmonic oscillator. Remaining details are the same as in Table I. A comparison between these figures and those of Table I clearly exhibits the power of the present approach.

λ_1	λ_2	Order	E_0	E_1	E_2	E_3	E_4
0.5	0.1	9	−0.188 984 161	0.510 600 803	1.412 304 628	2.640 505 191	4.231 411 920
		15	−0.255 238 015	0.452 560 098	1.197 893 436	2.196 807 038	3.341 295 809
		20	−0.255 475 475	0.452 240 913	1.196 160 880	2.191 578 062	3.328 841 987
1.0	0.1	9	−12.364 182 396	−3.179 437 044	0.287 488 097	1.501 283 262	3.463 540 344
		15	−30.555 552 733	−16.598 003 448	−7.449 297 818	−1.780 154 821	0.490 808 909
		20	−45.731 811 450	−30.474 727 330	−18.951 597 589	−10.246 080 887	−4.010 863 922
5.0	1.0	9	−27.202 764 358	−9.753 853 646	−0.722 642 967	1.899 561 869	5.315 416 301
		15	−49.543 372 341	−33.139 423 147	−18.316 871 720	−6.972 286 264	−0.268 318 570
		20	−55.186 151 814	−46.360 760 620	−34.770 228 680	−22.482 754 913	−11.560 141 898
10.0	1.0	9	−91.037 994 144	−34.111 004 781	−7.547 749 428	1.107 182 935	4.401 529 865
		15	−218.874 347 772	−127.290 830 875	−69.391 598 219	−32.168 229 220	−9.863 990 056
		20	−337.987 173 416	−227.806 937 773	−150.755 552 727	−94.514 306 884	−53.809 597 908
50.0	10.0	9	−140.370 963 595	−54.122 117 437	−11.444 774 449	2.490 753 579	9.105 856 656
		15	−309.515 338 747	−189.457 824 204	−106.253 456 581	−49.484 633 097	−14.179 096 541
		20	−440.825 803 444	−317.515 642 797	−219.135 110 879	−141.126 047 247	−81.257 768 708
100.	10.0	9	−367.792 836	−141.564 791	−38.098 112	−0.289 140	7.345 293
		15	−913.714 799	−524.588 021	−288.518 973	−140.709 534	−52.679 044
		20	−1459.029 605	−960.855 001	−629.765 501	−396.614 460	−232.232 550

The variational principle $dE_0/d\omega=0$ guarantees (as the general requirement for the Hartree approximation) that $h_2=h_3=0$ and $h_1=\omega=(1-\beta)/(1+\beta)$, so that

$$\hat{H}=E_0+\omega B^\dagger B+h_4{:}(B^\dagger+B)^3{:}+h_5{:}(B^\dagger+B)^4{:}\ , \quad (23)$$

and all that remains to be done is the diagonalization of $\hat{H}$ in the basis

$$B^{\dagger n}|\phi\rangle=\sqrt{n!}\,|n\rangle\ , \quad (24)$$

where the relevant matrix elements are

$$\langle n|\hat{H}|n\rangle=E_0+n\omega+6h_5 n(n-1)\ ,$$

$$\langle n|\hat{H}|n+1\rangle=3h_4 n(n+1)^{1/2}\ ,$$

$$\langle n|\hat{H}|n+2\rangle=4nh_5[(n+1)(n+2)]^{1/2}\ , \quad (25)$$

$$\langle n|\hat{H}|n+3\rangle=h_4[(n+1)(n+2)(n+3)]^{1/2}\ ,$$

$$\langle n|\hat{H}|n+4\rangle=h_5[(n+1)(n+2)(n+3)(n+4)]^{1/2}\ .$$

IV. RESULTS

Some illustrative results are exhibited in Tables I and II. When $\lambda_1=\lambda_2$ our approach and that of Ref. 13 coincide up to eight significant digits and the corresponding figures are not exhibited so as to save space.

Comparing Tables I and II it becomes immediately apparent that our modified Hsue and Chern approach is indeed a much more powerful one than the original method, both in respect to accuracy and convergence properties.

Summing up, we reinterpreted the treatment of Ref. 13 in clear physical terms that have allowed for a simple but powerful reformulation.

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