Simple procedure to compute accurate energy levels of a double-well anharmonic oscillator

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Accurate eigenvalues of the double-well anharmonic oscillator ($H=p^2-Z^2x^2+x^4$) are obtained in all regimes of the coupling constant Z^2. Tables of some eigenvalues up to $Z^2\leq 100$ are presented. The method is nonperturbative and involves the use of an appropriately scaled harmonic basis.

I. INTRODUCTION

Perhaps the most simple and successful method used in the literature to obtain accurate eigenvalues of the anharmonic oscillator[1]

$$H=p^2+x^2+\lambda x^4 ,$$
$$p=-i\frac{d}{dx} , \qquad (1)$$
$$\lambda\geq 0$$

is the variational procedure.[2] Take N members of some arbitrary complete orthonormal set of basic vectors $u_n(x)$. One then constructs the $N\times N$ matrix representation of H:

$$H_{ij}=\int u_i^* H u_j dx ,$$
$$\mathrm{Det}[H_{ij}-EI_{ij}]=0, \quad i,j=1,2,\ldots,N , \qquad (2)$$
$$I_{ij}=\delta_{ij} .$$

The eigenvalues are obtained at different levels of truncation and we search for the limit of successive estimates as the truncated determinants are increased in size.

The most natural basis[3] for this problem (1) is in terms of the harmonic oscillator

$$H_0=\frac{p^2}{2}+K\frac{x^2}{2} ,$$
$$u_n(x)=\left[\frac{\alpha}{\sqrt{\pi}2^n n!}\right]^{1/2} H_n(\alpha x)e^{-\alpha^2x^2/2} , \qquad (3)$$
$$\alpha^4=K ,$$

where $H_n(\alpha x)$ are the usual Hermite polynomials and α is some parameter to be determined. The simplest variational calculation is to just use a single eigenstate of H_0 and get a best fit to the corresponding ground state of an irreducible sector (n odd or even) of H by varying α.

Should one choose u_0 as the trial wave function

$$E_0=\int u_0^*(x)Hu_0(x)dx ,$$
$$\frac{dE_0}{d\alpha^2}=0 , \qquad (4)$$

it gives the condition

$$\alpha^6-\alpha^2-3\lambda=0 . \qquad (5)$$

In the subsequent calculation we keep α^2 fixed at that value and proceed as indicated in (2). The required matrix elements are

TABLE I. Convergence of some eigenvalues E_K of the anharmonic oscillator $H=p^2+x^2+\lambda x^4$ for $\lambda=10$. $N\times N$ is the size of the matrix.

N	$10^{-1}E_0$	$10^{-3}E_{21}$	$10^{-3}E_{38}$
10	0.244 917 414 796	. . .	. . .
20	0.244 917 407 212	0.290 889 187 347	4.275 220 568 94
40	0.244 917 407 212	0.283 879 305 446	0.775 211 251 430
60	0.244 917 407 212	0.283 879 305 433	0.615 623 574 398
80	0.244 917 407 212	0.283 879 305 433	0.615 577 264 638
90	0.244 917 407 212	0.283 879 305 433	0.615 577 264 599
95	0.244 917 407 212	0.283 879 305 433	0.615 577 264 599

TABLE II. Convergence of some eigenvalues E_K of the double-well oscillator $H=p^2-Z^2x^2+x^4$ for $Z^2=50$. $N\times N$ is the size of the matrix, and α^2 has been fixed by Eq. (4).

N	$10^{-3}E_0$	$10^{-3}E_{21}$	$10^{-4}E_{38}$
90	−0.610 742 213 410	−0.049 935 452 957 7	2.312 134 630 63
100	−0.612 072 333 718	−0.091 509 194 754 2	1.788 939 643 02
120	−0.613 040 968 777	−0.139 118 904 206	1.129 189 654 58
140	−0.613 554 919 533	−0.184 139 163 267	0.748 235 413 774
150	−0.614 000 551 485	−0.212 204 059 437	0.616 675 349 792
160	−0.614 219 966 345	−0.224 718 854 775	0.511 263 315 798

$$\langle n\mid H\mid n\rangle=\frac{\alpha^4+1}{2\alpha^2}(2n+1)+\frac{3\lambda}{4\alpha^4}(2n^2+2n+1)\ ,$$

$$\langle n\mid H\mid n+2\rangle=\left[-\frac{(\alpha^4-1)}{2\alpha^2}+\frac{\lambda}{4\alpha^4}(4n+6)\right]\times[(n+1)(n+2)]^{1/2}\ , \tag{6}$$

$$\langle n\mid H\mid n+4\rangle=\frac{\lambda}{4\alpha^4}[(n+1)(n+2)(n+3)(n+4)]^{1/2}$$

and the solution of the matrix eigenvalue problem (2) is easily done by machine. Because of the $(x\leftrightarrow -x)$ symmetry of H, even and odd states are obtained by a separate diagonalization.

In fact in the odd case it is better to fit α^2 by minimizing

$$E_1(\lambda)\equiv\int u_1^*(x)Hu_1(x)dx\ .$$

The new condition is

$$\alpha^6-\alpha^2-5\lambda=0\ . \tag{7}$$

The results converge exceedingly fast for any value of λ. In order to illustrate that convergence we show in Table I the energy eigenvalues corresponding to $K=0$, 21, and 38 at different levels of truncation for a coupling strength $\lambda=10$.

Obviously as K increases one needs a bigger and bigger matrix in order to reach a set of stable figures which one may believe to be the exact eigenvalues. However, the enormous advantage of this method lies in the fact that the process of increasing N is absolutely trivial because the matrix elements one has to put in are always of the type (6). In all our computations we have used the UNIVAC 1100, performing the diagonalizations by means of the standard routine JACOBI.

If one tries to perform the same job for the double-well anharmonic oscillator,[4,5,6]

$$H=p^2-Z^2x^2+x^4,\quad Z^2>0\ , \tag{8}$$

one easily recognizes that this method works only for small values of Z^2. That is easy to understand because as Z^2 grows the depth of the two wells becomes deeper and deeper and the actual low-lying energy eigenstates of the problem become radically different from the trial wave function offered by the harmonic basis; this fact handicaps severely the convergence. In principle the natural solution would be the simultaneous use of two harmonic bases centered around $x=\pm\mid Z\mid\sqrt{2}$, i.e., the positions of the two minima; however, the implementation of that idea although possible implies the use of nonorthogonal states, which is more cumbersome because one has to forget the simple scheme (6) for the Hamiltonian matrix. To illustrate the problems one finds with the convergence of the eigenvalues of (8), if α^2 is fixed by means of (4), we show in Table II the energies of the states $K=0$, 21, and 38 got at different levels N of truncation.

TABLE III. Convergence of some eigenvalues E_K of the double-well oscillator $H=p^2-Z^2x^2+x^4$ for $Z^2=50$. $N\times N$ is the size of the matrix and α^2 has been fixed by the criterion (14).

N	$10^{-3}E_0$	$10^{-3}E_1$	$10^{-3}E_{38}$	$10^{-3}E_{39}$
20	−0.351 752 165 698	−0.359 828 057 502	0.436 886 985 612	0.449 835 949 661
40	−0.575 113 242 590	−0.578 031 748 074	0.004 141 762 985	0.006 541 332 963
60	−0.615 012 840 616	−0.615 015 775 110	−0.151 848 042 313	−0.155 881 746 746
80	−0.615 020 090 903	−0.615 020 090 903	−0.260 462 072 450	−0.260 754 358 808
90	−0.615 020 090 903	−0.615 020 090 903	−0.261 112 800 933	−0.261 112 800 970
95	−0.615 020 090 903	−0.615 020 090 903	−0.261 112 800 977	−0.261 112 800 997
100	−0.615 020 090 903	−0.615 020 090 903	−0.261 112 800 977	−0.261 112 800 997

TABLE IV. Numerical values of some energy eigenvalues of the double-well oscillator $H=p^2-Z^2x^2+x^4$. (Exponential notation is used so that +01 means the number preceding is to be multiplied by 10^{+1}).

Z^2	E_0	E_1	E_{20}	E_{38}	E_{39}
0	0.106 036 209 048+01	0.379 967 302 980+01	0.122 654 639 001+03	0.284 068 590 581+03	0.293 948 458 266+03
0.5	0.870 017 518 372+00	0.333 377 932 989+01	0.120 063 175 836+03	0.280 206 152 559+03	0.290 019 627 484+03
1	0.657 653 005 191+00	0.283 453 620 212+01	0.117 498 096 009+03	0.276 320 189 466+03	0.286 067 274 589+03
2	0.137 785 848 189+00	0.171 302 789 777+01	0.112 296 111 820+03	0.268 477 022 249+03	0.278 091 347 173+03
4	−0.171 035 045 013+01	−0.124 792 249 207+01	0.101 599 114 965+03	0.252 501 468 994+03	0.261 850 409 125+03
5	−0.341 014 276 124+01	−0.325 067 536 229+01	0.961 017 378 427+02	0.244 366 964 365+03	0.253 583 300 288+03
7	−0.867 110 520 870+01	−0.866 245 222 488+01	0.848 074 609 803+02	0.227 800 501 793+03	0.236 751 799 512+03
10	−0.206 335 767 029+02	−0.206 335 468 844+02	0.671 368 007 617+02	0.202 202 092 716+03	0.210 755 910 287+03
15	−0.508 413 872 844+02	−0.508 413 872 842+02	0.361 032 401 550+02	0.157 581 244 216+03	0.165 467 937 839+03
50	−0.615 020 090 903+03	−0.615 020 090 903+03	−0.422 068 788 469+03	−0.261 112 800 997+03	−0.261 112 800 987+03
100	−0.248 586 788 034+04	−0.248 586 788 034+04	−0.220 639 793 309+04	−0.196 035 041 616+04	−0.196 035 041 616+04

Hence the specific problem we have faced has been the following: Is there any way of fixing α^2 in the harmonic basis (3) so that by using the general method (2) we may get accurate eigenvalues for the double-well oscillator[2]? In the next section we will show a simple way of doing it, which produces a very good convergence for any value of Z^2.

II. METHOD AND RESULTS

The fixing of α^2 for the single-well potential by (5) and (7) is so successful because $u_0(u_1)$ is always the best candidate among all the elements of the basis (3) as the trial wave function for the ground state of (1). In other words,

$$\begin{aligned}&\langle u_0 \mid p^2+x^2+\lambda x^4 \mid u_0\rangle \\ &\qquad \le \langle u_i \mid p^2+x^2+\lambda x^4 \mid u_i\rangle \quad \forall \text{ even } i\ , \\ &\langle u_1 \mid p^2+x^2+\lambda x^4 \mid u_1\rangle \\ &\qquad \le \langle u_i \mid p^2+x^2+\lambda x^4 \mid u_i\rangle \quad \forall \text{ odd } i\ .\end{aligned} \tag{9}$$

But this is not true any longer for the double-well potential because as Z^2 increases the minimum value of

$$\langle u_n \mid p^2-Z^2x^2+x^4 \mid u_n\rangle \tag{10}$$

is a nontrivial function of n and α^2. Qualitatively this is easy to understand because $\mid u_n \mid^2$ presents n nodes and the maximum of the probability density is coincident with the amplitude of the corresponding classical oscillator; i.e., the probability of finding the particle is maximal $x=\pm \mid d \mid$ with $\mid d \mid >0$. And this is just what must happen in this problem, as Z^2 grows a sensible description of its low energy should involve wave functions which present the maximal probability density at a position coincident with the minimum of the two wells. Although u_n, with $n\neq 0$, provides a bigger contribution than u_0 to the expectation value of the kinetic energy (because of their n nodes), the expectation value of the potential energy may be lower, which causes the existence of a competition between these two opposite effects. Therefore, one has to consider the possibility of varying also the n index to get a good variational parameter α^2. Specifically our proposal is to fix α^2 by imposing simultaneously the following two equations:

$$\begin{aligned}\frac{\partial\langle u_n \mid p^2-Z^2x^2+x^4 \mid u_n\rangle}{\partial\alpha^2}&=0\ , \\ \frac{\partial\langle u_n \mid p^2-Z^2x^2+x^4 \mid u_n\rangle}{\partial n}&=0\ ,\end{aligned} \tag{11}$$

which lead to

$$\alpha^6+Z^2\alpha^2-3\frac{(2n^2+2n+1)}{(2n+1)}=0\ ,$$
$$\alpha^6-Z^2\alpha^2+3(n+\tfrac{1}{2})=0\ . \tag{12}$$

By eliminating n the final equation for α^2 is

$$\alpha^{12}-Z^2\alpha^8+\tfrac{9}{8}=0\ . \tag{13}$$

From (13) two real and positive solutions for α^2 may be extracted. They provide similar efficiencies in the convergence process, but in order to obtain a simple criterion, easy to remember in practical calculations, Eq. (13) may be simplified. Should one skip the $\frac{9}{8}$ term, the solution of (13) is

$$\alpha^2=\sqrt{Z^2}\ . \tag{14}$$

The value provided by (14) is practically coincident with the bigger root of (13) when Z^2 is larger than say $Z_1{}^2=10$. In all practical cases (14) is an excellent recipe of convergence and has been used by us to get the numerical tables. In Table III we show the convergence of the method for $Z^2=50$, and $\alpha^2=\sqrt{Z^2}$. The ground states converge at about $N=75$, and when $N=100$ all 40 states are already stabilized.

In Table IV, just as an example, the numerical values of some energy eigenvalues for $0\leq Z^2\leq 100$ are presented. In all cases $N=100$ and we have checked its stability by computing later $N=130$. In the case $Z^2=100$ the convergence of the 40 states is reached at $N=220$.

For Z^2 lower than $Z_0{}^2=1.96$ Eqs. (12) admit only the trivial solution corresponding to $n=0$ (1). In that regime our calculations have been performed in the old ways (5) and (7). In that region Z^2 is reasonably small and therefore we do not find any problem for a fast convergence.

III. CONCLUDING REMARKS

Our main interest in this paper has been to obtain a simple and efficient procedure to obtain accurate eigenvalues of the double-well anharmonic oscillator. This problem has received great attention in the last years and it has been attacked by a broad range of methods; we believe, however, that the method developed here is perhaps the most simple and therefore the most economical; it may be summarized by Eq. (14). Our work remarks on the great importance of a good choice of the scale α^2 in order to get fast convergence. By quoting Cashwell,[7] but in an affirmative sense, "we believe that with our method, the evaluation of the DWP eigenvalues is already an industry." Now we try to extend these ideas to the problem of the two coupled anharmonic oscillators.[1]

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