Comment on "Simple procedure to calculate accurate energy levels of a double-well anharmonic oscillator"

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A simple method for obtaining the lower-lying eigenvalues of the double-well anharmonic oscillator, and the coupled-oscillator problem with a quartic coupling term, via a Rayleigh-Ritz-type variational procedure is discussed. It is shown numerically that the minimization of manifold energy is a simple means for determining the parametric dependence of the basis states, and that it is relatively insensitive to the number of basis states included. A rough estimate of the size of the Rayleigh-Ritz matrix and number of basis states to be included in the manifold are also obtained.

A simple method to obtain accurate eigenvalues for the double-well anharmonic oscillator

$$H=p^2-z^2x^2+x^4, \quad x^2>0 \ , \tag{1}$$

is a Rayleigh-Ritz-type variational procedure. One takes N basis states from an arbitrary complete orthonormal set $u_n(x)$. Then, using these states, one constructs an $N\times N$ matrix representation of the Hamiltonian and diagonalizes it to obtain the eigenvalues e_i $(i=1,\ldots,N)$,

$$H_{ij}=\int u_i^* H u_j dx \ , \quad \det(H_{ij}-eI_{ij})=0 \ . \tag{2}$$

It can be shown that the eigenvalues $\{e_i\}$ converge monotonically to the exact eigenvalues $\{E_i\}$ as N, the dimension of the representation, increases.

The basis commonly used for this problem (1) is the harmonic-oscillator basis

$$u_n(x)=\left(\frac{\alpha}{\sqrt{\pi}2^n n!}\right)^{1/2} H_n(\alpha x)e^{-\alpha^2x^2/2} \ , \tag{3}$$

where $H_n(\alpha x)$ are the Hermite polynomials and α is an oscillator parameter that must be predetermined. In the paper by Balsa, Plo, Esteve, and Pacheco,[1] the following procedure is suggested. The parameter α^2 is fixed by simultaneously solving the two equations

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

These lead to the following equations:

$$\begin{aligned}&\alpha^6+z^2\alpha^2-\frac{3(2n^2+2n+1)}{2n+1}=0 \ ,\\ &\alpha^6-z^2\alpha^2+3(n+\tfrac{1}{2})=0 \ .\end{aligned} \tag{5}$$

Eliminating n from these two equations yields the following equation for α:

$$\alpha^{12}-z^2\alpha^8+\tfrac{9}{8}=0 \ . \tag{6}$$

It should be noted that the quantum number n is not a continuous variable. But, in practice, substituting this solution for α back into Eq. (5), one obtains $n\approx-\frac{1}{2}$ (for $z^2\gtrsim 50$). This value cannot then be related to any physical harmonic-oscillator state. Thus, although the calculations are formally correct, the choice of α^2 has no simple physical interpretation.

As an alternative one could consider the following. Since one obtains the even- and odd-parity states by a separate diagonalization, two values of α^2 ($\alpha_e{}^2$ and $\alpha_o{}^2$) should be specified. If one chooses α^2 by minimizing the manifold energies of the first K odd-parity states and the first K even-parity states separately, one obtains the following equations:

$$\begin{aligned}&\frac{\partial}{\partial\alpha^2}\left(\sum_{n=1}^{K}\langle u_{2n-1}|p^2-z^2x^2+x^4|u_{2n-1}\rangle\right)_{\alpha^2=\alpha_0{}^2}=0 \ ,\\ &\frac{\partial}{\partial\alpha^2}\left(\sum_{n=0}^{K}\langle u_{2n}|p^2-z^2x^2+x^4|u_{2n}\rangle\right)_{\alpha^2=\alpha_e{}^2}=0 \ .\end{aligned} \tag{7}$$

These may be rewritten as

$$\begin{aligned}&\alpha_0{}^6+z^2\alpha_0{}^2-(4K+1)=0 \ ,\\ &\alpha_e{}^6+z^2\alpha_e{}^2-(4K-1)=0 \ .\end{aligned} \tag{8}$$

Such a choice is preferable because it is based on measurable quantities, namely, the manifold energies, which are invariant under similarity transforms. Moreover, if one requires several low-lying states, choosing α to minimize the manifold energy is more democratic than choosing α to minimize the energy of any one state.

The number K of states in the manifold must still be determined. However, our calculations indicate that there is no optimal choice for the value of K or α^2, but rather an optimal range. Since the method of Balsa *et al.* predicts a value of α^2 in this range, their rate of convergence is expected to be good. For comparison of the two methods one should note that the value of α^2 suggested by Balsa *et al.* corresponds to $K\approx 175$.

In principle one should choose α to minimize the energy of the lowest $K=N_{\max}$ states, where $N_{\max}$ is the dimension of the matrix ultimately used to obtain the eigenvalues. Fortunately, however, the rate of convergence appears to be insensitive to the choice of K. Thus, a crude estimate of the value $N_{\max}$ will suffice.

Tables I–IV show the rate of convergence as a function of

TABLE I. Convergence of the eigenvalue $E_0(\times 10^{-3})$ of the double-well anharmonic oscillator $H=p^2-50x^2+x^4$ vs K, the number of basis states in the manifold. $N\times N$ is the size of the matrix.

N \ K	40	50	60	75	100
20	−0.611 406 183 145	−0.587 803 637 959	−0.557 344 525 053	−0.514 494 589 368	−0.458 313 018 762
40	−0.615 020 090 896	−0.615 020 090 898	−0.615 020 090 873	−0.615 020 085 390	−0.614 665 165 496
60	−0.615 020 090 903	−0.615 020 090 903	−0.615 020 090 903	−0.615 020 090 903	−0.615 020 090 903
70	"	"	"	"	"
75	"	"	"	"	"
80	"	"	"	"	"
85	"	"	"	"	"
90	"	"	"	"	"
95	"	"	"	"	"
100	"	"	"	"	"

N \ K	125	150	175	200	Balsa *et al.* (Ref. 1)
20	−0.417 170 861 490	−0.385 884 536 054	−0.361 171 919 256	−0.341 037 439 622	−0.359 828 057 502
40	0.608 079 893 059	−0.594 707 319 002	−0.579 006 754 271	−0.563 172 219 517	−0.578 031 748 074
60	−0.615 020 090 903	−0.615 020 089 386	−0.615 016 871 801	−0.614 903 320 623	−0.615 015 775 110
70	"	−0.615 020 090 903	−0.615 020 090 903	−0.615 020 087 927	−0.615 202 090 902
75	"	"	"	−0.615 020 090 902	−0.615 020 090 903
80	"	"	"	−0.615 020 090 903	"
85	"	"	"	"	"
90	"	"	"	"	"
95	"	"	"	"	"
100	"	"	"	"	"

TABLE II. Convergence of the eigenvalue $E_{39}(\times 10^{-3})$ of the double-well anharmonic oscillator $H=p^2-50x^2+x^4$ vs K, the number of basis states in the manifold. $N\times N$ is the size of the matrix.

N \ K	40	50	60	75	100
20	0.150 141 739 894	0.185 883 272 941	0.217 886 801 729	0.260 158 283 474	0.319 220 210 926
40	−0.215 047 798 693	−0.211 278 113 096	−0.170 320 751 497	−0.120 229 637 764	−0.065 873 905 480
60	−0.260 929 233 497	−0.261 070 464 785	−0.261 086 492 625	−0.261 050 770 918	−0.260 080 830 324
70	−0.261 112 367 031	−0.261 112 782 065	−0.261 112 797 359	−0.261 112 798 372	−0.261 112 708 513
75	−0.261 112 785 429	−0.261 112 800 664	−0.261 112 800 928	−0.261 112 800 923	−0.261 112 800 792
80	−0.261 112 800 087	−0.261 112 800 992	−0.261 112 800 996	−0.261 112 800 997	−0.261 112 800 997
85	−0.261 112 800 970	−0.261 112 800 997	−0.261 112 800 997	"	"
90	−0.261 112 800 997	"	"	"	"
95	"	"	"	"	"
100	"	"	"	"	"

N \ K	125	150	175	200	Balsa *et al.* (Ref. 1)
20	0.368 328 923 392	0.410 538 096 627	0.447 702 996 630	0.481 019 897 099	0.449 835 949 661
40	−0.032 026 288 084	−0.010 007 010 036	0.005 670 371 244	0.019 588 164 449	0.006 541 332 963
60	−0.226 390 682 336	−0.188 673 596 387	−0.157 586 935 276	−0.113 984 549 603	−0.155 881 746 746
70	−0.261 087 715 984	−0.252 633 381 399	−0.227 841 092 220	−0.203 393 617 816	−0.226 293 951 411
75	−0.261 112 780 591	−0.261 100 892 759	−0.251 466 459 605	−0.231 603 747 430	−0.250 361 259 156
80	−0.261 112 800 984	−0.261 112 782 663	−0.260 892 663 564	−0.252 011 767 222	−0.260 754 358 808
85	−0.261 112 800 997	−0.261 112 800 979	−0.261 112 724 799	−0.260 674 602 360	−0.261 112 692 282
90	"	−0.261 112 800 997	−0.261 112 800 985	−0.261 112 785 225	−0.261 112 800 970
95	"	"	−0.261 112 800 997	−0.261 112 800 995	−0.261 112 800 997
100	"	"	"	−0.261 112 800 997	"

TABLE III. Convergence of the eigenvalue $E_{59}(\times 10^{-3})$ of the double-well anharmonic oscillator $H=p^2-50x^2+x^4$ vs K, the number of basis states in the manifold. $N\times N$ is the size of the matrix.

N \ K	50	60	75	90	100
85	−0.101 317 691 662	−0.101 317 711 071	−0.101 317 711 450	−0.101 317 711 530	−0.101 317 711 510
90	−0.101 317 711 206	−0.101 317 711 550	−0.101 317 711 556	−0.101 317 711 556	−0.101 317 711 556
95	−0.101 317 711 551	−0.101 317 711 556	"	"	"
100	−0.101 317 711 556	"	"	"	"
110	"	"	"	"	"
120	"	"	"	"	"
130	"	"	"	"	"
140	"	"	"	"	"

N \ K	125	150	175	200	Balsa *et al.* (Ref. 1)
85	−0.101 317 710 022	−0.101 316 827 614	−0.099 933 266 479	−0.084 930 430 116	−0.099 383 345 586
90	−0.101 317 711 554	−0.101 317 710 432	−0.101 315 505 973	−0.099 046 377 031	−0.101 314 623 609
95	−0.101 317 711 556	−0.101 317 711 555	−0.101 317 711 051	−0.101 317 323 562	−0.101 317 710 062
100	"	−0.101 317 711 556	−0.101 317 711 556	−0.101 317 711 353	−0.101 317 711 556
110	"	"	"	−0.101 317 711 556	"
120	"	"	"	"	"
130	"	"	"	"	"
140	"	"	"	"	"

K for the eigenvalues E_1, E_{39}, E_{59}, and E_{79}, respectively. (Calculations with the even-parity states yield similar results.) From these tables it is clear that the rate of convergence is insensitive to the choice of K, reflecting an underlying insensitivity to the choice of the parameter α (see Table V). Although in these calculations we have increased the dimension of the Rayleigh-Ritz matrix for fixed K until convergence was achieved, we note that if $N_{\max}$ is the number of Rayleigh states needed for convergence to a particular eigenvalue, choosing $K \approx N_{\max}$ yields good convergence to all lower-lying eigenvalues. In addition one notes that if one requires the lowest k eigenvalues ($k \geq 10$) a rough rule of thumb estimate is $N_{\max} \approx K \approx 2k$.

To clarify the role of K we have considered the problem

TABLE IV. Convergence of the eigenvalue $E_{79}(\times 10^{-2})$ of the double-well anharmonic oscillator $H=p^2-50x^2+x^4$ vs K, the number of basis states in the manifold. $N\times N$ is the size of the matrix.

N \ K	60	75	90	100	125
90	0.236 436 711 667	0.236 436 522 560	0.236 436 500 959	0.236 436 504 426	0.236 436 723 830
95	0.236 436 500 296	0.236 436 495 810	0.236 436 495 645	0.236 436 495 617	0.236 436 496 072
100	0.236 436 495 679	0.236 436 495 583	0.236 436 495 582	0.236 436 495 582	0.236 436 195 582
110	0.236 436 495 582	0.236 436 495 582	"	"	"
120	"	"	"	"	"
130	"	"	"	"	"
140	"	"	"	"	"
150	"	"	"	"	"

N \ K	150	160	175	200	Balsa *et al.* (Ref. 1)
90	0.236 465 761 256	−0.236 670 903 296	0.244 370 971 681	0.389 575 208 035	0.248 923 585 260
95	0.236 436 536 717	0.236 436 775 088	0.236 448 298 999	0.254 885 674 758	0.236 466 874 859
100	0.236 436 495 601	0.236 436 495 810	0.236 436 512 675	0.236 456 701 114	0.236 436 507 289
110	0.236 436 495 582	0.236 436 495 582	0.236 436 495 582	0.236 436 495 583	0.236 436 495 582
120	"	"	"	0.236 436 495 582	"
130	"	"	"	"	"
140	"	"	"	"	"
150	"	"	"	"	"

TABLE V. The value of the oscillator parameter α^2 as a function of K, the number of states in the manifold.

K	$\alpha_o{}^2$	$\alpha_e{}^2$
40	2.787 031 958 00	2.759 662 649 31
50	3.300 761 996 51	3.276 503 536 26
60	3.758 296 678 36	3.736 588 244 79
75	4.361 103 703 54	4.342 379 399 94
90	4.886 464 881 16	4.869 989 244 79
100	5.202 988 564 99	5.187 718 493 14
125	5.904 019 387 32	5.891 061 234 59
150	6.507 772 681 45	6.496 462 551 80
160	6.728 721 575 43	6.717 495 220 57
175	7.040 434 517 45	7.030 358 465 26
200	7.518 820 678 54	7.509 704 594 54
Balsa *et al.* (Ref. 1)	7.071 035 991 42	7.071 035 991 42

of two coupled harmonic oscillators with a quartic coupling term. The Hamiltonian is given by

$$H = -\frac{\hbar^2}{2m_1}\frac{d^2}{dx_1{}^2} - \frac{\hbar^2}{2m_2}\frac{d^2}{dx_2{}^2} + \tfrac{1}{2}m_1 w_1{}^2 x_1{}^2 + \tfrac{1}{2}m_2 w_2{}^2 x_2{}^2 + \gamma(x_1 - x_2)^4 \ . \tag{9}$$

Transforming to the center-of-mass and relative coordinates given by

$$X = \frac{m_1 x_1 + m_2 x_2}{m_1 + m_2} \ , \tag{10}$$

$$Y = x_1 - x_2 \ , \tag{11}$$

yields

$$H = -\frac{\hbar^2}{2M}\frac{d^2}{dX^2} - \frac{\hbar^2}{2m}\frac{d^2}{dY^2} + \tfrac{1}{2}M\Omega_1{}^2 X^2 + \tfrac{1}{2}m\Omega_2{}^2 Y^2 + m\Omega'^2 XY + \gamma Y^4 \ , \tag{12}$$

where M and m are the total and the reduced masses, respectively. Ω_1 and Ω_2 are the new angular frequencies. The relevant equations are given by

$$\Omega_1{}^2 = \frac{1}{M}(m_1 w_1{}^2 + m_2 w_2{}^2) \ , \tag{13}$$

$$\Omega_2{}^2 = m\left(\frac{w_1{}^2}{m_1} + \frac{w_2{}^2}{m_2}\right) = \frac{1}{M}(m_2 w_1{}^2 + m_1 w_2{}^2) \ , \tag{14}$$

$$\Omega'^2 = w_1{}^2 - w_2{}^2 \ . \tag{15}$$

If one makes the choice

$$m_1 = 2m_2 \text{ and } 2w_1{}^2 = 3w_2{}^2 \ ,$$

and introduces the conventional dimensionless variables,

$$\bar{X} = \tilde{\alpha}_1 X \text{ and } \bar{Y} = \tilde{\alpha}_2 Y \ ,$$

where

$$\tilde{\alpha}_1 = \left(\frac{M\Omega_1}{\hbar}\right)^{1/2}, \quad \tilde{\alpha}_2 = \left(\frac{m\Omega_2}{\hbar}\right)^{1/2} \ ,$$

one may rewrite the Schrödinger equation as

$$\left(-\frac{d^2}{d\bar{X}^2} + \bar{X}^2 - \tfrac{1}{2}(\tfrac{7}{2})^{1/2}\frac{d^2}{d\bar{Y}^2} + \tfrac{1}{2}(\tfrac{7}{2})^{1/2}\bar{Y}^2 + \tfrac{1}{2}(\tfrac{2}{7})^{1/4}\bar{X}\,\bar{Y} + \lambda\bar{Y}^4\right)\psi(\bar{X},\bar{Y}) = \bar{E}\psi(\bar{X},\bar{Y}) \ . \tag{16}$$

$\bar{E}$ is a dimensionless quantity related to the total energy by the equation $\bar{E} = 2E/\hbar\Omega_1$.

The basis used to diagonalize the Hamiltonian is simply given by

$$B = \{\psi_n(\alpha_1\bar{X})\psi_m(\alpha_2\bar{Y}) : n = 0, \ldots, N-1, \ m = 0, \ldots, M-1\} \ .$$

As before the oscillator scale parameters are chosen to minimize the manifold energy of the first K states. Since the diagonal matrix elements only depend on the harmonic piece of the Hamiltonian for the variable $\bar{X}$, α_1 is identically equal to 1, regardless of the number of states in the manifold. Minimizing the manifold energy,

$$E_m = \sum_{n=0}^{K_n - 1}\sum_{m=0}^{K_m - 1} \langle\psi_n(\bar{X})\psi_m(\alpha_2\bar{Y})|H|\psi_n(\bar{X})\psi_m(\alpha_2\bar{Y})\rangle \ , \tag{17}$$

TABLE VI. Convergence of the eigenvalue $E_0(\times 10^{-1})$ of coupled harmonic oscillators with quartic coupling vs K_m, the number of $\bar{Y}$ basis states in the manifold. $9M \times 9M$ is the size of the matrix. $\lambda = 10$.

M ($N=9$) \ K_m ($\alpha_2{}^2$)	10 (5.914 668 75)	20 (7.416 352 64)	30 (8.475 401 71)	40 (9.320 047 89)	50 (10.033 887 6)
6	0.328 981 811	0.330 294 445	0.334 006 697	0.338 863 058	0.344 181 269
8	0.328 973 656	0.328 979 717	0.329 357 856	0.330 295 102	0.331 705 166
10	0.328 960 310	0.328 960 898	0.328 972 569	0.329 070 170	0.329 308 617
12	0.328 960 288	0.328 960 322	0.328 960 246	0.328 964 886	0.328 989 617
14	0.328 960 218	0.328 960 217	0.328 960 233	0.328 960 272	0.328 961 701
16	0.328 960 217	"	0.328 960 217	0.328 960 218	0.328 960 250
18	"	"	"	0.328 960 217	0.328 960 217
20	"	"	"	"	"

TABLE VII. Convergence of the eigenvalue $E_9(\times 10^{-2})$ of coupled harmonic oscillators with quartic coupling vs K_m, the number of $\bar{Y}$ basis states in the manifold. $9M \times 9M$ is the size of the matrix. $\lambda = 10$.

K_m / α_2^2 / M ($N=9$)	10 5.914 668 75	20 7.416 352 64	30 8.475 401 71	40 9.320 047 89	50 10.033 997 6
6	0.150 459 900	0.150 710 242	0.151 793 286	0.153 350 334	0.154 212 614
8	0.150 437 034	0.150 436 268	0.150 533 039	0.150 830 911	0.151 314 892
10	0.150 434 145	0.150 434 424	0.150 436 285	0.150 464 866	0.150 546 132
12	0.150 433 992	0.150 433 999	0.150 433 996	0.150 435 081	0.150 443 001
14	0.150 433 978	0.150 433 977	0.150 433 983	0.150 433 984	0.150 434 380
16	0.150 433 976	0.150 433 976	0.150 433 976	0.150 433 977	0.150 433 983
18	"	"	"	0.150 433 976	0.150 433 976
20	"	"	"	"	"

with respect to α_2 yields

$$K_m(\alpha_2^6 - \alpha_2^2) - \lambda(2K_m^2 + 1) = 0 \ . \tag{18}$$

In Tables VI and VII we present the rate of convergence for a few representative eigenvalues both as a function of K_m, the number of states used to determine α_2, and of M, the number of states used in the diagonalization of the Hamiltonian. The results shown are for $\lambda = 10$. Unfortunately, owing to computer limitations, only 9-figure accuracy can be achieved. N has been chosen sufficiently large such that increasing N does not alter the eigenvalues to the accuracy shown.

We would like to emphasize that, as before, the convergence rate is uniformly good for a wide range of α_2 (and therefore K_m) values. The logical choice is $K_m = M$, but unfortunately one cannot predetermine how large M should be to obtain convergence to a specified accuracy. Fortunately, as in the previous case, the insensitivity to the precise value of K_m ensures that a reasonable estimate of M, and hence $K_m (= M)$, will still give a good rate of convergence. Again the rule-of-thumb estimate $K_m \approx M \approx 2k$ applies if one requires the lowest k eigenvalues ($k \gtrsim 10$).

To conclude we would like to point out that, although the work by Balsa *et al.* on the double-well anharmonic oscillator is correct, it lacks a simple physical explanation. If one is interested in obtaining the lower-lying eigenstates of the double-well anharmonic oscillator or the coupled oscillators via a Rayleigh-Ritz-type variational procedure, a simple means of determining the parametric dependence of the basis states is the minimization of the manifold energy. The good rate of convergence achieved in both the double-well anharmonic oscillator and the coupled oscillators is relatively insensitive to the choice of the number of states included in the calculation of the manifold energy. In both cases if one requires the lowest k eigenvalues ($k \geq 10$) our numerical work indicates that choosing both the size of the Rayleigh matrix and the number of states in the manifold roughly equal to $2k$ should yield a reasonably good convergence rate for the desired eigenvalues.

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[1]R. Balsa, M. Plo, J. G. Esteve, and A. F. Pacheco, Phys. Rev. D **28**, 1945 (1983).