Study of quantum anharmonic oscillators by state-dependent diagonalization

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In the present work, we propose the method of state-dependent diagonalization to find the energy eigenvalues and eigenstates of a quantum anharmonic oscillator. The example of a cubic-quartic anharmonic oscillator is used to illustrate its validity. Unlike the conventional exact diagonalization, this method is shown to be very efficient for calculating the energy eigenvalues of the excited states as well as the corresponding eigenfunctions. That is, no huge matrix needs to be diagonalized in this approach.

In recent years the problem of quantum oscillators has been a very active area of research [1]. The anharmonic oscillator model has the characteristic of being a rather simple model where many nontrivial features that are essential to understanding quite complicated systems may be implemented, and thus it has played a very significant role in the theoretical understanding of many branches of physics, e.g., nuclear and particle physics, atomic and molecular physics, solid-state physics, etc. This model also exhibits algebraically simple yet highly interesting properties so that various approximation schemes can be tested. For instance, it has been demonstrated by Bender and Wu that the application of a conventional perturbation method gives a divergent perturbation series for all values of the anharmonic coupling constant for a quartic anharmonic oscillator [2]. Besides, the problem of finding exact solutions for the anharmonic oscillator model is of considerable importance as well. Not only it is essential to some model field theories, but it is also useful in various applied contexts.

In the present work we develop the method of state-dependent diagonalization to determine the energy eigenvalues and eigenstates of a quantum anharmonic oscillator. Unlike the conventional numerical exact diagonalization, this approach is a very efficient method for calculating the energy eigenvalues of the excited states as well as the corresponding eigenfunctions. In other words, no huge matrix needs to be diagonalized in the method of state-dependent diagonalization. The basic idea of the method is very simple. Instead of diagonalizing the Hamiltonian of the anharmonic oscillator with a fixed basis set, we select different basis sets for different energy levels according to some optimization schemes, e.g., the operator method [3] or the variational principle of the "measure of nondiagonality [4]." With these optimal basis sets, the off-diagonal matrix elements of the Hamiltonian drop off very rapidly for each level. Even for the highly excited states, the size of the matrix is easily manageable. In the following sections we shall demonstrate the validity of the method of state-dependent diagonalization via the example of a cubic-quartic anharmonic oscillator.

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To begin with, we consider the one-dimensional cubic-quartic anharmonic oscillator described by the Hamiltonian,

$$H = \frac{p_x^2}{2} + A_2 x^2 + A_3 x^3 + A_4 x^4, \qquad (1)$$

where A_2, A_3, and A_4 are the coupling constants. By a simple change of variables, $y = x - s$, as well as the introduction of the annihilation operator, $a = (\mu y + i p_y)/\sqrt{2\hbar\mu}$, the Hamiltonian can be written in the form $H = H_0 + V$, with H_0 being the diagonal part and V the off-diagonal part:

$$H_0 = \left[\frac{\mu\hbar}{4} + \frac{\hbar}{2\mu}(A_2 + 3A_3 s + 6A_4 s^2) \right](2\hat{n}+1)$$
$$+ 3A_4 \left(\frac{\hbar}{2\mu} \right)^2 (2\hat{n}^2 + 2\hat{n} + 1) + A_2 s^2 + A_3 s^3 + A_4 s^4, \qquad (2)$$

where $\hat{n} = a^\dagger a$, and $V = \Sigma_{m=1}^4 a^{\dagger m} V_m + \text{H.c.}$ with

$$V_1 = \left(\frac{\hbar}{2\mu} \right)^{1/2} (2A_2 s + 3A_3 s^2 + 4A_4 s^3) + 3\left(\frac{\hbar}{2\mu} \right)^{3/2}$$
$$\times (A_3 + 4A_4 s)(\hat{n}+1),$$

$$V_2 = -\frac{\mu\hbar}{4} + \frac{\hbar}{2\mu}(A_2 + 3A_3 s + 6A_4 s^2)$$
$$+ 2A_4 \left(\frac{\hbar}{2\mu} \right)^2 (2\hat{n}+3),$$

$$V_3 = \left(\frac{\hbar}{2\mu} \right)^{3/2} (A_3 + 4A_4 s),$$

$$V_4 = A_4 \left(\frac{\hbar}{2\mu} \right)^2. \qquad (3)$$

It is obvious that the eigenstates of the diagonal term H_0 are basically the eigenstates of the simple harmonic oscillator associated with the Hamiltonian $H_{\text{SHO}} = \hbar\mu(a^\dagger a + \frac{1}{2})$. If V can be treated as a small perturbation, then H_0 will be an approximation to the Hamiltonian H. Besides, the oscillation theorem [5] states that the wave function of the nth excited
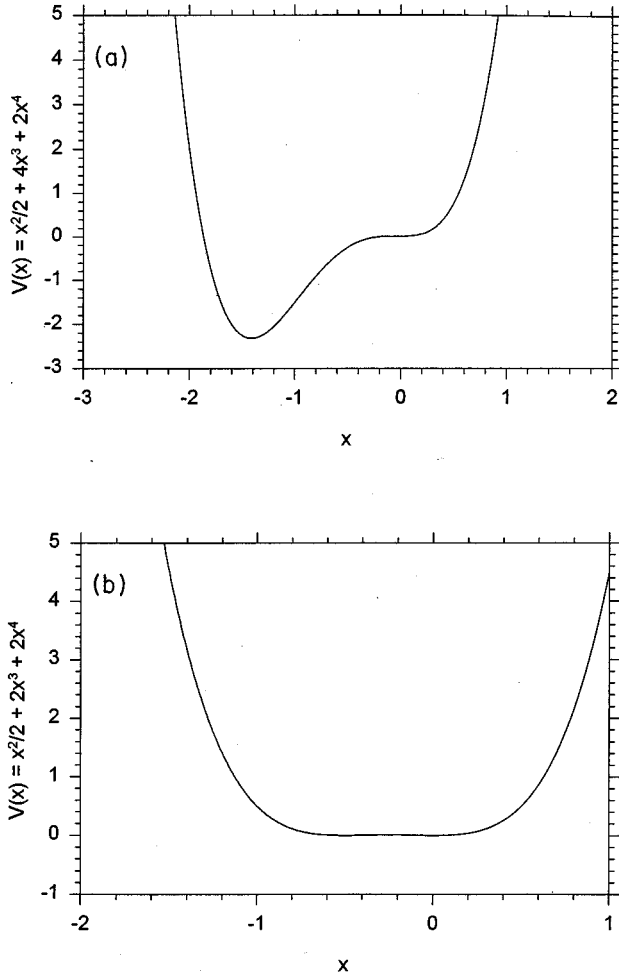
FIG. 1. (a) The cubic-quartic anharmonic oscillator potential $V(x)=x^2/2+4x^3+2x^4$; (b) the cubic-quartic anharmonic oscillator potential $V(x)=x^2/2+2x^3+2x^4$.

state of a bound system has exactly n nodes, and thus the nth excited state $|n\rangle$ of H_0 can be regarded as a first approximation to the corresponding nth excited state $|\psi_n\rangle$ of H. In accordance to this approximation, the zeroth-order estimate of the energy eigenvalue of $|\psi_n\rangle$ is given by $E_n^{(0)}=\langle n|H_0|n\rangle$, and the first-order correction $\Delta E_n^{(1)}=\langle n|V|n\rangle$ vanishes. So far the two parameters s and μ remain undetermined. Therefore, we now discuss how to fix these parameters according to three different optimization schemes, namely, the operator method, the variational principle of the "measure of nondiagonality," and the extremization method:

(i) *Operator method.* If we assume that the most important contribution of the off-diagonal term V comes from the terms V_1 and V_2, the operator method requires that $V_1|n\rangle=V_2|n\rangle=0$ so that the zeroth-order estimate of the energy eigenvalue $E_n^{(0)}$ may be improved. The two (coupled) algebraic equations will determine the two parameters s and μ. In previous studies of the anharmonic oscillators this method has proven to be able to give very good estimates of the energy eigenvalues [3].

(ii) *Variational principle of the "measure of nondiagonality."* If $|n\rangle$ is taken to approximate $|\psi_n\rangle$, then the nonnegative definite quantity $\Delta_n\equiv\sqrt{\langle n|[H-\langle n|H|n\rangle]^2|n\rangle}$ $=\sqrt{\langle n|H^2|n\rangle-E_n^{(0)2}}$ simply tells us how good the approximate wave function is. In the case where Δ_n vanishes, $|n\rangle$ indeed coincides with $|\psi_n\rangle$. Accordingly, we can minimize Δ_n by varying the parameters s and μ. With these optimal values of s and μ we can expect that $E_n^{(0)}$ provides a better estimate of the exact energy eigenvalue.

(iii) *Extremization method.* This method is a straightforward extension of the variational method for the ground-state energy in the sense that the parameters s and μ are chosen to extremize $E_n^{(0)}$. In other words, we vary the parameters to make the first-order variation of $E_n^{(0)}$ vanish. Unlike the case of the ground state, the resultant estimate of the energy eigenvalue of an excited state does not give any upper bound to the exact energy. Nevertheless, this approach has been

TABLE I. Comparison of the exact energy eigenvalues of the potential $(x^2/2+4x^3+2x^4)$, with the zeroth-order approximations based on three schemes: the operator method (OM), the variational principle of the measure of nondiagonality (MN), and the extremization method (EX).

State	OM	MN	EX	Exact	Error of OM (%)	Error of MN (%)	Error of EX (%)
0	−0.579 361	−0.542 866	−0.579 36	−0.671 324	−13.698 88	−19.135 07	−13.698 826
1	1.228 8059	1.189 4281	1.145 501 8	1.294 922 5	−5.105 835	−8.146 777	−11.538 966
2	3.483 898	3.461 298	3.417 077 6	3.529 314 1	−1.286 825	−1.927 174	−3.180 121 8
3	6.293 668	6.268 174 8	6.199 765 2	6.370 084 9	−1.199 622	−1.599 823	−2.673 742 4
4	9.511 7038	9.501 273 6	9.367 823 8	9.588 141 6	−0.797 212	−0.905 994	−2.297 815 6
5	13.060 149	13.068 733	12.852 358	13.124 747	−0.492 19	−0.426 78	−2.075 382 2
10	34.459 627	34.507 706	33.823 237	34.375 905	0.243 546 4	0.383 408 6	−1.607 718 3
30	155.647 67	155.391 16	152.544 26	154.485 39	0.752 353 6	0.586 311 9	−1.256 513 6
50	311.383 96	310.597 11	305.169 1	308.794 33	0.838 625 8	0.583 813	−1.173 996
70	490.781 7	489.356 31	481.022 33	486.544 7	0.870 836 1	0.577 872 8	−1.135 018 1
100	793.984 39	791.460 82	778.283 88	786.965 73	0.891 863	0.571 192 7	−1.103 205 7
500	6 886.744 2	6 861.853 2	6 754.029 7	6 824.260 4	0.915 612 5	0.550 869 96	−1.029 132 5
1000	17 405.395	17 341.941	17 072.504	17 247.66	0.914 532 29	0.546 633 89	−1.015 533 4

TABLE II. Same as in Table I except for the potential $(x^2/2 + 2x^3 + 2x^4)$.

State	OM	MN	EX	Exact	Error of OM (%)	Error of MN (%)	Error of EX (%)
0	0.810 862 7	0.815 034 6	0.810 862 7	0.791 295 7	2.472 768 53	2.999 998 73	2.472 768 53
1	2.921 794 8	2.927 527 7	2.921 794 8	2.879 789 9	1.458 610 03	1.657 682 81	1.458 610 03
2	5.718 668	5.713 514 9	5.710 321 7	5.727 911 9	−0.161 383 1	−0.251 348 3	−0.307 097 3
3	8.975 867 3	8.976 968 5	8.942 285 2	9.003 418 5	−0.306 007 5	−0.293 777 2	−0.679 001 1
4	12.591 02	12.606 57	12.518 644	12.623 325	−0.255 913 9	−0.132 731 1	−0.829 265 1
5	16.504 369	16.535 132	16.382 681	16.531 733	−0.165 520 8	0.020 564 92	−0.901 607 4
10	39.463 855	39.530 482	38.992 4	39.384 652	0.201 101 18	0.370 271 44	−0.995 951 5
30	165.274 65	165.102 16	162.581 79	164.242 01	0.628 725 42	0.523 704 52	−1.010 841 6
50	324.653 54	324.011 34	319.036 12	322.283 07	0.735 525 02	0.536 260 46	−1.007 483 3
70	507.233 67	506.004 95	498.232 12	503.290 65	0.783 448 58	0.539 310 98	−1.005 091 7
100	814.694 46	812.435 68	799.963 93	808.067 17	0.820 141 03	0.540 612 26	−1.002 792 7
500	6 946.262 1	6 922.226 3	6 816.414 1	6 885.016 7	0.889 545 35	0.540 442 64	−0.996 404 9
1000	17 499.589	17 437.506	17 171.246	17 343.835	0.898 037 58	0.540 081 19	−0.995 104 1

applied to a number of examples quite successfully, and the estimates of the energy eigenvalues are remarkably good [6].

Furthermore, it should be noted that in all these three approaches, the optimal parameters s and μ as well as the resultant Hamiltonian H_0 are all state-dependent.

The above three methods give us criteria for selecting optimal values of s and μ for each energy level, and they enable us to obtain good estimates of the exact energy eigenvalues. To further improve the results, we shall apply the method of state-dependent diagonalization. Suppose that we are interested in determining the energy eigenvalue of the level n and the corresponding wave function. We first define a basis set $\{|\phi_k(s_n,\mu_n)\rangle; k=1,2,3, \dots\}$ as follows:

$$|\phi_k(s_n,\mu_n)\rangle = \begin{cases} |n+(-1)^k[\frac{k}{2}]\rangle, & \text{if } k \leq 2n+1 \\ |k-1\rangle, & \text{if } k > 2n+1, \end{cases}$$

where $[k/2]$ equals the integral part of $k/2$. The states $\{|k\rangle; k=1,2,3, \dots\}$ are the eigenstates of the diagonal term

TABLE III. The dimensions of the matrices of the state-dependent diagonalization method required for the energy eigenvalues to converge to five significant figures. The potential is $(x^2/2 + 4x^3 + 2x^4)$. The schemes OM, MN, and EX are used to determine s_n and μ_n.

$H_0(s_n,\mu_n)$ associated with the energy level n. In terms of this basis we can expand the actual state vector $|\psi_n\rangle$ as a linear combination of the basis vectors: $|\psi_n\rangle = \Sigma_{k=1}^{\infty} C_k |\phi_k(s_n,\mu_n)\rangle$. Since we expect that $|\psi_n\rangle$ has the largest overlap with $|\phi_1(s_n,\mu_n)\rangle$, C_k should be small for large k. Then the summation can be truncated at a large enough value of k; in other words, we can write $|\psi_n\rangle = \Sigma_{k=1}^{K} C_k |\phi_k(s_n,\mu_n)\rangle$. The time-independent Schrödinger equation becomes

$$\sum_{m=1}^{K} (H_{mk} - E\delta_{mk})C_m = 0, \quad k=1,2,3, \dots K. \quad (4)$$

H_{mk} is a $K \times K$ symmetric matrix whose matrix elements are $H_{mk} \equiv \langle \phi_m(s_n,\mu_n)|H|\phi_k(s_n,\mu_n)\rangle = E_m^{(0)}(s_n,\mu_n)\delta_{mk} + V_{mk}$, and it can be diagonalized very easily because the off-diagonal elements V_{mk} are expected to be small. If we denote the eigenvalues of H_{mk} in ascending order by $\lambda_1, \lambda_2, \lambda_3, \dots, \lambda_K$, and the normalized eigenfunctions by $|\varphi_1\rangle, |\varphi_2\rangle, |\varphi_3\rangle, \dots, |\varphi_K\rangle$, then the approximate energy ei-

TABLE IV. Same as in Table III except for the potential $(x^2/2 + 2x^3 + 2x^4)$.

State	OM	MN	EX		State	OM	MN	EX
0	13	13	13		0	11	13	13
1	15	15	17		1	13	13	13
2	17	17	17		2	13	13	13
3	17	17	17		3	15	15	15
4	21	21	19		4	15	15	17
5	17	17	15		5	17	17	15
10	23	23	23		10	21	21	21
30	25	25	33		30	29	29	29
50	45	41	41		50	37	33	41
70	53	53	53		70	41	41	53
100	49	53	77		100	49	53	73
500	181	191	291		500	181	181	281
1000	311	331	531		1000	301	321	521

genvalue for the state $|\psi_n\rangle$ and the corresponding approximate eigenfunction will be given by

$$E_{n,K} = \begin{cases} \lambda_{r+1}, & \text{if } n > r \\ \lambda_{n+1}, & \text{if } n \leq r \end{cases}$$

and

$$|\psi_{n,K}\rangle = \begin{cases} |\varphi_{r+1}\rangle, & \text{if } n > r \\ |\varphi_{n+1}\rangle, & \text{if } n \leq r, \end{cases}$$

respectively, where $r = [(K-1)/2]$. When K increases, $E_{n,K}$ and $|\psi_{n,K}\rangle$ will converge to the exact results. Unlike the conventional exact diagonalization, the approximate estimate $E_{n,K}$ is, in general, not an upper bound of E_n. Nevertheless, when K is so large that the state $|0\rangle$ is included in the summation, the state-dependent diagonalization becomes exactly the same as the conventional exact diagonalization. Then $E_{n,K}$ will be an upper bound of E_n. Furthermore, it should be noted that if the anharmonic oscillator potential does not contain the cubic term, i.e., $A_3 = 0$, the potential will be an even function of x and the eigenfunctions will have definite parity. Hence, the numerical diagonalization can be simplified by choosing the subspace of basis vectors with appropriate parity.

To illustrate the validity of the method of state-dependent diagonalization, we perform the explicit numerical calculations for two special cases of the cubic-quartic anharmonic potential model, namely, (i) $A_2 = \frac{1}{2}$, $A_3 = 4$, and $A_4 = 2$, and (ii) $A_2 = \frac{1}{2}$, $A_3 = 2$, and $A_4 = 2$. As shown in Fig. 1, the former case corresponds to that of an asymmetrical double-well potential, while the latter is essentially a single-well potential with a shallow hump at the center of the well. First, we apply the three optimization schemes to determine the zeroth-order estimates of the energy eigenvalues of the cubic-quartic anharmonic oscillator and tabulate the results in Tables I and II. Then we evaluate the exact eigenenergies and eigenfunctions by the method of state-dependent diagonalization. For easy comparison, we list the exact energies in Tables I and II as well. It is clear that the zeroth-order estimates are satisfactory for all energy levels, especially for the highly excited states. The discrepancies that occur in the low-lying eigenstates are due to the fact that the asymmetry of the potential well becomes significant for these states, and our approximation of the potential well by a simple harmonic oscillator potential thus fails, no matter how we tune the parameters s and μ. The numerical results also indciate that for the low-lying eigenstates the operator method is able to give better estimates of the eigenenergies than the other two methods, whereas the variational method of the "measure of nondiagonality" proves to be a better approach for the highly excited states. Besides, both the operator method and the extremization method give exactly identical ground-state results; in fact, both methods yield the same set of two (coupled) algebraic equations in s and μ, as well as the same expression for $E_0^{(0)}$. This interesting feature was observed in previous studies of the quartic anharmonic oscillator as well [3].

Tables III and IV show the matrix size required to achieve the converged results for each energy level by the method of state-dependent diagonalization. It is remarkable that each of

TABLE V. State-dependent diagonalization with (s,μ) fixed at their ground-state values given by the extremization method. The "matrix size" is the dimension of the matrix required for the energy eigenvalue to converge to five significant figures. Results are shown for two potentials: $(A_2,A_3,A_4)=(1/2,4,2)$ and $(A_2,A_3,A_4)=(1/2,2,2)$.

	Matrix size	
State	$A_3=4$	$A_3=2$
0	13	13
1	15	15
2	17	19
3	19	23
4	23	19
5	19	21
10	31	35
30	73	101
50	141	181
70	211	271
100	301	421

the eigenenergies of the first 50 states can be accurately calculated by simply diagonalizing a matrix of the size less than 50×50. On the other hand, by using the basis of the simple harmonic oscillator $H = p_x^2/2 + A_2 x^2$, the conventional exact diagonalization will need a 50×50 matrix in order to give the energy eigenvalues of the first eight levels [7]. Therefore, finding the eigenenergies of the higher levels by the conventional approach seems not feasible at all because a very huge matrix is needed, whereas our approach is able to accomplish the task with very modest effort. Furthermore, it should be noted that for low-lying eigenstates all the three different optimization schemes provide equally good basis sets for diagonalization, but the performance of the extremization method starts to deteriorate as we go to the higher levels. It seems to suggest that the matrix size required to achieve the converged results is not sensitive to the parameters s and μ for the low-lying states. In fact, if those parameters of the ground state determined by the extremization method are used for all energy levels, the speed of convergence is about the same for the low-lying eigenstates. Nevertheless, as shown in Table V, the matrix size needed for convergence increases dramatically as we go to the higher levels.

In summary, we have proposed a different approach—the method of state-dependent diagonalization—to find the energy eigenvalues and eigenstates of a quantum anharmonic oscillator, and the example of a cubic-quartic anharmonic oscillator has been used to illustrate its validity. It has been shown that unlike the conventional exact diagonalization, this approach is a very efficient method for calculating the energy eigenvalues of the excited states, as well as the corresponding eigenfunctions. The method of state-dependent diagonalization is so simple that it can be easily applied to more complicated anharmonic oscillator potentials. We are currently pursuing this direction, and the results will be published elsewhere.

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