PHYSICAL REVIEW D VOLUME 12, NUMBER 8 15 OCTOBER 1975

Matrix mechanics as a practical tool in quantum theory: The anharmonic oscillator*

Ching-Teh Li, Abraham Klein, and Franz Krejs
Department of Physics, University of Pennsylvania, Philadelphia, Pennsylvania 19174
(Received 7 April 1975)

For an anharmonic oscillator, it follows from the number of zeros of the exact wave functions as functions of the quantum number n that the matrix elements $\langle n|x|n'\rangle$ and $\langle n|p|n'\rangle$ should be rapidly decreasing functions of $|n-n'|$. Matrix elements of polynomials in x and p should therefore be well approximated by a finite number of terms in their sum-rule decomposition. From the matrix elements of the equations of motion for x and for p and of the commutator $[x,p]$, one thereby obtains closed sets of nonlinear algebraic equations to characterize subspaces of the Hilbert space of exact eigenfunctions. The approximations are also derived from a novel variational principle, and numerous variant approximation schemes are suggested. Essentially exact numerical results are obtained and compared with previous work. The broad applicability of the techniques is emphasized.

I. INTRODUCTION

For more than a decade, one of the authors (A. K.) and his associates have been studying problems of nuclear and other collective motion utilizing, among other variants, a calculus derived from matrix elements of the Heisenberg equations of motion and of the commutation relations.[1] When tested on exactly soluble models, these methods of matrix mechanics have proved to be convenient and accurate means of computing both eigenvalues and matrix elements of operators.

It has recently occurred to the authors that the characteristic manner in which the concept of collectivity defines a viable approximation scheme may render the method more widely applicable to problems in the quantum mechanics of particles and fields than was originally contemplated. In this paper we shall illustrate this thesis by studying the anharmonic oscillator with quartic interaction, defined by the Hamiltonian

$$H=\tfrac{1}{2}(p^2+x^2)+\tfrac{1}{4}\lambda x^4 . \tag{1.1}$$

This Hamiltonian has received a surprising amount of attention in recent years directed toward both theoretical and numerical aspects of the problem.[2-8] On the whole, our own efforts have a practical orientation. Our aim is to develop a complete calculational scheme that is neither the direct numerical integration of the Schrödinger equation nor the diagonalization of the Hamiltonian, in a definite preselected basis. In Sec. II we describe a straightforward and systematic version of the method and the one we have exploited numerically: From the equations of motion

$$[x,H]=ip , \tag{1.2}$$

$$[p,H]=-ix-i\lambda x^3 , \tag{1.3}$$

and from the commutation relation

$$[x,p]=i , \tag{1.4}$$

we simply form matrix elements between the *exact* eigenstates of H. By the use of sum rules to evaluate the matrix elements of polynomials of x and p and the assumption, which is the *sine qua non*, that these sum rules saturate rapidly, we derive a closed approximate set of nonlinear algebraic equations for a finite set of matrix elements of x and p. The elementary argument for anticipating convergence is given and the method for solution is described (in the Appendix).

In Sec. IV we present the results of our calculation, which are seen to justify our previous optimism; the results converge as anticipated for any value of λ, clearly exhibiting the nonperturbative character of our method. Some comparison with previous work is presented.

In Sec. III we adjoin some theoretical considerations. We show how the calculational scheme of the previous section can be derived from a novel variational principle. We also discuss briefly a number of variants of our scheme. We conclude in Sec. V with a brief discussion.

In this paper we have emphasized methods appropriate to low-lying states; higher approximations proceed by adding states of higher energy. The methods are, however, readily adapted to the study of the semiclassical limit, and thus provide a powerful alternative to the WKB approximation. This remark forms the basis of the work of Halpern,[8] whose approach is closest in spirit to our own. It is our intention to return to the semiclassical limit in a separate publication.

II. A COMPUTATIONAL SCHEME BASED ON MATRIX MECHANICS

A. General equations

Let $|n\rangle$, with $n=0,1,2,\ldots$, be the exact normalized eigenstates of the Hamiltonian (1.1),

$$H|n\rangle = E_n|n\rangle \tag{2.1}$$

and

$$\langle n|H|n'\rangle = 0 \quad \text{if } n \neq n'. \tag{2.2}$$

In this representation, Eq. (1.4) becomes

$$\sum_{n''} (\langle n|x|n''\rangle\langle n''|p|n'\rangle - \langle n|p|n''\rangle\langle n''|x|n'\rangle) = i\delta_{nn'}. \tag{2.3}$$

Equations (1.2) and (1.3) become

$$(E_{n'} - E_n)\langle n|x|n'\rangle = i\langle n|p|n'\rangle, \tag{2.4}$$

$$(E_{n'} - E_n)\langle n|p|n'\rangle = -i\langle n|x|n'\rangle - i\lambda \sum_{n''}\sum_{n'''} \langle n|x|n''\rangle\langle n''|x|n'''\rangle\langle n'''|x|n'\rangle. \tag{2.5}$$

We emphasize that the conditions $\langle n|H|n'\rangle = E_n\delta_{nn'}$ expressing (2.1) and (2.2) have been used in deriving the equations above.

It is convenient to eliminate the energies as variables between the above two equations of motion. Thus, we find

$$\langle n|p|n'\rangle^2 = -\langle n|x|n'\rangle^2 - \lambda\langle n|x|n'\rangle \sum_{n''}\sum_{n'''} \langle n|x|n''\rangle\langle n''|x|n'''\rangle\langle n'''|x|n'\rangle. \tag{2.6}$$

If we apply the assumption that sum rules are saturated by a reasonable number of states, Eqs. (2.2), (2.3), and (2.6) then constitute a closed set of nonlinear algebraic equations to be satisfied by all the matrix elements $\langle n|x|n'\rangle$ and $\langle n|p|n'\rangle$ between these states.

As in the case of the harmonic oscillator, the energy eigenstates have definite parities which alternate. Hence

$$\langle n|x|n'\rangle = \langle n|p|n'\rangle = 0, \quad |n-n'| \text{ even}. \tag{2.7}$$

In addition, time-reversal invariance allows us to choose

$$\langle n|x|n'\rangle = \langle n'|x|n\rangle, \qquad \langle n|p|n'\rangle = -\langle n'|p|n\rangle. \tag{2.8}$$

For numerical purposes it is convenient to express these restrictions by a change of notation. With $n = 2I-2$ and $n' = 2J-1$, we set

$$X(I,J) = \langle n|x|n'\rangle = \langle n'|x|n\rangle, \qquad Y(I,J) = -i\langle n|p|n'\rangle = i\langle n'|p|n\rangle. \tag{2.9}$$

The first index of $X(I,J)$ and $Y(I,J)$ refers to the Ith even-parity states and the second refers to the Jth odd-parity state. In this new notation, Eq. (2.6) becomes

$$-Y(I,J)^2 + X(I,J)^2 + \lambda X(I,J)\sum_{I'}\sum_{J'} X(I,J')X(I',J')X(I',J) \equiv E_M(I,J) = 0, \tag{2.10}$$

and Eq. (2.3) divides into two sets, one for each parity, namely,

$$\sum_{J} [X(I,J)Y(I',J) + Y(I,J)X(I',J)] + \delta(I,I') \equiv C_E(I,I') = 0 \tag{2.11}$$

and

$$\sum_{I} [X(I,J)Y(I,J') + Y(I,J)X(I,J')] - \delta(J,J') \equiv C_O(J,J') = 0. \tag{2.12}$$

B. Approximation scheme based on the ground state

We first describe an approximation scheme which starts with the ground state and works up in energy. Actually we can start at an excited state, if we assume we know all the relevant matrix elements to lower states. This idea will allow us later to reach rather high states in the spectrum without having to consider at one time all states below.

The basic physical idea behind the construction of an approximation scheme is that the matrix elements $\langle n|x|n'\rangle$ and $\langle n|p|n'\rangle$ decrease rapidly with increasing $|n-n'|$. That this should be so is intuitively clear from the standard consideration of the number of zeros for different n of the wave functions in coordinate space (or momentum space). By considering the matrix element $\langle 0|x^3|1\rangle$ which enters into $E_M(1,1)$, the first equation of motion considered, we see that

$$\langle 0|x^3|1\rangle \cong \langle 0|x|1\rangle\langle 1|x|0\rangle\langle 0|x|1\rangle + \langle 0|x|1\rangle\langle 1|x|2\rangle\langle 2|x|1\rangle + \cdots, \tag{2.13}$$

where $\cdots$ refers to smaller terms. Since $\langle 0|x|1\rangle$ is of the same order as $\langle 1|x|2\rangle$, we conclude that the lowest order of approximation which

makes physical sense *in this problem* is to work with three states 0, 1, 2.

Owing to the parity consideration, it is easy to see that we must include two more states, one of each parity, for each further step of approximation. Thus, in the νth order of approximation we have $2\nu+1$ states, $\nu+1$ of even parity and ν of odd parity. At this stage we have $2\nu(\nu+1)$ variables, namely $X(I,J)$ and $Y(I,J)$ with $1 \leq I \leq \nu+1$, $1 \leq J \leq \nu$. Hence, to find the solutions for these matrix elements, we also need $2\nu(\nu+1)$ independent equations. In fact, for every possible order of approximation, we always have more than enough equations to be satisfied by the matrix elements. This redundancy is a general feature of the present algebraic method. It gives us alternatives for selecting a closed set of equations to determine the relevant variables and provides us room for self-consistent checks.

Since the diagonalization of the Hamiltonian has already been used in deriving the equations of motion (2.10), we leave the conditions (2.2) as the set of self-consistent checks to the final solutions. Thus, Eqs. (2.10)–(2.12) are the remaining equations available. Totally there are still $\nu+1$ equations more than necessary. To carry through a general scheme, we omit those even commutator equations in (2.11) which most severely involve the boundary $I=\nu+1$, $I'=1,2,\ldots,\nu+1$. This is sensible since the main truncation errors come from matrix elements involving boundary states. However, as we shall note in the next section, this was not the only possible course open to us.

In the νth order of approximation, therefore, we solve the following three sets of equations:

$$E_M(I,J)=0\,,\quad 1 \leq I \leq \nu+1\,,\quad 1 \leq J \leq \nu\,, \tag{2.14}$$

$$C_E(I,I')=0\,,\quad 1 \leq I' \leq I \leq \nu\,, \tag{2.15}$$

$$C_O(J,J')=0\,,\quad 1 \leq J' \leq J \leq \nu\,, \tag{2.16}$$

which comprise $\nu(\nu+1)$, $\frac{1}{2}\nu(\nu+1)$, and $\frac{1}{2}\nu(\nu+1)$ equations, respectively. The basic method utilized in solving these nonlinear equations, which has been described previously,[9] is summarized and extended in the Appendix. The technique described therein allows us to write a program suitable for every possible order of approximation. The results of our calculation are given in Sec. IV.

Of course, ν will have some upper limit for the above program determined by computer capacity or economics, or both. The structure of the problem allows us to overcome these limitations to a considerable extent in seeking information about high-lying states. To within the preassigned accuracy of the solutions of (2.14)–(2.16), we should and do find that there is a ν_0 such that for $\nu > \nu_0$ the matrix elements $X(1,1)$ and $Y(1,1)$ are independent of ν, i.e., we have found their exact value. For a still greater ν_0, others of the matrix elements relating to the lowest-lying states will have converged to their exact values. Treating these matrix elements as *known constants,* we can increase ν commensurately without thereby increasing the number of variables in the problem defined by (2.14)–(2.16). If carried out systematically, such a procedure can carry us as high into the spectrum as we have patience to probe. The results of a specific procedure of this type will also be described in Sec. V.

III. VARIATIONAL CONSIDERATIONS

The starting point of such considerations was the thought that the matrix elements $\langle n|x|n'\rangle$ and $\langle n|p|n'\rangle$ might be useful as variational parameters for a Rayleigh-Ritz principle.[10] The stimulus for such a suggestion comes from the application of sum rules to the evaluation of $\langle n|H|n\rangle$,

$$\langle n|H|n\rangle=\sum_{n'}\left(\tfrac{1}{2}\langle n|p|n'\rangle\langle n'|p|n\rangle+\tfrac{1}{2}\langle n|x|n'\rangle\langle n'|x|n\rangle\right)+\tfrac{1}{4}\lambda\sum_{n'n''n'''}\left(\langle n|x|n'\rangle\langle n'|x|n''\rangle\langle n''|x|n'''\rangle\langle n'''|x|n\rangle\right), \tag{3.1}$$

and the desire to study the condition that $\langle n|H|n\rangle$ be stationary.

One is, however, confronted with two obvious difficulties:

(i) How many of the matrix elements are independent variables?

(ii) The same matrix elements recur in different energy functionals. Thus $\langle n|x|n'\rangle$ occurs in both $\langle n|H|n\rangle$ and $\langle n'|H|n'\rangle$. This is to be expected since this matrix element helps determine two wave functions.

A symmetrical solution to the second problem is to form the trace of H over the subspace considered and to require

$$\delta\,\mathrm{Tr}H=\delta\sum_n\langle n|H|n\rangle=0\,. \tag{3.2}$$

A solution to the first problem is to impose all

the kinematical constraints within the subspace, namely

$$\delta\langle n|[x,p]|n'\rangle=0\,. \tag{3.3}$$

To exploit (3.3), we multiply by a Lagrange multiplier $i\langle n'|h|n\rangle$, sum over n,n', and subtract the results from (3.2). (Note that the elements $\langle n'|h|n\rangle$ form a Hermitian matrix.) We are thus led to a master variational principle,

$$\delta\,\mathrm{Tr}\{H-ip[h,x]\}=\delta\,\mathrm{Tr}\{H-ix[p,h]\}=0\,. \tag{3.4}$$

This yields the equations

$$\langle n|p|n'\rangle-i\langle n|[h,x]|n'\rangle=0\,, \tag{3.5}$$

$$\langle n|x|n'\rangle+\lambda\langle n|x^3|n'\rangle+i\langle n|[h,p]|n'\rangle=0\,. \tag{3.6}$$

Up to now the basis $|n\rangle$ was arbitrary (because of the invariance of the trace), but the most convenient choice is the one in which h is diagonal. Equivalently, identifying h with the Hamiltonian certifies (3.5) and (3.6) as the equations of motion.

As we have asserted in the previous section, this formulation provides a convenient basis for a systematic numerical treatment of the problem. There are, however, infinitely many variants, several of which have been found useful in the applications to the many-body problem.[11] It is perhaps worth listing some of these variants in order to emphasize the flexibility of the method. In comparing this listing with the method described in the previous section, we keep in mind that in the latter we use all the equations derived from the variational principle (3.4) and *most* but not all of the commutation relations. The variants are the following.

(i) Substitute conditions $\langle n|H|n'\rangle=0$, $n\neq n'$, for the least accurate equations of motion. For instance, for $\nu=1$, we normally use two equations of motion $(n,n')=(0,1)$ and $(1,2)$ and two commutation relations $(0,0)$ and $(1,1)$. For the equation of motion $(1,2)$ we would substitute the condition $\langle 0|H|2\rangle=0$. As Halpern has noted,[8] if we use *all* the kinematical constraints the conditions that the Hamiltonian be diagonal completely define the dynamics. For the case $\nu=1$, we would adjoin to the condition $\langle 0|H|2\rangle=0$ the three commutation relations $(0,0),(1,1),(0,2)$.

The following further possibilities arise.

(ii) There was no compulsion to form the trace in (3.2). Thus we consider more generally, with arbitrary α_n,

$$\delta\sum_n \alpha_n\langle n|H|n\rangle=0\,. \tag{3.7}$$

A rationale for choosing a weighted average exists. It is that in any given order of approximation the energies of the lower states are more accurately determined and therefore should be emphasized in the variational method. Proceeding as before we see that there follow again "equations of motion" but these are no longer recognized as the Heisenberg equations of motion. Therefore, $h\neq H$. If we insist that h be diagonal we determine a representation of x and p, but after all this we must take the further steps of constructing the Hamiltonian matrix in our subspace and diagonalizing it, thus carrying out a unitary transformation on x and p.

Again the double procedure just described may be avoided by not insisting that h be diagonal, and including the H diagonal conditions as part of the nonlinear system, either in place of some of the equations of motion or in place of some of the off-diagonal commutation relations.

The variants just described subsume, except for purely technical differences, all the cases which have been considered by us in the past.

IV. CONVERGENCE AND APPLICATION TO HIGHER-STATE CALCULATIONS

A. Convergence of the numerical results

In this subsection we present some of the computer solutions of Eqs. (2.14)–(2.16) for various orders of approximation to show the rapid convergence of the method. From the wide range of anharmonicity for which these results were calculated, one can clearly see that our method is nonperturbative in spirit.

In Table I some of the matrix elements relating to the lowest states are given. For a given order of approximation, it is clear that the least accurate results are those matrix elements $X(I,J)$ and $Y(I,J)$ for which $I\cong\nu+1$ and $J\cong\nu$. But when they recur in the calculations of the next orders of approximation, they also converge very rapidly. Although we have only listed the results for $\lambda=1.0$, the rapid convergence of the numerical results is a general feature of our method for the whole range of anharmonicity. This feature can also be seen from the results of the energies shown in Table II. The basic physical idea of the method is thus well verified.

Once the most significant matrix elements have been found we can actually calculate all other physical quantities of interest to us, especially the energy eigenvalues. Usually the $2\nu+1$ energies in the νth order of approximation can be calculated from the expressions of the diagonal Hamiltonian matrix elements in terms of $X(I,J)$ and $Y(I,J)$. However, in what follows the results evaluated from $(0|H|0)$ and the equations of motion (2.4) are much more accurate, especially

TABLE I. Convergence of the results for the matrix elements $X(I,J)$ and $Y(I,J)$ calculated in the first six orders of approximation; $\lambda = 1.0$.

Matrix elements \ ν	1	2	3	4	5	6
$X(1,1)$	0.591 079 49	0.595 336 63	0.595 343 89	0.595 343 90	0.595 343 90	0.585 343 90
$Y(1,1)$	−0.845 909 91	−0.836 529 38	−0.836 481 59	−0.836 481 48	−0.836 481 48	−0.836 481 48
$X(2,1)$	0.835 912 64	0.771 097 32	0.770 988 14	0.770 876 78	0.770 876 78	0.770 876 78
$Y(2,1)$	1.196 297 26	1.288 027 30	1.289 275 35	1.289 279 20	1.289 279 20	1.289 279 20
$X(1,2)$		0.019 981 37	0.020 133 97	0.020 134 22	0.020 134 22	0.020 134 22
$Y(1,2)$		−0.099 263 45	−0.099 396 90	−0.099 395 62	−0.099 395 62	−0.099 395 62
$X(2,2)$		0.888 311 69	0.894 473 22	0.894 483 48	0.894 483 50	0.894 483 50
$Y(2,2)$		−1.680 935 21	−1.663 056 71	−1.662 958 52	−1.662 958 27	−1.662 958 27
$X(3,1)$		0.030 205 06	0.027 237 04	0.027 228 59	0.027 228 57	0.027 228 57
$Y(3,1)$		0.159 647 95	0.150 892 70	0.150 913 07	0.150 913 19	0.150 913 19
$X(3,2)$		1.076 148 96	0.992 766 90	0.992 484 34	0.992 483 87	0.992 483 87
$Y(3,2)$		1.853 997 65	1.993 718 39	1.995 725 54	1.995 731 95	1.995 731 96
$X(1,3)$			0.000 705 54	0.000 710 92	0.000 710 93	0.000 710 93
$Y(1,3)$			−0.006 437 72	−0.006 461 12	−0.006 461 10	−0.006 461 10
$X(2,3)$			0.032 311 19	0.032 557 76	0.032 558 16	0.032 558 17
$Y(2,3)$			−0.195 387 66	−0.195 699 75	−0.195 697 29	−0.195 697 29
$X(3,3)$			1.067 431 37	1.074 935 58	1.074 948 04	1.074 948 06
$Y(3,3)$			−2.326 526 54	−2.301 311 93	−2.301 168 56	−2.301 168 18
$X(4,1)$			0.001 088 35	0.000 981 54	0.000 981 23	0.000 981 23
$Y(4,1)$			0.010 502 57	0.009 752 30	0.009 752 05	0.009 752 06
$X(4,2)$			0.040 957 32	0.036 939 74	0.036 928 22	0.036 928 20
$Y(4,2)$			0.250 587 90	0.236 566 09	0.236 597 54	0.236 597 73
$X(4,3)$			1.244 469 23	1.147 155 00	1.146 823 75	1.146 823 20
$Y(4,3)$			2.402 409 88	2.583 836 12	2.586 531 35	2.586 540 15

for lower orders and the boundary states in a given order. We thus write

$$E(0) = (0|H|0)$$
$$= \tfrac{1}{2}\sum_{J=1}^{\nu}[Y(1,J)^2 + X(1,J)^2]$$
$$+ \frac{\lambda}{4}\sum_{J=1}^{\nu}\sum_{I=1}^{\nu+1}\sum_{J'=1}^{\nu} X(1,J)X(I,J)X(I,J')X(1,J') . \tag{4.1}$$

The odd-parity-state energies are given by

$$E(2J-1) = E(0) - \frac{Y(1,J)}{X(1,J)}, \quad J = 1, \ldots, \nu \tag{4.2}$$

and the even-parity-state energies by

$$E(2I-2) = E(1) + \frac{Y(I,1)}{X(I,1)}, \quad I = 2, \ldots, \nu+1 . \tag{4.3}$$

In Table II we show the first eleven energy eigenvalues evaluated with (4.1)–(4.3) in the first six orders of approximation for four different values of λ, i.e., $\lambda = 0.01$, 0.10, 1.00, and 10.0. It can be clearly seen that the energies of the lower states converge very rapidly to their exact values. The results for the upper states are less accurate, as anticipated. In prinicple we can find their exact values by successively increasing the level of approximation. However, in practice, this has an upper limit set by computer capacity or economy. In the next subsection, we shall develop a general scheme which will enable us to evaluate accurately the matrix elements and energies of the upper states for large n. All further results reported below were calculated with this scheme.

As mentioned before, we use the off-diagonal Hamiltonian equations (2.2) as self-consistency checks of our results. For those not seriously involving the boundary states, these checks are always very good. They also improve as we increase the order of approximation.

B. Application to the calculations of higher states

As asserted at the end of Sec. II and justified by the numerical results in the previous subsection, the most significant matrix elements relating to

TABLE II. Convergence of the results for the energies calculated in the first six orders of approximation; $\lambda = 0.01, 0.10, 1.00, 10.0$.

n \ ν	1	2	3	4	5	6
			$\lambda = 0.01$			
0	0.501 861 14	0.501 858 91	0.501 858 91	0.501 858 91	0.501 858 91	0.501 858 91
1	1.509 278 42	1.509 249 77	1.509 249 77	1.509 249 77	1.509 249 77	1.509 249 77
2	2.516 695 69	2.523 912 82	2.523 913 12	2.523 913 12	2.523 913 12	2.523 913 12
3		3.545 787 73	3.545 705 52	3.545 705 51	3.545 705 51	3.545 705 51
4		4.563 823 17	4.574 489 71	4.574 490 63	4.574 490 63	4.574 490 63
5			5.610 300 64	5.610 138 73	5.610 138 72	5.610 138 72
6			6.636 628 70	6.652 524 08	6.652 526 08	6.652 526 08
7				7.701 795 78	7.701 534 68	7.701 534 66
8				8.737 216 53	8.757 048 04	8.757 051 62
9					9.819 345 37	9.818 969 10
10					10.863 576 56	10.887 177 61
			$\lambda = 0.10$			
0	0.517 520 77	0.517 364 89	0.517 364 85	0.517 364 85	0.517 364 85	0.517 364 85
1	1.585 443 78	1.583 613 97	1.583 612 68	1.583 612 68	1.583 612 68	1.583 612 68
2	2.653 366 79	2.708 542 86	2.708 630 65	2.708 630 71	2.708 630 71	2.708 630 71
3		3.888 753 14	3.885 139 47	3.885 135 64	3.885 135 64	3.885 135 64
4		5.030 360 34	5.107 657 44	5.107 834 92	5.107 835 08	5.107 835 08
5			6.378 161 14	6.372 669 65	6.372 662 36	6.372 662 35
6			7.581 662 64	7.676 096 04	7.676 369 91	7.676 370 19
7				9.023 536 49	9.016 302 43	9.016 291 21
8				10.281 182 41	10.389 814 24	10.390 185 53
9					11.805 000 65	11.796 156 89
10					13.111 195 96	13.232 032 33
			$\lambda = 1.00$			
0	0.624 016 42	0.620 932 21	0.620 927 04	0.620 927 03	0.620 927 03	0.620 927 03
1	2.055 143 57	2.026 068 96	2.025 966 40	2.025 966 16	2.025 966 16	2.025 966 16
2	3.486 270 71	3.696 451 23	3.698 444 77	3.698 450 31	3.698 450 32	3.698 450 32
3		5.588 732 08	5.557 703 02	5.557 577 44	5.557 577 14	5.557 577 14
4		7.311 539 57	7.565 947 15	7.568 415 77	7.568 422 86	7.568 422 87
5			9.745 503 22	9.709 299 35	9.709 148 25	9.709 147 88
6			11.675 972 04	11.961 685 58	11.964 535 24	11.964 543 60
7				14.363 953 09	14.323 438 33	14.323 265 64
8				16.461 447 00	16.773 268 33	16.776 443 29
9					19.361 378 43	19.317 146 36
10					21.600 952 68	21.935 378 04
			$\lambda = 10.00$			
0	1.023 520 50	1.009 209 33	1.009 170 42	1.009 170 32	1.009 170 32	1.009 170 32
1	3.624 764 68	3.507 370 35	3.506 741 63	3.506 739 60	3.506 739 59	3.506 739 59
2	6.226 008 87	6.725 769 82	6.733 833 30	6.733 865 11	6.733 865 21	6.733 865 21
3		10.503 964 29	10.407 532 41	10.406 985 25	10.406 983 48	10.406 983 47
4		13.830 874 63	14.428 932 83	14.437 465 33	14.437 498 08	14.437 498 18
5			18.873 384 74	18.769 981 36	18.769 409 46	18.769 407 63
6			22.696 179 57	23.355 780 38	23.364 818 23	23.364 852 35
7				28.307 008 70	28.196 686 78	28.196 086 71
8				32.520 186 47	33.232 154 32	33.241 685 92
9					38.602 019 36	38.485 308 31
10					43.143 035 43	43.900 897 78

the lowest states converge very rapidly and, to within the preassigned accuracy, become independent of further levels of approximation. By treating them as known constants we can enlarge the level of approximation without at the same time increasing the number of equations to be solved. This feature then enables us to evaluate the matrix elements, and thereby the energies of the upper states, essentially with the same ease as before.

Suppose that we have found the matrix elements of the lowest states by the νth-order approximation and consider the most significant matrix elements relating to the lowest two states as essentially exact. In the next step of calculation we include two more upper states, one for each parity. This time we are going to solve for the $2\nu(\nu+1)$ matrix elements $X(I,J)$ and $Y(I,J)$ with $I=2,\ldots,\nu+2$ and $J=2,\ldots,\nu+1$ from the following equations:

$$E_M(I,J) = -Y(I,J)^2 + X(I,J)^2 + \lambda X(I,J) \sum_{I'=1}^{\nu+2} \sum_{J'=1}^{\nu+1} X(I,J')X(I',J')X(I',J) = 0 ,$$

where (4.4)

$$I=2,\ldots,\nu+2 ,$$

$$J=2,\ldots,\nu+1 ,$$

$$C_E(I,I') = \sum_{J=1}^{\nu+1} [X(I,J)Y(I',J) + Y(I,J)X(I',J)] + \delta(I,I') = 0 ,$$

where (4.5)

$$I=2,\ldots,\nu+1 ,$$

$$I'=2,\ldots,I ,$$

$$C_O(J,J') = \sum_{I=1}^{\nu+2} [X(I,J)Y(I,J') + Y(I,J)X(I,J')] - \delta(J,J') = 0 ,$$

where (4.6)

$$J=2,\ldots,\nu+1 ,$$

$$J'=2,\ldots,J .$$

The matrix elements $X(1,J)$, $Y(1,J)$ and $X(I,1)$, $Y(I,1)$ with $J=1,\ldots,\nu$, $I=1,\ldots,\nu+1$ are included in all the above intermediate summations but are regarded as known constants. $X(1,\nu+1)$, $Y(1,\nu+1)$ and $X(\nu+2,1)$, $Y(\nu+2,1)$ occur in the sums but are set to zero because they are not in the range of the previous νth-order calculation and are usually very small. The previous results for $X(I,J)$, $Y(I,J)$ with $I,J \geq 2$ are to be used as starting values for the solution of Eqs. (4.4)–(4.6). For those matrix elements relating to the two upper states which have just been added to the set of variables, the method of assigning proper initial values described in (A5) was used.

The procedure described above can be successively applied to calculate the matrix elements for more and more higher states. However, because of the rapidly decreasing nature of the matrix elements, it is not necessary that the intermediate summations always start from the lowest even-parity or odd-parity state. Therefore, at the lth step of such a calculation we solve for $X(I,J)$, $Y(I,J)$ with $I=l,\ldots,\nu+l$, $J=l,\ldots,\nu+l-1$ from

$$E_M(I,J) = -Y(I,J)^2 + X(I,J)^2 + \lambda X(I,J) \sum_{I'=I_0}^{\nu+l} \sum_{J'=J_0}^{\nu+l-1} X(I,J')X(I',J')X(I',J) = 0 ,$$

with (4.7)

$$l \leq I \leq \nu+l ; \quad l \leq J \leq \nu+l-1 ,$$

$$C_E(I,I') = \sum_{J=J_0}^{\nu+l-1} [X(I,J)Y(I',J) + Y(I,J)X(I',J)] + \delta(I,I' = 0 ,$$

with (4.8)

$$l \leq I' \leq I \leq \nu+l-1 ,$$

and

$$C_O(J,J') = \sum_{I=I_0}^{\nu+l} [X(I,J)Y(I,J') + Y(I,J)X(I,J')] - \delta(J,J') = 0$$

with (4.9)

$$l \leq J' \leq J \leq \nu+l-1 ,$$

where $I_0 = J_0 =$ maximum $(1, l-\nu)$. At each step we include at most ν possible lower states for all the dummy indices I and J. This is sufficient to take the lower boundary effects properly into account. Since at each step we are primarily interested in results relating to the lth even-parity and odd-parity states, which are already nested in the center of all the states included in the intermediate sums in this way, it appears that there is no need to sum over more lower states.

The energies for the $2\nu+1$ states at the lth-step calculation are evaluated from the formulas

$$\omega_1 = E(2l-2)$$
$$= \tfrac{1}{2}\sum_{J=J_0}^{\nu+l-1}[Y(l,J)^2 + X(l,J)^2]$$
$$+ \frac{\lambda}{4}\sum_{J=J_0}^{\nu+l-1}\sum_{I=I_0}^{\nu+l}\sum_{J'=J_0}^{\nu+l-1} X(l,J)X(I,J)X(I,J')X(l,J'),$$

where (4.10)

$$I_0 = J_0 = \mathrm{Max}(1, l-\nu),$$

$$E(2J-1) = \omega_1 - \frac{Y(l,J)}{X(l,J)} \quad \text{for } J = l, \ldots, \nu+l-1; \tag{4.11}$$

and

$$\omega_2 = E(2l-1), \tag{4.12}$$

$$E(2I-2) = \omega_2 + \frac{Y(I,l)}{X(I,l)} \quad \text{for } I = l+1, \ldots, \nu+l. \tag{4.13}$$

For any two successive steps of such a calculation there are always $2\nu-1$ energies in common being evaluated from (4.10)–(4.13). This provides us consistency checks on the results of the two steps. By picking up the first two energies calculated at each step, we can find the energy eigenvalues of all the states up to very large n. Besides, we have found that if the third energy of the $(l-1)$st step is the same as the first one of the lth step to some decimal digit, then, to a very good approximation, the first two energies calculated at the lth step are also accurate to that digit.

In Table III the results for some of the energies calculated with this step-by-step procedure are given. In Table IV we compare our results with the previous work done by Chan, Stelman, and Thompson.[3] To be consistent we transform the operators x and p into the operators X and P used in their work. Besides, we include another parameter μ before the harmonic interaction term. This requires a trivial modification of our method. Hence the Hamiltonian becomes

$$H = \tfrac{1}{2}p^2 + \tfrac{1}{2}\mu x^2 + \tfrac{1}{4}\lambda x^4. \tag{4.14}$$

By setting

$$x = (k/\sqrt{2})X, \qquad p = (1/k\sqrt{2})P, \tag{4.15}$$

we have the correct commutation rule for X and P, i.e.,

$$[X, P] = 2i.$$

Also, this brings our Hamiltonian (4.14) into the form

TABLE III. Results of the first 22 energies calculated by the step-by-step procedure with $\nu = 5$; $\lambda = 0.01, 0.10, 1.00, 10.0$.

n \ λ	0.01	0.10	1.0	10.0
0	0.501 858 91	0.517 364 85	0.620 927 03	1.009 170 32
1	1.509 249 77	1.583 612 68	2.025 966 16	3.506 739 59
2	2.523 913 12	2.708 630 71	3.698 450 32	6.733 865 21
3	3.545 705 51	3.885 135 64	5.557 577 14	10.406 983 47
4	4.574 490 63	5.107 835 08	7.568 422 87	14.437 498 18
5	5.610 138 72	6.372 662 35	9.709 147 88	18.769 407 62
6	6.652 526 08	7.676 370 19	11.964 543 62	23.364 852 45
7	7.701 534 66	9.016 291 20	14.323 265 20	28.196 084 80
8	8.757 051 62	10.390 185 96	16.776 452 79	33.241 721 60
9	9.818 968 97	11.796 141 46	19.316 954 30	38.484 678 62
10	10.887 183 27	13.232 500 16	21.938 849 36	43.910 930 43
11	11.961 595 30	14.697 808 87	24.637 139 38	49.508 715 76
12	13.042 109 79	16.190 780 74	27.407 536 16	55.268 002 41
13	14.128 635 18	17.710 266 47	30.246 312 16	61.180 112 30
14	15.221 083 39	19.255 231 93	33.150 191 14	67.237 450 19
15	16.319 369 61	20.824 740 57	36.116 266 23	73.433 302 00
16	17.423 412 12	22.417 939 35	39.141 937 24	79.761 681 63
17	18.533 132 09	24.034 047 29	42.224 861 72	86.217 212 03
18	19.648 453 42	25.672 346 12	45.362 916 26	92.795 031 69
19	20.769 302 62	27.332 172 53	48.554 165 32	99.490 719 62
20	21.895 608 63	29.012 911 67	51.796 835 85	106.300 234 78
21	23.027 302 72	30.713 991 67	55.089 296 47	113.219 866 21

TABLE IV. Comparison of Chan-Stelman-Thompson (CST) method with present work for the energy eigenvalues.

n \ α	$\alpha=0.0$	$\alpha=0.1$		$\alpha=0.5$		$\alpha=1.0$	
		CST	Present work	CST	Present work	CST	Present work
0	2	1.991 99	1.991 985 28	2.273 41	2.273 406 71	2.671 95	2.671 945 0
1	6	6.141 95	6.141 947 51	7.743 93	7.743 928 76	9.574 58	9.574 576 1
2	10	10.5953	10.595 274 01	14.6492	14.649 249 0	18.7872	18.787 182
3	14	15.3050	15.304 967 43	22.4645	22.464 510 9	29.3429	29.342 920
4	18	20.2396	20.239 575 9	31.0097	31.009 695 8	40.9773	40.977 234
5	22	25.3761	25.376 133 6	40.1725	40.172 543 9	53.5174	53.517 346
6	26	30.6969	30.696 941 8	49.8766	49.876 622 7	66.8476	66.847 558
7	30	36.1878	36.187 839 8	60.0657	60.065 710 0	80.8835	80.883 398
8	34	41.8376	41.837 179 0	70.6963	70.696 355 9	95.5600	95.559 974
9	38	47.6367	47.635 169 9	81.7337	81.733 768 6	110.8256	110.825 57

$$H=\frac{1}{4k^2}(P^2+\mu k^4X^2+\tfrac{1}{4}\lambda k^6X^4)\,. \tag{4.16}$$

With

$$\mu=1,\ \lambda=4\left(\frac{\alpha}{1-\alpha}\right)^{3/2},\ \text{and}\ k=(1-\alpha)^{1/4}, \tag{4.17}$$

or

$$\mu=\frac{1-\alpha}{\alpha},\ \lambda=4,\ \text{and}\ k=\alpha^{1/4}, \tag{4.18}$$

(4.16) becomes

$$4k^2H=P^2+(1-\alpha)X^2+\alpha^{3/2}X^4\,, \tag{4.19}$$

which is just the reduced Hamiltonian used in Ref. 3. In our method (4.17) and (4.18) are equivalent within a canonical transformation, and exactly the same results are obtained for (4.19), for $\alpha\neq1$. Because of the singularity of λ in (4.17) at $\alpha=1$, for this pure quartic interaction case we can only use (4.18). From Table IV it can be seen that the numerical results obtained for the energy eigenvalues by the present approach are in very good agreement with those obtained by the Chan-Stelman-Thompson method. The technique of directly diagonalizing the Hamiltonian matrix of finite dimension in some selected representation was used by these authors. The results thereby obtained are usually representation-dependent and less accurate for higher eigenvalues, as can be seen from the slight discrepancies (especially for $\alpha=0.1$, because the harmonic-oscillator representation was used in this case, instead of the quartic-oscillator representation in other cases). The present approach works directly with matrix elements in the exact energy eigenstate representation and, because of the good behavior of the matrix elements, should give more accurate results.

In Fig. 1 the most significant matrix elements $X(I,J)$ with $J=I, I-1$ and relating to the lowest 14 states are plotted against the anharmonicity parameter λ. It can be seen that these matrix elements decrease rapidly for small anharmonicity and behave as $\lambda^{-1/6}$ for large anharmonicity. The asymptotic behavior can be easily shown to be so from Eqs. (2.10)–(2.12) by considering only those matrix elements $X(I,J)$, $Y(I,J)$ with $J=I$ and $I-1$, namely the lowest order of approximation. From the diagonal commutator equations of (2.11) and (2.12), we have

$$X(I,I)\,Y(I,I)+X(I,I-1)\,Y(I,I-1)\cong-\tfrac{1}{2}\,, \tag{4.20}$$

$$X(I,I-1)\,Y(I,I-1)+X(I-1,I-1)\,Y(I-1,I-1)\cong\tfrac{1}{2}\,, \tag{4.21}$$

and

$$X(1,1)\,Y(1,1)\cong-\tfrac{1}{2}\,. \tag{4.22}$$

Knowing (4.22) we can successively determine $X(I,I-1)\,Y(I,I-1)$ and $X(I,I)\,Y(I,I)$ for $I=2,3,\ldots$ from the recursion relations (4.20) and (4.21). Thus,

$$X(I,I-1)\,Y(I,I-1)\cong I-1\,, \tag{4.23}$$

$$X(I,I)\,Y(I,I)\cong-(I-\tfrac{1}{2})\,. \tag{4.24}$$

The off-diagonal commutator equations yield less accurate information about the products of the leading matrix elements because of the cancellations between them, and in fact there is no need to use these equations in the following proof.

In the lowest order of approximation we consider only Ith and $(I+1)$st even-parity states and Ith odd-parity states at one time. Therefore, by neglecting the harmonic term and using (4.23), (4.24), the equations of motion become

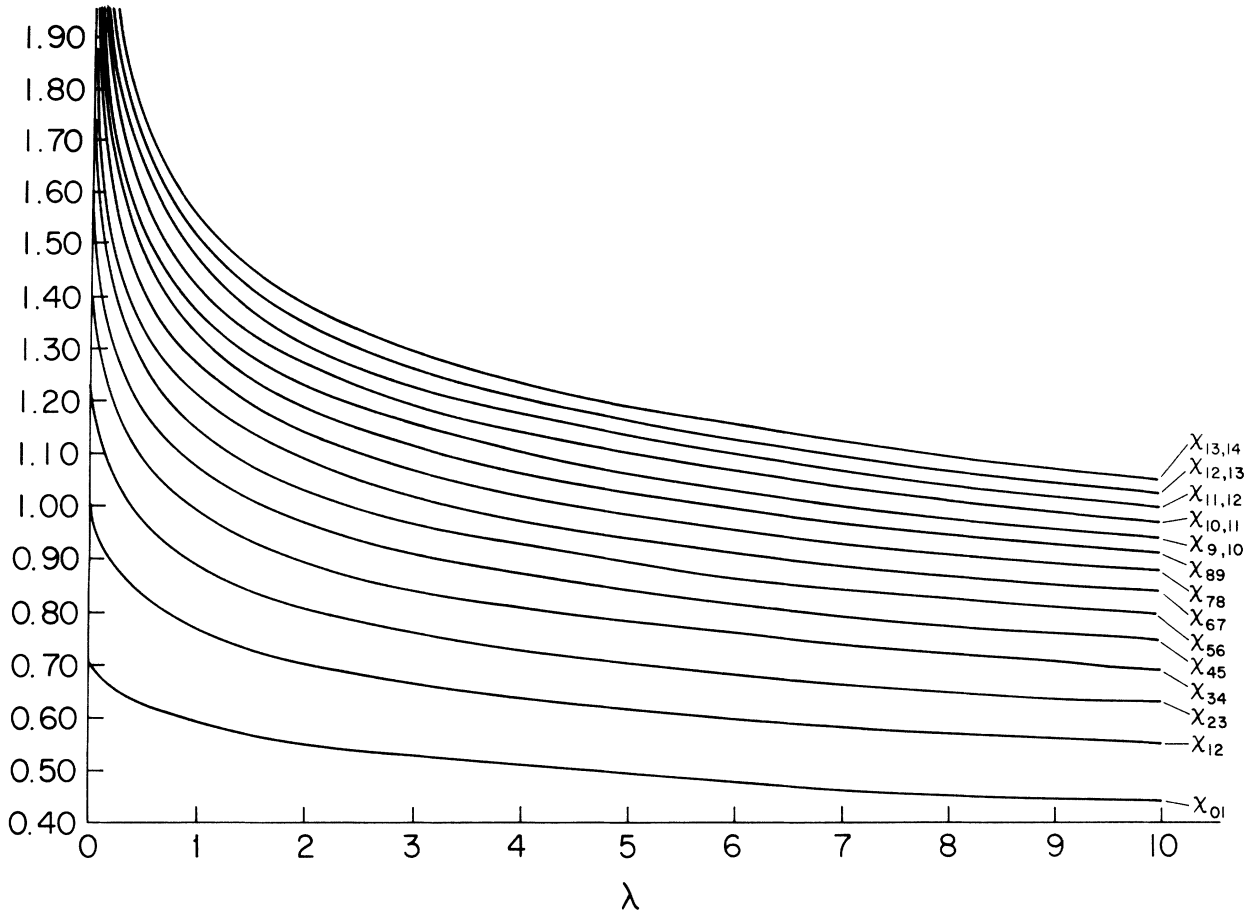

FIG. 1. The most significant matrix elements $\chi_{n,n\pm1}$ relating to 14 lower states plotted against λ for the anharmonic oscillator with $H=\frac{1}{2}(p^2+x^2)+\frac{1}{4}\lambda x^4$.

$$-\frac{(I-\frac{1}{2})^2}{X(I,I)^2}+\lambda X(I,I)^2[X(I,I)^2+X(I+1,I)^2]\cong 0 \tag{4.25}$$

and

$$-\frac{I^2}{X(I+1,I)^2}+\lambda X(I+1,I)^2[X(I+1,I)^2+X(I,I)^2]\cong 0. \tag{4.26}$$

These readily yield the results that

$$X(I,I)\cong\left[\frac{(I-\frac{1}{2})^3}{(2I-\frac{1}{2})\lambda}\right]^{1/6} \tag{4.27}$$

and

$$X(I+1,I)\cong\left[\frac{I^3}{(2I-\frac{1}{2})\lambda}\right]^{1/6}. \tag{4.28}$$

Thus, as $\lambda\to\infty$

$$X(I,I), X(I+1,I)\sim\lambda^{-1/6}, \tag{4.29}$$

and

$$Y(I,I), Y(I+1,I)\sim\lambda^{1/6}. \tag{4.30}$$

Although the conclusions above follow from the lowest-order consideration, it is plausible to expect they are true to every order of approximation because, as $\lambda\to\infty$, if $X(I,J)$ and $Y(I,J)$ are the solution of Eqs. (2.10)–(2.12) for $\lambda=\lambda_0$, it is easy to see that $(\lambda_0/\lambda_1)^{1/6}X(I,J)$ and $(\lambda_1/\lambda_0)^{1/6}Y(I,J)$ also satisfy Eqs. (2.10)–(2.12) for $\lambda=\lambda_1$.

In Fig. 2 some matrix elements $(n|x|n\pm3)$ are plotted against λ. It is seen that these matrix elements increase rapidly from zero to some maximum values and then decrease smoothly also as $\lambda^{-1/6}$. In Fig. 3 the first 14 energy eigenvalues are shown as functions of λ. Their asymptotic behavior is $E_n\sim\lambda^{1/3}$ as $\lambda\to\infty$. In fact, the correct asymptotic behaviors of the matrix elements and the energies have been checked numerically up to $\lambda=100$.

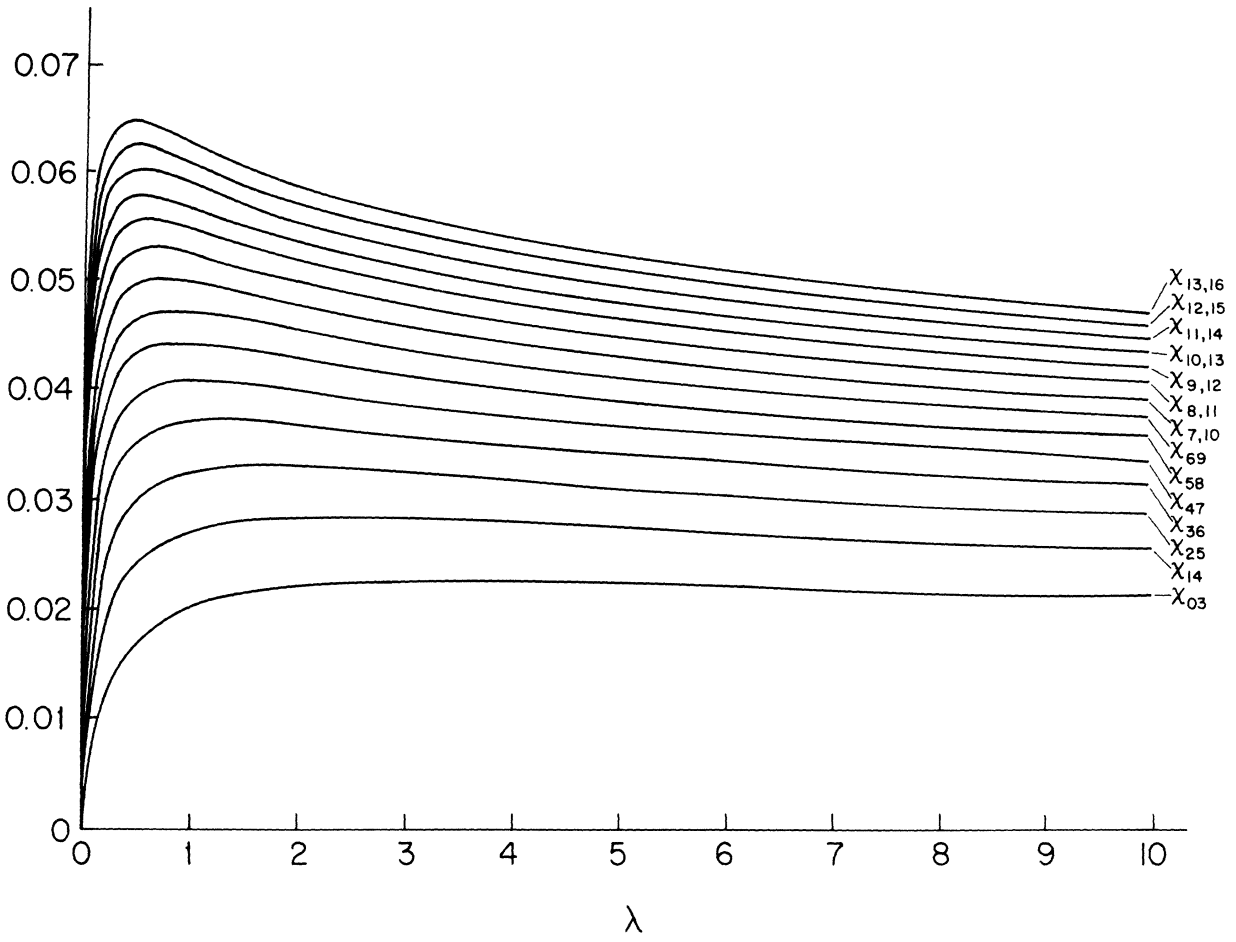

FIG. 2. The matrix elements $\chi_{n,n\pm3}$ relating to 14 lower states plotted against λ for the anharmonic oscillator with $H=\frac{1}{2}(p^2+x^2)+\frac{1}{4}\lambda x^4$.

V. DISCUSSION

In principle, the systematic scheme set up in the previous sections can readily be applied to finding the relevant matrix elements and the energy eigenvalues for the potential well of any even-power polynomial in x. In particular, for the anharmonic oscillator characterized by the Hamiltonian

$$H=\tfrac{1}{2}(p^2+x^2)+\tfrac{1}{6}\lambda x^6,$$

we have found rapidly convergent results in exact agreement with those obtained by direct numerical integration[7] to the accuracy limit of the latter. The general features of this problem are essentially the same as those of the anharmonic oscillator considered in the previous sections except that it takes a little more time to find the solution because there are more intermediate summations now.

One may wonder why we did not apply Eqs. (2.10)–(2.12) directly to any subspace of states not starting from the ground state and solve the problem locally without having to sum over states outside this subspace for the intermediate summations. If we had solved this problem in that way, then for all such subspaces selected we would have used essentially the same set of equations and would have obtained the same results even for entirely different subspaces selected. This should not be surprising from the variational-principle point of view. As asserted in Sec. III, our method can be derived from a novel variational principle. For a variational calculation for the energies of higher excited states, these states cannot be arbitrary. In fact, the coupling of these states with all the lower states through the commutator equations (2.11), (2.12) must be properly taken into account as in the step-by-step procedures of Sec. IV B or, more primitively, as in the successive

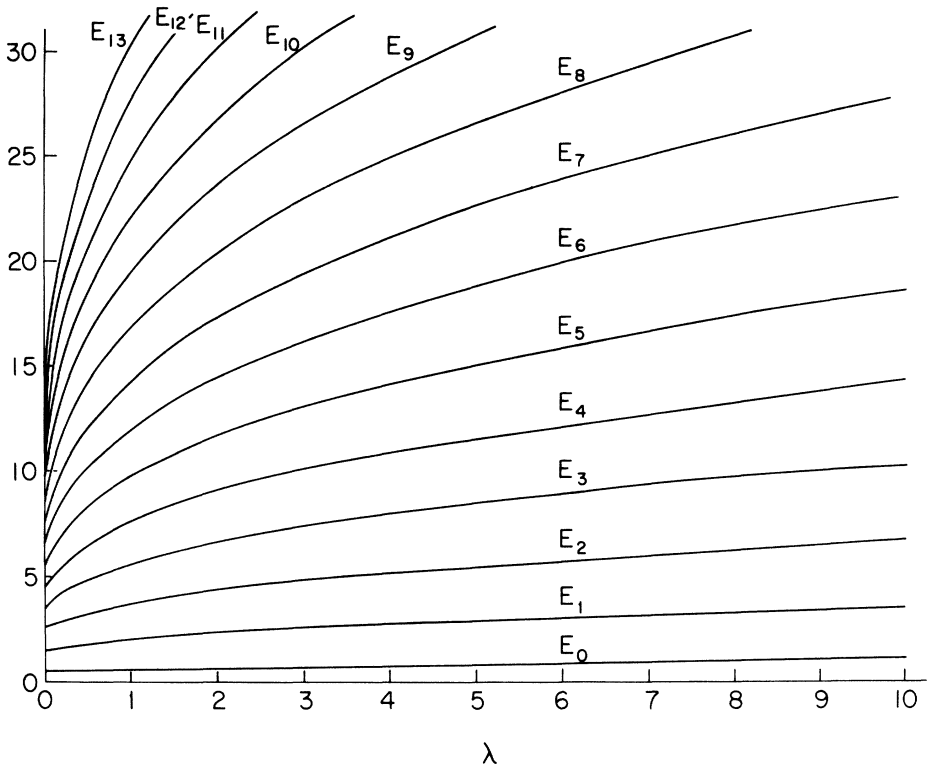

FIG. 3. Energy-level correlation diagram for the anharmonic oscillator with $H=\frac{1}{2}(p^2+x^2)+\frac{1}{4}\lambda x^4$.

determinations of $X(I,I)Y(I,I)$ and $X(I,I-1)Y(I,I-1)$ for $I>2$ beginning with $X(1,1)Y(1,1)$ calculated from (4.20)–(4.22) in the lowest-order calculation. Tentatively, we have added the lowest-order result $X(I,I-1)Y(I,I-1)\cong I-\frac{1}{2}$ to the first even commutator equation $C_E(I,I)=0$ of the $2\nu+1$ states starting from the Ith even-parity state and successfully solved the problem locally without having to include any lower state in the intermediate sums. For $\nu=5$ or 6, the energies and the matrix elements for the centered states are exactly the same as those obtained by the step-by-step procedure within the accuracy of our calculations. We shall also elaborate on this in the separate paper mentioned in Sec. I.

APPENDIX

We wish to solve a set of nonlinear equations

$$F_i(x_j)=0, \quad i,j=1,\ldots,N \tag{A1}$$

which also contains at least one coupling parameter λ. Suppose that for $\lambda=\lambda_0$ an approximate solution $x_j^{(0)}$ is known and

$$F_i(x_j^{(0)})=-B_i. \tag{A2}$$

Then from (A1) and (A2) we have approximately, with $\delta x_j^{(0)}=x_j-x_j^{(0)}$,

$$\sum_j\left(\frac{\partial F_i}{\partial x_j^{(0)}}\right)\delta x_j^{(0)}=\sum_j A_{ij}\delta x_j^{(0)}\cong B_i. \tag{A3}$$

Then

$$x_j^{(1)}=x_j^{(0)}+\delta x_j^{(0)} \tag{A4}$$

is our first approximation. We repeat the process to obtain $x_j^{(2)}$ etc. until convergence. It may happen that if $x_j^{(0)}$ is too far from the correct solution, one may have to proceed cautiously and allow only a fraction of the change $\delta x_j^{(0)}$ in defining $x_j^{(1)}$.

Assuming one has found the solution of (A1) for $\lambda=\lambda_0$, one takes this to be the approximate solution for $\lambda=\lambda_0+\delta\lambda$ and proceeds as before. For the anharmonic oscillator we have started from $\lambda=0$, the harmonic-oscillator limit, and have found that this method permits us to continue without hin-

drance to arbitrarily large λ. If one is primarily interested in large λ, it is more efficient to start from an approximate large-λ solution which can be readily obtained from our equations by omitting the harmonic interaction and using the lowest (equivalently $\nu=1$) level of approximation. Then one enlarges the level of approximation to $\nu'=\nu+1$ by using the results of the previous order as part of the initial values for the variables. For those most significant matrix elements not previously covered, one sets

$$X(I,\nu')\cong X(I-1,\nu'-1),$$
$$Y(I,\nu')\cong Y(I-1,\nu'-1) \text{ for } I=\nu' \text{ and } \nu'+1. \tag{A5}$$

Other less important matrix elements can be conveniently assigned some small numbers of correct signs. Note that under the usual phase convention

$$X(I,J)>0 \text{ for all } I \text{ and } J,$$

but

$$Y(I,J)>0 \text{ if } I>J,$$
$$Y(I,J)<0 \text{ if } I\leq J. \tag{A6}$$

This procedure can then carry one successively to the desired order of approximation for this particular λ.

In the method described by (A1)–(A4) to solve a set of nonlinear equations, before we really define $x_j^{(1)}$ in each iteration we have to determine the correct change $\delta x_j^{(0)}$ from (A3). This is usually achieved by using the routine based on the normal Gauss elimination method. Of course, the derivatives A_{ij} and the functions B_i should be evaluated beforehand. For the anharmonic-oscillator problem, the following is the most efficient way to do it:

Because of the linear storage nature of computer memory for matrices, the variables and the equations in (A1)–(A4) can be labeled equivalently well by a set of indices instead of just a single subscript i or j, provided that the total number of the variables (or equations) specified by the multiple indices is the same as that originally specified. This feature allows us to redefine the matrix elements $X(I,J)$ and $Y(I,J)$, and similarly the three types of equations, into a compact set by using an additional index, and thereby the procedure (A1)–(A4) applies more readily. Thus we set

$$V(I,J,1)\equiv X(I,J),$$
$$V(I,J,2)\equiv Y(I,J) \tag{A7}$$

and

$$F(I,J,1)\equiv E_M(I,J)=0,$$
$$F(I'',I',2)\equiv C_E(I',I'')=0,$$
$$F(J+1,J',2)\equiv C_O(J,J')=0,$$

with (A8)

$$1\leq I\leq \nu+1,$$
$$1\leq J'\leq J\leq \nu,$$
$$1\leq I''\leq I'\leq \nu.$$

Hence the $2\nu(\nu+1)$ equations $F(I,J,K)=0$ are what we have to solve for the $2\nu(\nu+1)$ matrix elements $V(I,J,K)$. The matrices B_i and A_{ij} then take the following forms:

$$B(I,J,K)=-F(I,J,K) \tag{A9}$$

and

$$A(I,J,K,M,N,L)=\partial F(I,J,K)/\partial V(M,N,L),$$

with (A10)

$$1\leq I,M\leq \nu+1,$$
$$1\leq J,N\leq \nu,\ 1\leq K,L\leq 2.$$

When written out explicitly by using the definitions (A7), (A8) and the fact that $\partial X(I,J)/\partial X(M,N)=\partial Y(I,J)/\partial Y(M,N)=\delta(I,M)\delta(J,N)$ etc. the resulting expressions for (A9) and (A10) in $X(I,J)$, $Y(I,J)$ and appropriate Kronecker δ's can be directly programmed for every order of approximation. Note that when the previously mentioned routine is called, the matrices $A(I,J,K,M,N,L)$ and $B(I,J,K)$ are automatically viewed as a $2\nu(\nu+1)\times 2\nu(\nu+1)$ two-dimensional matrix and a $2\nu(\nu+1)\times 1$ column matrix, respectively, by the computer. Equations (A7) – (A10) can readily be applied to the step-by-step procedure described in Sec. IV B if at each step of calculation we properly take care that the ranges of those indices in A and B of (A9) and (A10) do not increase. For instance, at the lth step, with other things unchanged, A and B can be set to be $A(I-l+1,J-l+1,K,M-l+1,N-l+1,L)$ and $B(I-l+1,J-l+1,K)$, respectively.

In more general cases it might be difficult to redefine the variables or the equations in such fashions as described in (A7) and (A8). When this happens, after performing the necessary intermediate summations and derivatives by the help of two-subscript variables, we can then transform these subscripts into a single one at each appropriate step. This can be carried out as $K=\nu(I-1)+J$ for $X(I,J)$ and $K'=\nu(\nu+1)+\nu(I-1)+J$ for $Y(I,J)$ and similar transformations for the equations. The resulting matrices A, B are then two-subscript and one-subscript, respectively, as usual.

*Work supported in part by the U. S. Energy Research and Development Administration.

[1]An early reference is A. K. Kerman and A. Klein, Phys. Rev. 132, 1326 (1963). For surveys consult A. Klein, in *Quantum Fields and Nuclear Matter*, 1968 Boulder Lectures, edited by W. E. Brittin *et al.*, Vol. XIB (Gordon and Breach, New York, 1969); A. Klein, in *Dynamical Structure of Nuclear Structure of Nuclear States* (Univ. of Toronto Press, Toronto, 1972); A. Klein, Rev. Mex. Fis. 23, 59 (1974).

[2]C. M. Bender and T. T. Wu, Phys. Rev. 184, 1231 (1969); Phys. Rev. D 7, 1620 (1973). These papers contain an elaborate investigation of the properties of the solutions of the Hamiltonian (1.1), given below, as a function of the anharmonic parameter λ.

[3]S. I. Chan, D. Stelman, and L. E. Thompson, J. Chem. Phys. 41, 2828 (1964). [Diagonalizes the Hamiltonian (1.1) using various basic systems.]

[4]J. J. Loeffel, A. Martin, B. Simon, and A. S. Wightman, Phys. Lett. 30B, 656 (1969). (Applies Padê approximants to the calculation of energy levels.)

[5]S. N. Biswas, K. Datta, R. P. Saxena, P. K. Srivastava, and V. S. Varma, Phys. Rev. D 4, 3617 (1971). (Applies the method of the Hill determinant to the calculation of energy levels.)

[6]P. Lu, S. S. Wald, and B.-L. Young, Phys. Rev. D 7, 1701 (1973). (Contains higher approximations of the WKB method.)

[7]C. A. Uzes and J. H. Henkel, Phys. Rev. D 8, 1067 (1973). (Contains a version of the new Tamm-Dancoff method.)

[8]F. R. Halpern, J. Math. Phys. 14, 219 (1973); 15, 733 (1974); F. R. Halpern and T. W. Yonkman, *ibid.* 15, 1718 (1974). In the last of the these references, in particular, the general idea is closely similar to the one we propose. We have embedded the approach of Halpern and Yonkman in an infinite matrix of variant procedures. Also, these authors have studied the semi-classical approximation, whereas we shall emphasize (in this paper) how to utilize the method as an exact numerical procedure to calculate properties from the ground state up.

[9]G. J. Dreiss and A. Klein, Nucl. Phys. A139, 81 (1969).

[10]Similar variational ideas in the nuclear many-body problem were first proposed by R. M. Dreizler, G. J. Dreiss, G. Do Dang, A. Klein, and C. S. Wu, Nucl. Phys. A114, 501 (1968).

[11]For example, see M. Vallieres, A. Klein, and R. M. Dreizler, Phys. Rev. C 7, 2188 (1973).