Moment method for eigenvalues and expectation values

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We present a simple technique for performing accurate calculations of the eigenvalues of quantum systems whose potential energy is a polynomial in the coordinates. The method involves the study of recursion relations between matrix elements of powers of the coordinate operator between the exact eigenstate and a conveniently chosen basis state. The general theory is developed and applied to three examples: the quartic oscillator, the octic oscillator, and two coupled quartic oscillators. Numerical results are given.

I. INTRODUCTION

In this paper we present a new technique for making accurate calculations of the energy levels of quantum-mechanical systems whose potential energy is a polynomial in the components of the coordinate operator. The basic idea is to study the matrix elements of powers of the coordinate operator between the exact energy eigenstate and a trial state. We show that these matrix elements are readily calculable and that the coupled (difference) equations which they satisfy yield a very accurate evaluation of the energy eigenvalues.

Our procedure is a straightforward generalization of earlier work[1] in which matrix elements of powers of the coordinate operator between exact energy eigenstates were studied. Our new approach has the advantage that the trial state can be adjusted to ensure rapid convergence. In addition our technique can be readily applied to systems with more than one degree of freedom in contrast to the method of Ref. 1. We should also add that this technique seems to be easier to implement and of greater range of validity than either Borel resummation[2] or perturbation around instanton solutions[3] to the classical equations of motion.

In Sec. II we present our general technique and apply it to three examples: the quartic oscillator, the octic oscillator $V(x)\sim x^8$, and two coupled quartic oscillators. In Sec. III we present our numerical results and briefly discuss their application to the study of systems with many degrees of freedom.

II. MOMENT RECURSION RELATIONS

We wish to solve for the eigenvalues of the Schrödinger equation

$$H|\psi\rangle = E|\psi\rangle\,, \tag{1}$$

where

$$H=\sum_{i=1}^{N} p_i{}^2 + V\,, \tag{2}$$

and V is a polynomial in the components of the coordinate operator, $\vec{\mathbf{x}}=(x_1,\ldots,x_N)$. To this end we introduce the moments

$$S_{n_1 n_2\cdots n_N} = \langle\varphi|x_1{}^{n_1}x_2{}^{n_2}\cdots x_N{}^{n_N}|\psi\rangle\,, \tag{3}$$

where $|\psi\rangle$ is an exact eigenstate of H and $|\varphi\rangle$ is a trial state which is at our disposal. It is convenient to choose $|\varphi\rangle$ so that

$$\varphi(x)=\langle\vec{\mathbf{x}}|\varphi\rangle=\exp\left[-\int_0^{\vec{\mathbf{x}}} d\vec{\mathbf{x}}'\cdot\vec{\mathbf{g}}(\vec{\mathbf{x}}')\right]. \tag{4}$$

Then

$$\vec{\nabla}\varphi(x)=-\vec{\mathbf{g}}(x)\,\varphi(x)\,, \tag{5}$$

and

$$\nabla^2\varphi(x)=(\vec{\mathbf{g}}\cdot\vec{\mathbf{g}}-\nabla\cdot g)\,\varphi(x)\,.$$

Taking the matrix element of Eq. (1) with the state $\langle\varphi|x_1{}^{n_1}\cdots x_N{}^{n_N}$ gives

$$ES_{n_1\cdots n_N}=\left\langle\varphi\left|\left((\nabla\cdot g)-\vec{\mathbf{g}}\cdot\vec{\mathbf{g}}+V+\sum_{i=1}^{N}[2g_i(x)n_i x_i{}^{-1} - n_i(n_i-1)x_i{}^{-2}]\right)x_1{}^{n_1}\cdots x_N{}^{n_N}\right|\psi\right\rangle. \tag{6}$$

If both V and g are polynomials in the x_i, then Eq. (6) is a recursion relation among the $S_{n_1\cdots n_N}$. To show how this recursion relation can be used to calculate the energy eigenvalues it is helpful to consider some examples.

A. The quartic oscillator

We start with the one-dimensional quartic oscillator whose Hamiltonian can be written in the form

$$H=p^2+\lambda(x^2-f^2)^2\,. \tag{7}$$

Since λ and f^2 have the dimensions x^{-6} and x^2, respectively, the energy eigenvalues must satisfy the scaling relation

$$E(\lambda, f^2) = \lambda^{1/3} \epsilon(\lambda^{1/3} f^2) . \tag{8}$$

So, we can set $\lambda = 1$ without any loss of generality.

A particularly simple choice for the trial state is

$$\begin{aligned} g(x) &= bx , \\ \varphi(x) &= \exp(-\tfrac{1}{2} b x^2) , \end{aligned} \tag{9}$$

where the parameter b is at our disposal, subject to a few minor constraints which will be elaborated below. Substituting Eqs. (7) and (9) into Eq. (6) with $N = 1$ gives the recursion relation

$$S_{n+4} - (2f^2 + b^2) S_{n+2} + [(2n+1) b + f^4 - E] S_n - n(n-1) S_{n-2} = 0 , \tag{10}$$

with the boundary condition that $n(n-1) S_{n-2} = 0$ at $n = 0, 1$. Since $\varphi(x)$ is an even-parity state, the S_n vanish for odd n if $\psi(x)$ has even parity, and for even n if $\psi(x)$ has odd parity.

Our program for determining the energy eigenvalues from Eq. (10) is as follows. We start by obtaining an asymptotic expansion for the S_n valid when $n \geq M \gg 1$. We then determine the S_n for $n < M$ by Eq. (10). For the even-parity states we determine S_0 from Eq. (10) with $n = 2$. Setting $n = 0$ in Eq. (10) yields

$$S_4 / S_0 - (2f^2 + b^2) S_2 / S_0 + b + f^4 - E = 0 . \tag{11}$$

For the odd-parity states S_1 is determined from Eq. (10) with $n = 3$. Setting $n = 1$ in Eq. (10) then yields

$$S_5 / S_1 - (2f^2 + b^2) S_3 / S_1 + 3b + f^4 - E = 0 . \tag{12}$$

Since the S_n are all determined at this point, Eqs. (11) and (12) will only be satisfied for certain values of E, namely the eigenvalues. Therefore, we need only plot the left-hand sides of Eqs. (11) and (12) as a function of E (the S_n are, of course, functions of E), and search for their zeros.

The asymptotic expansion of the S_n can be read off directly from Eq. (10); however, it is instructive to return to the original definition. The nonzero S_n can be written in the form

$$S_n = 2 \int_0^\infty dx \, \varphi(x) \psi(x) e^{n \ln(x)} . \tag{13}$$

Since $\varphi(x)$ and $\psi(x)$ are decreasing functions of x for large x, this integral can be evaluated by the saddle-point method for large n, where only the large-x behavior of $\psi(x)$ is needed to determine S_n. It can easily be obtained by writing $\psi(x) = e^{-\chi(x)}$ and substituting into the Schrödinger equation to get an equation for χ:

$$\chi'' - \chi'^2 + (x^2 - f^2)^2 - E = 0 . \tag{14}$$

For large positive x we find

$$\chi(x) = \tfrac{1}{3} x^3 - f^2 x + O(\ln x) . \tag{15}$$

Thus for large n the integrand of Eq. (13) has saddle points when

$$x^3 + bx - f^2 - n/x \approx 0 . \tag{16}$$

The only saddle point relevant to our integral is the one at $x \approx n^{1/3} - b/3$, which gives[4]

$$S_n = n^{n/3} e^{-n/3} \exp[-\tfrac{1}{2} b n^{2/3} + (f^2 + \tfrac{2}{3} b^2) n^{1/3} + O(n^{-1/3})] . \tag{17}$$

Equation (16) of course has three independent solutions. The other two have integral representations similar to Eq. (13), but with contours of integration running through the saddle points at $x_\pm \sim e^{\pm 2\pi i/3} (n^{1/3} - b/3)$. These solutions have asymptotic expansions of the form

$$S_n^\pm = e^{\pm 2\pi i n/3} n^{n/3} e^{-n/3} \exp[-\tfrac{1}{2} b n^{2/3} e^{\pm 4\pi i n/3} + n^{1/3} e^{\pm 2\pi i n/3} (f^2 + \tfrac{1}{3} b^2 e^{\pm 2\pi i n/3} - \tfrac{1}{6} b^2 e^{\pm 2\pi i n/3}) + O(n^{-1/3})] , \tag{18}$$

as can be verified by direct substitution into Eq. (10).

The fact that the solution of physical interest has the subdominant, i.e., smallest, asymptotic behavior is crucial to obtaining accurate numerical results. In approximating the S_n for $n \geq M$ by the asymptotic expression of Eq. (17), we are of course introducing an error. It corresponds to having admixtures of the unwanted solutions $S_n^\pm$, but only with weights of the order of $\exp(-\tfrac{3}{4} b M^{2/3})$ relative to the desired solutions. Thus as long as $b > 0$, we can make this error arbitrarily small by taking M sufficiently large. In practice we can make very accurate evaluations of the energy eigenvalues even with very crude approximations to the asymptotic behavior of the S_n, as is illustrated in Table I.

It should be noted that if we had used the diagonal moments $\langle \psi | \chi^n | \psi \rangle$, then we would have obtained asymptotic solutions analogous to Eqs. (17) and (18), with $b = 0$. Thus the solution of interest would not have the subdominant asymptotic behavior for the interesting case of $f^2 > 0$, and we would therefore require a very accurate evaluation of the as-

TABLE I. Ground-state energies for the anharmonic oscillator, calculated using different values of M and different forms for the asymptotic ratio R_M. For $M=200$, our results are accurate to several more significant figures than we have bothered to write out.

	E_0 ($f^2=2$)			
R_M	$M=10$	$M=20$	$M=50$	$M=200$
R_M [Eq. (20)]	2.30	2.283	2.289 649 7	2.289 649 5
$R_M=M^{2/3}$	2.37	2.280	2.289 650	2.289 649 5
$R_M=2M^{2/3}$	3.04	2.276	2.289 652	2.289 649 5
$R_M=0$	2.54	2.31	2.289 650	2.289 649 5

R_M	$M=10$	$M=20$	$M=50$	$M=200$
R_M [Eq. (20)]	1.063	1.060 37	1.060 362 1	1.060 362 1
$R_M=M^{2/3}$	1.064	1.060 38	1.060 362 1	1.060 362 1
$R_M=2M^{2/3}$	1.059	1.060 35	1.060 362 1	1.060 362 1
$R_M=0$	1.054	1.060 30	1.060 362 1	1.060 362 1

ymptotic form of the S_n.

Since Eq. (19) is linear, we only acutally need to evaluate the ratios

$$R_n \equiv S_{n+2}/S_n . \tag{19}$$

Equation (10) can be rewritten in the form

$$R_{n-2} = n(n-1)[(2n+1)b + f^2 - E - (2f^2+b^2)R_n + R_n R_{n+2}]^{-1} \tag{20}$$

for $n \geq 2$. The eigenvalue conditions are

$$b + f^4 - E - (2f^2+b^2)R_0 + R_0 R_2 = 0$$

and

$$b + f^4 - E - (2f^2+b)R_1 + R_1 R_3 = 0 .$$

The R_n's have the asymptotic expansion

$$R_n = n^{2/3}[1 - \tfrac{2}{3}bn^{-1/3} + \tfrac{1}{3}(2f^2+b^2)n^{-2/3} + O(n^{-1})] . \tag{21}$$

The R_n's are more convenient for numerical calculations because they grow much more slowly with n than the S_n. We have used Eqs. (20) and (21) to calculate the ground-state and first-excited-state energies as a function of f^2. The results are recorded in Table II and Fig. 1, and are discussed in Sec. III.

TABLE II. Ground-state and first-excited-state energies of the anharmonic oscillator.

f^2	E_0	E_1
5	4.366 423 29	4.366 453 1
4	3.863 666 9	3.865 185 7
3	3.251 809 5	3.293 207 5
2	2.289 649 5	2.752 077 1
1	1.137 785 8	2.713 027 9
0	1.060 362 1	3.799 673 0
−1	2.677 826 5	6.409 828 0

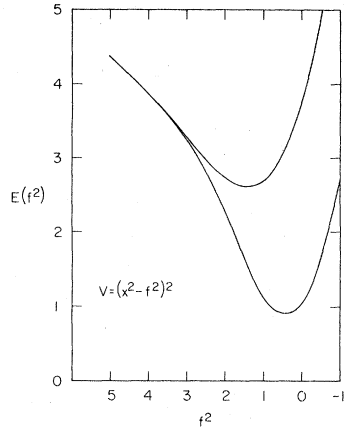

FIG. 1. Energies of the ground state and first excited state of the anharmonic oscillator, $V=(x^2-f^2)^2$.

In the preceding discussion we have used a Gaussian trial function for simplicity. We have tried a variety of other forms for the trial function which lead to equally good results. A natural choice is to build the large-x behavior of $\psi(x)$ into $\varphi(x)$. This can be done in the present example by taking

$$\begin{aligned} g(x) &= x|x| + bx , \\ \varphi(x) &= \exp(-\tfrac{1}{3}|x|^3 - \tfrac{1}{2}bx^2) . \end{aligned} \tag{22}$$

We define the moments for even-parity eigenstates to be

$$S_n = \langle \varphi | |x|^n | \psi \rangle = 2\int_0^\infty dx\, \varphi(x)\psi(x)x^n , \tag{23}$$

and for odd-parity states to be

$$S_n = \langle \varphi | |x|^n \epsilon(x) | \psi \rangle = 2\int_0^\infty dx\, \varphi(x)\psi(x)x^n , \tag{24}$$

where $\epsilon(x) = \pm 1$ for $x \gtrless 0$. In either case the S_n satisfy the recursion relation

$$2bS_{n+3} + (2f^2+b^2)S_{n+2} - 2(n+1)S_{n+1} + [E - f^4 - (2n+1)b]S_n + n(n-1)S_{n-2} = 0 , \tag{25}$$

for $n \geq 2$. For even-parity states Eq. (25) is also valid for $n=0$, and for odd-parity states it is valid for $n=1$. These two equations provide the eigenvalue conditions. The S_n have the asymptotic expansion

$$S_n = (n/2)^{n/3} e^{-n/3} \exp[-\tfrac{1}{2}b(n/2)^{2/3} + (f^2 - b^2/12)(n/2)^{1/3} + O((n/2)^{-1/3})] . \tag{26}$$

We have used Eqs. (25) and (26) to calculate the energies of the ground state and first excited state of the quartic oscillator, and they yield results in

complete agreement with those obtained using the Gaussian trial function. The rate of convergence of the energy using $g(x)$ given by (9) and by (22) are comparable.

B. The octic oscillator

We next consider the one-dimensional octic oscillator with the Hamiltonian

$$H = p^2 + \lambda(x^2 - f^2)^4 . \tag{27}$$

This potential is of some interest because, unlike the quartic oscillator, the energy gap between the ground state and the first excited state cannot be calculated simply from instanton effects, even for large positive f^2 which yields a potential with deep double minima.

As for the quartic oscillator, the energy eigenvalues satisfy a scaling law,

$$E(\lambda, f^2) = \lambda^{1/5} \epsilon(\lambda^{1/5} f^2) , \tag{28}$$

so we can again set $\lambda = 1$ without loss of information.

For large x, $\psi(x)$ has the asymptotic expansion

$$\psi(x) = \exp[-\tfrac{1}{5}|x|^5 + \tfrac{2}{3} f^2 |x|^3 + O(|x|)] . \tag{29}$$

So, in analogy with Eq. (22) we define $\varphi(x)$ by writing

$$\begin{aligned} g(x) &= x|x|(x^2 + 2f^2 b) , \\ \varphi(x) &= \exp[-\tfrac{1}{5}|x|^5 - \tfrac{2}{3} f^2 b |x|^3] . \end{aligned} \tag{30}$$

Defining the moments by Eqs. (23) and (24), we obtain the recursion relation

$$\begin{aligned} &4f^2(b+1) S_{n+6} - 2f^4(3 - 2b^2) S_{n+4} \\ &\quad - 2(n+2) S_{n+3} + 4f^6 S_{n+2} - 4f^2 b(n+1) S_{n+1} \\ &\quad + (E - f^8) S_n + n(n-1) S_{n-2} = 0 , \end{aligned} \tag{31}$$

which is valid for either-parity eigenstates when $n \geq 2$, for the even-parity states when $n = 0$, and for the odd-parity states when $n = 1$. The S_n have

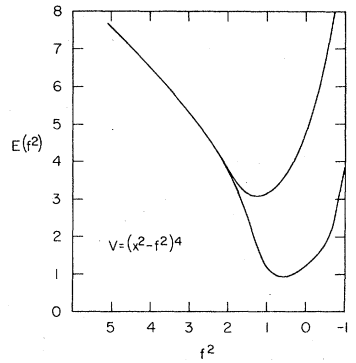

FIG. 2. Energies of the ground state and first excited state of the octic oscillator, $V = (x^2 - f^2)^4$.

TABLE III. Ground-state and first-excited-state energies of the octic oscillator.

f^2	E_0	E_1
4	6.517 5	6.5175
3	5.275 3	5.2753
2	3.743	3.800
1	1.170 4	3.14
0	1.225 826	4.80
−1	3.841 2	10.1583

the asymptotic expansion

$$S_n = (n/2)^{n/5} e^{-n/5} \exp[-\tfrac{2}{5} f^2 (b-1)(n/2)^{3/5} + O((n/2)^{2/5})] . \tag{32}$$

We have used Eqs. (31) and (32) to calculate the energies of the ground state and first excited state of the octic oscillator. The results are given in Fig. 2 and Table III.

C. Coupled quartic oscillators

As our final example we consider the problem of two coupled quartic oscillators with the Hamiltonian

$$H = p_x^2 + p_y^2 + \lambda(x^2 - f^2)^2 + \lambda(y^2 - f^2)^2 + \Delta(x - y)^2 . \tag{33}$$

This problem is interesting in its own right, and it is a first step in generalizing our technique to systems with many degrees of freedom.

As usual we can set $\lambda = 1$, since the energy eigenvalues satisfy the scaling relation

$$E(\lambda, f^2, \Delta) = \lambda^{1/3} \epsilon(\lambda^{1/3} f^2, \lambda^{-2/3} \Delta) . \tag{34}$$

It is convenient to introduce the variables

$$\begin{aligned} p_{1,2} &= 2^{-1/2}(p_x \pm p_y) , \\ x_{1,2} &= 2^{-1/2}(x \pm y) , \end{aligned} \tag{35}$$

and rewrite the Hamiltonian in the form

$$\begin{aligned} H = {} & p_1^2 + p_2^2 + \tfrac{1}{2}(x_1^2 - 2f^2)^2 \\ & + \tfrac{1}{2}[x_2^2 - 2(f^2 - \Delta)]^2 + 3x_1^2 x_2^2 - 2(f^2 - \Delta)^2 . \end{aligned} \tag{36}$$

Clearly the energy eigenstates $\psi(x_1, x_2)$ will be either even or odd under the separate symmetry operations $x_1 \to -x_1$ and $x_2 \to -x_2$. The former corresponds to the ordinary parity operation and the latter to the interchange of the two oscillators. If we now define the trial function by

$$\vec{g} = (g_1, g_2) = (b_1 x_1, b_2 x_2) , \tag{37}$$

or

$$\varphi(x_1, x_2) = \exp(-\tfrac{1}{2} b_1 x_1^2 - \tfrac{1}{2} b_2 x_2^2) ,$$

then the moments

$$S_{n_1 n_2} = \langle \varphi | x_1^{n_1} x_2^{n_2} | \psi \rangle \tag{38}$$

will be nonzero only for n_1 even or odd, but not both, and similarly for n_2. Substituting Eqs. (36) and (37) into Eq. (6) gives the recursion relation

$$\tfrac{1}{2}(S_{n_1+4,n_2}+6S_{n_1+2,n_2+2}+S_{n_1,n_2+4})-(2f^2+b_1^2)S_{n_1+2,n_2}-(2f^2-2\Delta+b_2^2)S_{n_1,n_2+2}$$
$$+[(2n_1+1)b_1+(2n_2+1)b_2+2f^4]S_{n_1,n_2}-n_1(n_1-1)S_{n_1-2,n_2}-n_2(n_2-1)S_{n_1,n_2-2}=ES_{n_1,n_2}, \quad (39)$$

which is valid for all (n_1, n_2).

Our strategy for obtaining the energy eigenvalues from Eq. (39) is as follows. We first obtain an asymptotic approximation for S_{n_1,n_2} valid for $n_1+n_2 \geq M \gg 0$, which we denote by $\tilde{S}_{n_1,n_2}$. We then demand that Eq. (39) be satisfied inside the triangle bounded by the lines $n_1=0$, $n_2=0$, $n_1+n_2=M$. For $n_1+n_2 \leq M-4$, Eq. (39) can be used directly. For the diagonal $n_1+n_2=M-2$ we must make use of our asymptotic approximation to write

$$(\tfrac{1}{2}R^1_{n_1+2,n_2}+\tfrac{3}{2}R^2_{n_1+2,n_2}-2f^2-b_1^2)S_{n_1+2,n_2}+(\tfrac{1}{2}R^2_{n_1,n_2+2}+\tfrac{3}{2}R^1_{n_1,n_2+2}-2f^2+2\Delta-b_2^2)S_{n_1,n_2+2}$$
$$+[b_1(2n_1+1)+b_2(2n_2+1)+2f^4]S_{n_1,n_2}-n_1(n_1-1)S_{n_1-2,n_2}-n_2(n_2-1)S_{n_1,n_2-2}=ES_{n_1,n_2}, \quad (40)$$

where

$$R^1_{n_1,n_2}=\tilde{S}_{n_1+2,n_2}/\tilde{S}_{n_1,n_2},$$
$$R^2_{n_1n_2}=\tilde{S}_{n_1,n_2+2}/\tilde{S}_{n_1,n_2}. \quad (41)$$

Similarly for $n_1+n_2=M$, we have

$$[b_1(2n_1+1)+b_2(2n_2+1)+2f^4-(2f^2+b_1^2)R^1_{n_1,n_2}-(2f^2-\Delta+b_2^2)R^2_{n_1,n_2}+\tfrac{1}{2}R^1_{n_1,n_2}R^1_{n_1+2,n_2}+\tfrac{1}{2}R^2_{n_1,n_2}R^2_{n_1,n_2+2}$$
$$+\tfrac{3}{2}R^1_{n_1n_2}R^2_{n_1+2,n_2}+\tfrac{3}{2}R^2_{n_1n_2}R^1_{n_1,n_2+2}]S_{n_1n_2}-n_1(n_1-1)S_{n_1-2,n_2}-n_2(n_2-1)S_{n_1,n_2-2}=ES_{n_1,n_2}. \quad (42)$$

Equation (39) for $n_1+n_2 \leq M-4$, together with Eqs. (40) and (42), form a set of $(M+2)(M+4)/8$ homogeneous, linear equations for the $S_{n_1n_2}$. If we regard the S_{n_1,n_2} as elements of an $(M+2)(M+4)/8$ dimensional column vector S, then these equations can be written in the matrix form

$$\tilde{H}S=ES, \quad (43)$$

where the elements of the matrix H can be read off from Eqs. (39)–(42). Thus by our knowledge of the asymptotic behavior of the S_{n_1,n_2}, we have reduced an infinite-dimensional eigenvalue problem to a finite-dimensional one. The latter can of

TABLE IV. Ground-state and first-excited-state energies of the coupled anharmonic oscillators at $\Delta=1$ and $f^2=0$ and 2, versus M, showing the convergence of the recursion relations.

	$\Delta=1.0$	
M	E_0 $(f^2=0)$	E_1 $(f^2=0)$
8	2.74	5.340 9
10	2.726 0	5.341 7
12	2.725 1	5.340 3
14	2.725 66	5.340 079
16	2.725 67	5.340 083
18	2.725 630	5.340 090
20	2.725 635 0	5.340 093 6
22	2.725 636 4	5.340 093 8
24	2.725 635 3	5.340 093 5
M	E_0 $(f^2=2)$	E_1 $(f^2=2)$
8	5.95	5.36
10	5.49	5.43
12	5.48	5.46
14	5.417	5.481
16	5.400	5.490
18	5.393	5.493 6
20	5.390 6	5.494 55
22	5.390 92	5.494 46
24	5.391 49	5.494 29

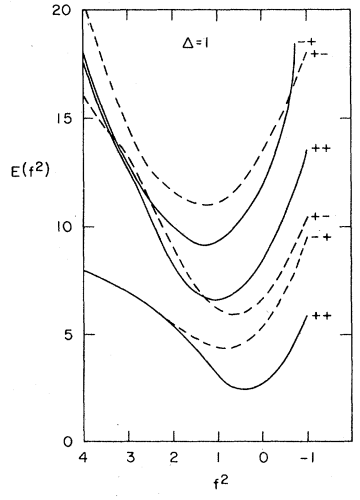

FIG. 3. Energies of the ground state and first few excited states of the coupled anharmonic oscillators, with H given by Eq. (33) and $\Delta=1$, as a function of f^2.

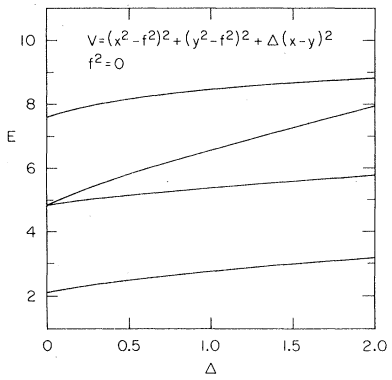

FIG. 4. Energies of the ground state and first few excited states of the coupled anharmonic oscillators with $f^2=0$ as a function of Δ.

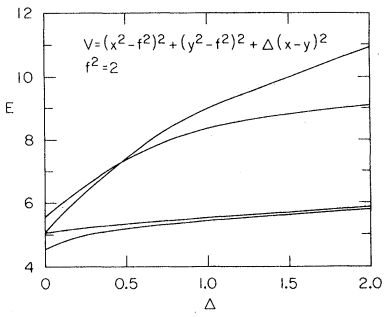

FIG. 5. Energies of the ground state and first few excited states of the coupled anharmonic oscillators with $f^2=2$ as a function of Δ.

course be solved by using canned computer subroutines, provided M is not too large.

We could of course have used the same procedure to solve the one-dimensional problems discussed earlier. In those cases the structure of H was so simple that $\det[H-E]$ could be computed iteratively.

Since the dimension of H grows as $M^2/8$, it is essential that the $\tilde{S}_{n_1,n_2}$ approach the S_{n_1,n_2} rapidly as n_1+n_2 increases. The first step in obtaining the $\tilde{S}_{n_1,n_2}$ is to notice that

$$\psi(x,y)\approx\exp\left[-\tfrac{1}{3}(x^3+y^3)+(f^2-\tfrac{1}{2}\Delta)(x+y)+\Delta(xy(x-y)^{-1})\ln(x/y)\right], \tag{44}$$

for $x,y\gg 0$. By substituting Eq. (44) into Eq. (38), one can obtain an asymptotic expansion for S_{n_1,n_2}, the relevant saddle point being at $x_1\sim 2^{-1/6}(2n_1-n_2)^{1/3}$, $x_2\sim(4n_1-2n_2)^{-1/6}n_2^{1/2}$ for $n_1\geq n_2$; and at $x_2\sim 2^{-1/6}(2n_2-n_1)^{1/3}$, $x_1\sim(4n_2-2n_1)^{-1/6}n_1^{1/2}$ for $n_2\geq n_1$. However, we can do much better by making use of our previous calculation of the moments of the one-dimensional oscillator.

We rewrite Eq. (33) in the form

$$H=H_0-2\Delta xy, \tag{45}$$

and Eq. (37) as

$$\varphi(x_1,x_2)=\varphi_0(x,y)\exp\left[-\tfrac{1}{2}(b_1-b_2)xy\right]. \tag{46}$$

The exact moments for the Hamiltonian H_0 and the trial function φ_0 are

$$S^0_{n_1,n_2}=\langle\varphi|x^{n_1}x^{n_2}|\psi_0\rangle=\left\langle\varphi_0\left|\left(\frac{x+y}{\sqrt{2}}\right)^{n_1}\left(\frac{x-y}{\sqrt{2}}\right)^{n_2}\right|\psi_0\right\rangle$$
$$=2^{(n_1+n_2)/2}\sum_{k_1=0}^{n_1}\sum_{k_2=0}^{n_2}S_{k_1+k_2}S_{n_1+n_2-k_1-k_2}(-1)^{n_2-k_2}n_1!\,n_2!\Big/[k_1!\,k_2!\,(n_1-k_1)!\,(n_2-k_2)!\,], \tag{47}$$

where the S_n are the moments for the one-dimensional Hamiltonian $p^2+(x^2-f^2+\Delta/2)^2$ with the trial function $\exp[-\frac{1}{4}(b_1+b_2)x^2]$.

We use the saddle point only to calculate the ratio $\tilde{S}_{n_1n_2}/S^0_{n_1n_2}$. Our final result is

$$\tilde{S}_{n_1,n_2}=S^0_{n_1,n_2}\exp\{\Delta(n_1-n_2)(8n_1-4n_2)^{-1/6}n_2^{-1/2}\times\ln[(n_1+(2n_1n_2-n_2^2)^{1/2})\times(n_1-n_2)^{-1/2}]-(b_1-b_2)(n_1-n_2)(4n_1-2n_2)^{-1/3}\}. \tag{48}$$

Equation (48) provides a very useful asymptotic approximation as long as $\Delta/M^{2/3}$ and $(b_1-b_2)/M^{2/3}$ are less than one. In practice we have taken $b_1=b_2$.

We have used Eqs. (39), (40), (42), and (48) to calculate the four lowest energy levels of the coupled oscillators. The results are shown in Table IV, and Figs. 3–5.

III. DISCUSSION

Our numerical results are presented in Tables I and II, and in Figs. 1 and 2. It is clear that for any one-dimensional problem with a potential of the form

$$V(x)=\sum_{n=0}^{2N}a_nx^n, \tag{49}$$

the energy levels can be easily computed to any

desired accuracy using the moment method. Our procedure is very simple to apply and the calculations require a trivial amount of computer time. Since the approach is nonperturbative, it can be applied equally well to cases in which the potential has one or several minima. From a calculational point of view it seems far superior to the numerical integration of the Schrödinger equation, or to procedures based on perturbation theory such as Padé approximates or Borel resummation. Finally, we should note that although we have only presented results for the two lowest energy levels in the one-dimensional problems, there is no difficulty in calculating the energies of higher excited states. In addition by combining our results with the techniques of Ref. 1, one can calculate matrix elements such as $\langle\psi|x^n|\psi\rangle$ and $\psi(0)$ to very high accuracy.

Problems involving more than one degree of freedom cannot be overpowered to the same extent as the one-dimensional problems. In the one-dimensional case we approximated the moments S_n by the first few terms in an asymptotic expansion for $n \geq M \gg 1$, and then determined the S_n for $n<M$ iteratively. Since this calculation could be done very rapidly and did not require the storage of large arrays of numbers, we could ensure high accuracy by simply taking M to be reasonably large.

For problems with more than one degree of freedom the equations relating the moments could not be solved quite so simply. One is faced with a finite-dimensional eigenvalue problem whose dimensionality increases rapidly with M; thus there is a practical limit on the size of M and the resultant accuracy.

For the problem of two coupled quartic oscillators we used our knowledge of the one-dimensional oscillator to obtain asymptotic moments which gave a good approximation to the exact ones even at moderate values of M. As can be seen from Table III, our calculation converges quite rapidly. We are not aware of any other calculation of the energy levels of coupled anharmonic oscillators which gives comparable accuracy. If even greater accuracy were wanted, one could either increase M, or improve the approximate moments $\tilde{S}_{n_1 n_2}$ by solving Eq. (39) iteratively for $n_1 + n_2 \approx M$ with the $\tilde{S}_{n_1 n_2}$ as the zero-order approximation.

It is clear that it will not be practical to solve the moment recursion relations directly for systems such as lattice field theories, which involve large numbers of coupled anharmonic oscillators. One approach to the lattice field theory problem is to make a real-space renormalization-group calculation in which blocks of oscillators are replaced by a single average oscillator.[5] The ability to make accurate calculations of the one-dimensional oscillator is crucial for these calculations. It is also possible to treat two coupled oscillators as the exactly solvable "base" problem using the methods described here. We hope to return to this calculation in the future.

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[4] Note the approximate equality: We have required that x be large compared to b or f^2. This requirement translates into limits on the size of b: $b<M^{1/3}$, and on n, for given f^2: $M^{2/3}>f^2$. If these constraints are not satisfied, the evaluation of S_n by steepest descent which gives Eq. (17) will not be accurate and the moment recursion relations might not yield good energy eigenvalues.

[5] See, for instance, J. Richardson and R. Blankenbecler, Phys. Rev. D 20, 1351 (1979).