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Generalized moment method for eigenvalues

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We present a new technique for making accurate calculations of the energy eigenvalues of quantum systems whose potential energy is a polynomial in the coordinate operator. This technique can be applied to arbitrary polynomial potentials whether or not they conserve parity. The problem of an anharmonic oscillator in an external field is studied as an example.

I. INTRODUCTION

Recently a new technique was presented for making accurate calculations of the energy levels of quantum-mechanical systems whose potential energy is a polynomial in the coordinate operator.[1] In the specific examples addressed in I, only potentials which are even under parity were considered. However, in some applications, such as an anharmonic oscillator in an external field or variational calculations in lattice field theories,[2] it is necessary to consider potentials involving odd powers of the coordinate operator. In this note we extend the moment method to such potentials. The extension is not completely straightforward, and we believe that it gives additional insight into the moment method.

We start with the Hamiltonian

$$H=p^2+\sum_{n=1}^{4}c_n x^n\,, \qquad (1)$$

although the extension to potentials with higher powers of x is straightforward. By making the change of variables $x\to c_4^{-1/6}(x-c_3c_4^{-5/6}/4)$, this Hamiltonian can be reduced to the form

$$H=p^2+Ax+Bx^2+x^4 \qquad (2)$$

aside from an additive and a multiplicative constant. It is the Hamiltonian of Eq. (2) which we study in detail. In Sec. II we present our calculational technique, and in Sec. III we discuss our results.

II. THE MOMENT METHOD

We wish to find the eigenvalues of the Schrödinger equation

$$H|\psi\rangle=E|\psi\rangle \qquad (3)$$

with H given by Eq. (2). To this end we introduce the moments

$$S_n=\langle\phi|x^n|\psi\rangle\,, \qquad (4)$$

where $|\phi\rangle$ is a trial state at our disposal. For concreteness we shall take

$$\phi(x)=\exp(-\tfrac{1}{2}bx^2)\,, \qquad (5)$$

but as is discussed in I, the exact functional form of $\phi(x)$ is not important.

Taking the matrix element of Eq. (3) with the state $\langle\phi|x^n$, we obtain after an integration by parts

$$S_{n+4}+(B-b^2)S_{n+2}+AS_{n+1}+[(2n+1)b-E]S_n-n(n-1)S_{n-2}=0\,. \qquad (6)$$

Our strategy for solving the moment recursion relations, Eq. (6), is as follows. We first obtain an asymptotic expansion of the S_n valid for n larger than or equal to some fixed value N. We then obtain the S_n for $n<N$ by repeated application of Eq. (6). A solution valid for all n is, of course, possible only for certain discrete values of E, namely the eigenvalues of Eq. (3).

To obtain the asymptotic expansion of S_n for large n, we try the ansatz

$$S_n\sim\exp[\alpha n\ln(n)+\beta n+\gamma n^{2/3}+\delta n^{1/3}+\epsilon\ln(n)+O(1/n)]\,. \qquad (7)$$

Substituting into Eq. (6), we find six independent solutions of the form

$$S_n^m=n^{n/3}e^{i\pi mn/3}\exp[-\tfrac{1}{3}n-\tfrac{1}{2}be^{2\pi im/3}n^{2/3}+\tfrac{1}{2}(\tfrac{1}{3}b^2-B)e^{-2\pi im/3}n^{1/3}-(\tfrac{1}{2}+\tfrac{1}{6}Ae^{i\pi m})\ln(n)+O(1/n)]\,,\quad m=0,1,\ldots,5\,. \qquad (8)$$

In order to understand which of these solutions is relevant, we return to Eq. (4), and notice that for large n the integral defining S_n must be dominated by large values of $|x|$. We can obtain an asymptotic expansion of the wave function $\psi(x)$ by writing $\psi(x)=e^{\chi(x)}$. Upon substituting into the Schrödinger equation we find

$$-\chi'' - (\chi')^2 + Ax + Bx^2 + x^4 = E \,, \tag{9}$$

which yields for large $|x|$

$$\chi(x) \sim -[\tfrac{1}{3}|x|^3 + \tfrac{1}{2}B|x| + O(\ln x)] \,. \tag{10}$$

Thus, for large values of n the integrand of the right-hand side of Eq. (4) has two saddle points along the real x axis at $|x| \simeq n^{1/3}$. The contributions of these saddle points correspond to the asymptotic solutions S_n^0 and S_n^3 of Eq. (8), so the desired S_n is a linear combination of these two solutions.

Notice that for large n

$$S_n^m/S_n^0 \sim e^{i\pi mn/3}\exp[\tfrac{1}{2}bn^{2/3}(1-e^{2\pi i m/3})] \tag{11}$$

for $m \neq 0,3$ and

$$S_n^3/S_n^0 \sim (-)^n n^{A/3} \,. \tag{12}$$

So the desired solutions S_n^0 and S_n^3 are the subdominant ones at large n. Our one requirement on the trial function $\phi(x)$ is that it be chosen so that this is the case. If the physical solution did contain admixtures of S_n^m, $m \neq 0,3$, then our approach would fail because we would not be able to determine how much S_n^0 and S_n^3 components were present in S_n at large n.

We are now prepared to calculate S_n^0 and S_n^3. We use the asymptotic expression of Eq. (8) for $n \geq N$, and then obtain S_n^0 and S_n^3 for $n<N$ by making repeated use of Eq. (6). Of course, in using the asymptotic formula for $n \geq N$, we are introducing an error in the form of admixtures of the unwanted solutions. From Eq. (11) we see that admixtures of S_n^m, $m \neq 0,3$ can at most be of order $\exp(-\frac{1}{4}bN^{2/3})$, so by choosing N to be sufficiently large they can be made negligible. If A is sufficiently large our solution for S_n^0 may contain a significant admixture of S_n^3 or vice versa; however, that is irrelevant as long as we obtain two linearly independent solutions of Eq. (6) with negligible admixtures of S_n^m, $m \neq 0,3$.

Starting with the asymptotic expressions for S_n^0 and S_n^3 for $n \geq N$, we obtain S_{n-1}^0 and S_{n-1}^3 using Eq. (6) with $n=N+1$. Continuing on down, we finally obtain S_0^0 and S_0^3 from Eq. (6) with $n=2$. At this point all the moments are determined, but in general neither the set S_n^0 nor S_n^3 will satisfy Eq. (6) for either $n=1$ or $n=0$. We must take a linear combination of these solutions which we write in the form

$$\bar{S}_n = S_n^0 + \alpha S_n^3 \,. \tag{13}$$

This explains why there is no loss in accuracy if our solution for S_n^0 contains an admixture of S_n^3 or vice versa.

The $\bar{S}_n$ will satisfy the two equations

$$\begin{aligned} &\bar{S}_5 + (B-b^2)\bar{S}_3 + A\bar{S}_2 + (5b-E)\bar{S}_1 = 0 \,, \\ &\bar{S}_4 + (B-b^2)\bar{S}_2 + A\bar{S}_1 + (3b-E)\bar{S}_0 = 0 \end{aligned} \tag{14}$$

only for discrete values of E. Substituting Eq. (13) into Eq. (14) and eliminating α gives the eigenvalue equation

$$F(E) \equiv Q^0(E)P^3(E) - Q^3(E)P^0(E) = 0 \,, \tag{15}$$

where

$$\begin{aligned} &Q^m(E) = S_4^m + (B-b^2)S_2^m + AS_1^m + (3b-E)S_0^m \,, \\ &P^n(E) = S_5^n + (B-b^2)S_3^n + AS_2^n + (5b-E)S_1^n \,. \end{aligned} \tag{16}$$

We need only plot $F(E)$ as a function of E and search for its zeros which can be determined with great accuracy using Newton's method.

Notice that for $A=0$ we have from parity conservation that $S_n^0 = (-)^n S_n^3$. As a result, $\alpha = \pm 1$, and either the even or the odd moments vanish. This fact was used in I where only potentials which are even under parity were considered. One then had only one nontrivial subdominant solution to the difference equation, but a different eigenvalue equation for the even- and odd-parity states. In the present formulation, Eq. (15) is the eigenvalue equation for all cases.

In practical calculations it is convenient to work with ratios of moments. Defining

$$R_n^m = S_{n+1}^m/S_n^m \,, \tag{17}$$

Eq. (6) can be rewritten in the form

$$R_{n-1}^m = n(n-1)(R_n^m\{(2n+1)b - E + R_{n+1}^m[A + R_{n+2}^m(B - b^2 + R_{n+3}^m R_{n+4}^m)]\})^{-1} \,. \tag{18}$$

From Eq. (8) we see that for large n

$$R_n^m = n^{1/3}e^{i\pi m/3}[1 - \tfrac{1}{3}be^{2\pi i m/3}n^{-1/3} + (\tfrac{1}{9}b^2 - \tfrac{1}{6}B)e^{-2\pi i m/3}n^{-2/3} - (\tfrac{2}{81}b^3 - \tfrac{1}{18}bB + \tfrac{1}{3} + \tfrac{1}{6}Ae^{i\pi m})n^{-1} + O(n^{-4/3})] \,. \tag{19}$$

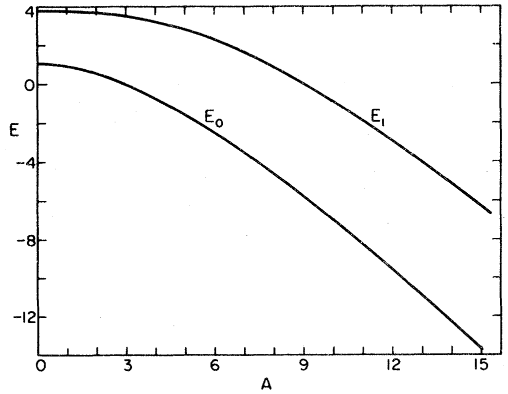

FIG. 1. The two lowest energy levels of the potential $V=Ax+x^4$ as a function of A.

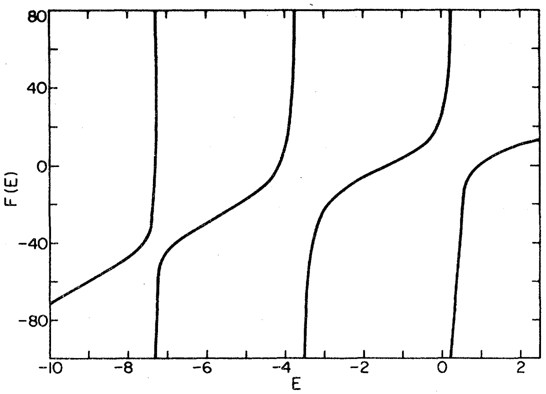

FIG. 3. The function $F(E)$, defined in Eq. (15), for the potential $V=x-6x^2+x^4$.

If we normalize the moments so that $S_0^m=1$, we can recover the low-order moments from the relation $S_{n+1}^m=R_n^mS_n^m$. Then the energy eigenvalues can be obtained from Eqs. (15) and (16).

III. NUMERICAL RESULTS

Examples of our calculations are shown in Figs. 1–4 and in Tables I–III.

In Fig. 1 we plot the energies of the ground state and first excited state of the potential $V(x)=Ax+x^4$ as functions of A. Energy eigenvalues for specific values of A are given in Table I. The results are quite unexceptional. For $A=0$ the potential has a single minimum at $x=0$ and the two lowest energy states are well separated. For small A the energy eigenvalues vary as A^2, as one expects from perturbation theory.

In Table II we illustrate the rate of convergence of our calculational scheme. The convergence is clearly very rapid for small to moderate values of A. However, for A larger than 15, we rapidly lose accuracy. The difficulty can be read off from Eq. (8). We see that for large n

$$S_n^3/S_n^0\sim(-)^n n^{A/3}\,. \tag{20}$$

Thus in our solution for S_n^0 we can expect an admixture of S_n^3 of order $N^{-A/3}$, while in our solution for S_n^3, we can expect an admixture of S_n^0 of order $N^{A/3}$. From Eqs. (15) and (16) we see that such admixtures will not effect the accuracy with which we compute the energy eigenvalues so long as we obtain two linearly independent solutions to the difference equation, one of which has a finite component of S_n^0 and the other of which has a finite component of S_n^3. The difficulty is that for A large and positive (negative) S_n^0 (S_n^3) dominates both of our solutions. As a result, $Q^0(E)P^3(E)$ is almost equal to $Q^3(E)P^0(E)$ for all E, and we lose accuracy by taking their difference in Eq. (15).

Fortunately for A larger than or of order 15, we can obtain an asymptotic expansion of the energy eigenvalues by expanding the potential about its minimum value $x=-(A/4)^{1/3}$. We find that the kth eigenvalue is given by

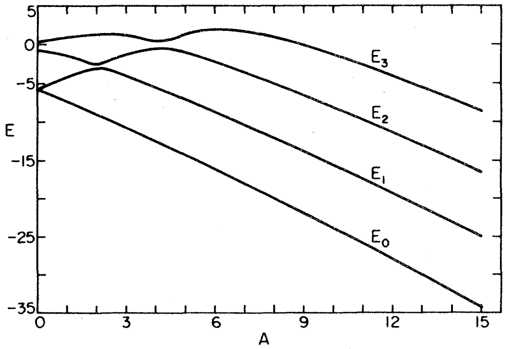

FIG. 2. The four lowest energy levels of the potential $V=Ax-6x^2+x^4$ as a function of A.

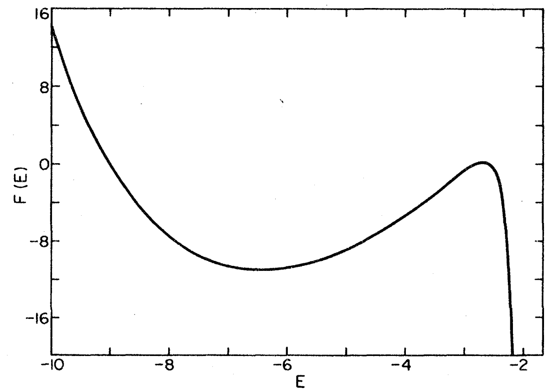

FIG. 4. The function $F(E)$ for the potential $V=2x-6x^2+x^4$.

TABLE I. Energy levels of the potential $V=Ax+x^4$.

A	E_0	E_1
0	1.060 362 09	3.799 673 01
1	0.930 546 03	3.781 896 25
5	−1.547 077 68	2.835 738 65
10	−6.951 328 43	−0.940 998 30
15	−13.747 006	−6.627 207

TABLE III. Energy levels of the potential $V=Ax-6x^2+x^4$.

A	E_0	E_1
0	−5.748 190 5	−5.706 792 5
1	−7.337 195 8	−4.180 640 3
5	−14.257 928 2	−7.070 244 4
10	−23.749 394 7	−15.536 874 0
15	−33.974 6	−24.980

$$\begin{aligned} E_k = & -3(A/4)^{4/3}+(2k+1)6^{1/2}(A/4)^{1/3} \\ & +\tfrac{1}{8}(2k^2+2k+1)(A/4)^{-2/3} \\ & +\tfrac{1}{36}\sum_{l\neq k}\left|\langle l|(a+a^\dagger)^3|k\rangle\right|^2(k-l)^{-1}(A/4)^{-2/3} \\ & +O((A/4)^{-5/3}). \end{aligned} \tag{21}$$

Here a and $a^\dagger$ are the usual harmonic-oscillator raising and lowering operators and $a^\dagger a|k\rangle=k|k\rangle$. For $A=15$, Eq. (21) yields $E_0\simeq-13.736$, $E_1\simeq-6.620$, each within 0.1 percent of the "exact" results given in Table I.

In Fig. 2 we plot the four lowest eigenvalues of the potential $V=Ax-bx^2+x^4$ as a function of A. Typical numerical results are given in Table III. In this case, at $A=0$, V has double minima at $x=\pm 3^{1/2}$, and the two lowest energy levels are almost degenerate. For A less than two, E_0 and E_1 appear to vary linearly with A. This is easily understood from nearly degenerate perturbation theory. If we denote the values of E_0 and E_1 at $A=0$ by ϵ and $\epsilon+\Delta\epsilon$, respectively, then, taking into account only the mixing between these two states, we find

$$\begin{aligned} E_0 &= \epsilon+\tfrac{1}{2}\Delta\epsilon-\tfrac{1}{2}(\Delta\epsilon^2+4A^2{x_{01}}^2)^{1/2} \\ &\simeq \epsilon-A|x_{01}|, \\ E_1 &= \epsilon+\tfrac{1}{2}\Delta\epsilon+\tfrac{1}{2}(\Delta\epsilon^2+4A^2{x_{01}}^2)^{1/2} \\ &\simeq \epsilon+A|x_{01}|, \end{aligned} \tag{22}$$

where x_{01} is the matrix element of the coordinate operator between the ground state and the first excited state at $A=0$.

Figure 2 provides beautiful examples of the repulsion of nearly degenerate energy levels in one-dimensional quantum mechanics. The fact that E_1 and E_2 become so nearly equal can also be explained from almost degenerate perturbation theory. For small A the wave functions for these states are approximately $|\psi_1\rangle=2^{-1/2}[|0\rangle+|1\rangle]$ and $|\psi_2\rangle=2^{-1/2}[|2\rangle-|3\rangle]$. Here $|n\rangle$ are the eigenstates of the Hamiltonian at $A=0$. The states $|n\rangle$ of course have definite parity. The matrix element which controls the mixing between these states is

$$\langle\psi_2|x|\psi_1\rangle=\tfrac{1}{2}[\langle 2|x|1\rangle-\langle 3|x|0\rangle]. \tag{23}$$

Since $\langle 2|x|1\rangle\simeq\langle 3|x|0\rangle$, the mixing is very small except when the states are almost exactly degenerate.

For large A the rate of convergence deteriorates just as in the case $B=0$, but one can once again obtain an asymptotic expansion for the energy levels by expanding the potential about its minimum.

In Figs. 3 and 4 we plot the function $F(E)$ vs E for two typical values of the parameters. $F(E)$ can have poles as well as zeros, but in general the poles are not so symmetrically spaced between the zeros as in Fig. 3. The poles in $F(E)$ cause no difficulty except when one of them is very close to a zero. If one has written a computer code which automatically searches for the zeros, for example by Newton's method, a zero near a pole can be easily missed. This problem can be overcome simply by plotting $F(E)$ as in Figs. 3 and 4.

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TABLE II. The ground-state energy of the potential $V=Ax+x^4$ calculated for various values of N. N is the value of n above which we use the asymptotic expansion for the moments S_n^m.

N	$A=0$	$A=5$	$A=10$	$A=15$
50	1.060 363	−1.547 8	−7.08	−12.4
100	1.060 362 09	−1.547 097	−6.950	−13.68
500	1.060 362 09	−1.547 077 67	−6.951 328 43	−13.747 006 9
1000	1.060 362 09	−1.547 077 67	−6.951 328 43	−13.747 010 4

[1] R. Blankenbecler, T. DeGrand, and R. L. Sugar, Phys. Rev. D 21, 1055 (1980), hereafter referred to as I. See also, J. L. Richardson and R. Blankenbecler, Phys. Rev. D 19, 496 (1979) and references contained therein.

[2] J. B. Bronzan (unpublished).