

## MOMENT RECURSIONS AND THE SCHRÖDINGER PROBLEM\*

John L. Richardson and Richard Blankenbecler  
Stanford Linear Accelerator Center  
Stanford University, Stanford, California 94305

## ABSTRACT

We present new techniques for attacking the Schrödinger eigenvalue problem. They are based on asymptotic solutions to an exact set of recursion relations satisfied by moments of the coordinate operator. We apply these techniques to the generalized anharmonic oscillator  $H = P^2 + X^{2M}$  and show how to compute the energy levels, all of the moments  $\langle X^N \rangle$ , and the value of the wave function and its derivatives at the origin. We specialize to the case  $M = 2$  to obtain accurate numerical results for the low lying energy levels as well as (all) the moments. We also discuss the case  $V(x) = dx^2 + x^4$ . Transition moments are then treated in the same manner.

Submitted to Physical Review

---

\*Work supported by the Department of Energy

## I. INTRODUCTION

In this paper we present a general yet practical (and simple) method for the computation of energy eigenvalues and physically interesting observables with equivalent accuracy. Because of the recent interest in the anharmonic oscillator from both a mathematical<sup>1-6</sup> and a computational<sup>7-9</sup> point of view, the moment method will be applied to polynomial potentials in this paper in order to illustrate its use. Power behaved potentials, such as the coulomb interaction, can be included in this class.

Elegant and simple evaluations of certain perturbation expansions using recursive methods have been discussed by Swenson and Danforth<sup>10</sup> and Killingbeck.<sup>11</sup> The evaluation of high moments of the coordinate operation in terms of its lowest moments has been described by Banerjee.<sup>12</sup> In this paper these recursive methods are generalized and are shown to determine the energy eigenvalues as well as the coordinate moments.

## II. RECURSION RELATIONS

The derivation of generalized virial theorems has been well discussed. Here we shall discuss a restricted class of relations that are of immediate interest to the problem at hand. Consider a one-dimensional Schrödinger problem and the double commutator

$$\left[ H, [H, g(x)] \right] \quad (1)$$

where

$$H = \frac{-d^2}{dx^2} + V(x)$$

Taking the matrix elements of (1) between eigenstates of H, and

symmetrizing, one finds

$$\begin{aligned} & (E_\ell - E_m)^2 \langle \ell | g | m \rangle + 2(E_\ell + E_m) \langle \ell | g'' | m \rangle \\ & = \langle \ell | 2g'v' + 4g''v | m \rangle - \langle \ell | g'''' | m \rangle, \end{aligned} \quad (2)$$

where the prime denotes differentiation with respect to the argument  $x$ . This is exactly the relation derived and discussed by Banerjee.<sup>12</sup>

The matrix elements of (2) take on the particularly useful form if the potential is a polynomial. Although other cases can be treated, we will restrict ourselves to polynomial potentials here. For example, by setting  $\ell = m$  (and dropping explicitly the label  $\ell$  from now on), one finds for the case of a pure power,

$$V(x) = x^{2M}, \quad (3)$$

(any coefficient can be scaled to unity) and with

$$g(x) = \frac{x^{N+2}}{(N+2)}, \quad (4)$$

that Eq. (2) becomes

$$4E(N+1)Q^N = 4(N+M+1)Q^{N+2M} - (N+1)N(N-1)Q^{N-2}, \quad (5)$$

where

$$Q^N = \langle \ell | x^N | \ell \rangle.$$

The discussion for  $\ell \neq m$  will be given in Section VI.

Equation (5) and its obvious generalizations form the basis of this method. The familiar virial theorem is achieved by choosing  $N = 0$ ,

$$E = (M+1)Q^{2M} \quad (6)$$

As Banerjee has discussed, knowledge of the even moments from  $N = 0$  to  $N = 2M$  allows one to compute all of the higher even moments by repeated applications of Eq. (5).

Let us define the odd moments by

$$Q^N \equiv \langle \ell | |x|^N | \ell \rangle \quad (7)$$

which also obey the relation (5) for  $N \geq 3$ . For smaller  $N$ , a simple integration by parts for  $N > 1$  yields the relation

$$\begin{aligned} (N-1)Q^{N-2} &= 2 \int_0^{\infty} dx (N-1) x^{N-2} \psi^2(x) \\ &= -2 \int_0^{\infty} dx x^{N-1} \frac{d}{dx} (\psi^2(x)). \end{aligned}$$

Thus

$$\lim_{N \rightarrow 1+} (N-1) Q^{N-2} = 2 \psi^2(0),$$

and one finds

$$\psi^2(0) = (M+2)Q^{2M+1} - 2EQ^1. \quad (8)$$

Proceeding one step further

$$\left. \frac{d^2}{dx^2} \psi^2(x) \right|_{x=0} = 2MQ^{2M-1} - 4E \psi^2(0).$$

It is convenient to rewrite the last equation using  $V(0) = 0$

$$\left. \frac{d^2}{dx^2} \psi^2(x) \right|_{x=0} = 2 (\psi'(0))^2 - 2E (\psi(0))^2,$$

in the form

$$\left(\psi'(0)\right)^2 + E\left(\psi(0)\right)^2 = M Q^{2M-1} . \quad (9)$$

Since the states have a given parity, only one term on the left of Eq. (9) can contribute at a time. Incidentally, note that the value of Eq. (8), i.e.,  $\psi^2(0)$ , indicates whether or not one is dealing with an even or an odd state. We see that the value of the wave function and its derivatives at the origin can be determined from a knowledge of the odd positive moments. Note also that for a symmetric state, Eq. (8) and (9) imply a relation between  $E$ ,  $Q^1$ ,  $Q^{2M-1}$ , and  $Q^{2M+1}$ .

Higher derivatives of the wave function at the origin  $\psi^{(k)}(0)$  can be computed by continuing the moment recursion relations to more negative  $N$  values. Alternatively one may use the differential equation with the initial condition given by Eq. (9);

$$\psi^{(k+2)}(0) = \frac{k!}{(k-2M)!} \psi^{(k-2M)}(0) - E\psi^{(k)}(0). \quad (10)$$

This relation will be applied to the quartic oscillator in Section IV.

### III. ASYMPTOTIC BEHAVIOR AND EIGENVALUE CONDITION

In the previous section, a knowledge of  $E$  and the low moments was shown to be sufficient for determining all higher moments recursively. Actually a study of the behavior of (5) for large  $N$  will lead us to a convenient method for determining  $E$  and the lower moments as well.

That the large  $N$  behavior of  $Q^N$  is connected to the eigenvalue condition should come as no surprise. Imagine solving the Schrödinger equation in coordinate space. The wave function must be finite at the

origin and for a potential that behaves asymptotically as  $V \sim X^{2M}$ , fall at large distances as

$$\psi(x) \sim \exp \left[ \frac{-|x|^{M+1}}{M+1} \right]$$

Since the moments are controlled at large  $N$  by the large  $x$  behavior of  $\psi(x)$ , one finds that

$$Q^N \sim 2 \int_0^\infty dx x^N \exp \left[ -\frac{2}{M+1} x^{M+1} \right]$$

or

$$\begin{aligned} Q^N &\sim \left( \frac{M+1}{2} \right)^N \Gamma \left( \frac{N+1}{M+1} \right) \\ &\sim \left( \frac{N}{2} \right)^{N/M+1} \end{aligned} \tag{11}$$

for large  $N$ . More accurate estimates will be given shortly for the asymptotic behavior of  $Q^N$ .

The important point is the following. If a sequence of  $(M+1)$  even moments of  $Q^N$  are known at some (large) value of  $N$ , say  $N_\infty$ , the recursion relation (5) with an arbitrary  $E$  can be used to compute the  $Q^N$  down to  $N=0$ . The demand that Eq. (5) for  $N=0$  (the virial condition) is consistent then determines  $E$ . Actually one does not need to know all  $M+1$  moments but only  $M$  ratios since their overall normalization is fixed by requiring that  $Q^0 = 1$ .

Our procedure in practice is as follows. Derive an asymptotic expansion for  $Q^N$  at large  $N$ . Then choose a sufficiently large value of

$N_\infty$  so that the fractional errors in  $Q^N$  are acceptable. Then use these approximate values to start off the recursion relations. Since the recursion relations are linear, one finds that the fractional errors propagate approximately linearly. Hence the fractional errors in  $Q^2, \dots, Q^{2M}$  (and  $E$ ) are roughly the same as those in  $Q^N$  (and these can be made arbitrarily small by choosing  $N_\infty$  to be sufficiently large. Once the even moments have been used to determine  $E$ , the odd moments can be properly normalized and  $\psi^2(0)$ , etc., can be computed.

This procedure is simpler than its description, so let us turn to an example which clarifies it. Numerical results and examples will be given.

#### IV. ANHARMONIC OSCILLATOR

For this case the recursion relation can be written as

$$E = \frac{N + M + 1}{N + 1} \frac{Q^{N+2M}}{Q^N} - \frac{N(N - 1)}{4} \frac{Q^{N-2}}{Q^N} \quad (12)$$

From Eq. (11) we know that

$$Q^N \sim \left(\frac{N}{2}\right)^{\frac{N}{M+1}}$$

and hence the  $E$  term is nonleading in Eq. (12). Define  $q^N$  to be the solution of Eq. (12) when  $E = 0$ . One finds that

$$q^N = (M + 1)^{\frac{N}{M+1}} \frac{\Gamma\left(\frac{N + 1}{2M + 2}\right) \Gamma\left(\frac{N + 2}{2M + 2}\right) \Gamma\left(\frac{N + 3}{2M + 2}\right)}{\Gamma\left(\frac{N + M + 1}{2M + 2}\right)} \quad (13)$$

Introducing  $F(N)$  through the relation

$$Q^N = q^N \exp \{ -F(N) \} , \quad (14)$$

then  $F(N)$  is determined by the relation

$$e^{F(N) - F(N+2M)} - e^{F(N) - F(N-2)} = E R(N). \quad (15)$$

where

$$R(N) = (M+1)^{\frac{-2M}{M+1}} \frac{\Gamma\left(\frac{N+M+1}{2M+2}\right) \Gamma\left(\frac{N+2}{2M+2}\right) \Gamma\left(\frac{N+3}{2M+2}\right)}{\Gamma\left(\frac{N+2M+1}{2M+2}\right) \Gamma\left(\frac{N+2M+2}{2M+2}\right) \Gamma\left(\frac{N+M+3}{2M+2}\right)} .$$

For large  $N$ ,  $R(N)$  can be expanded in an asymptotic series and  $R(N) \sim (2/N)^r$ ,  $r = \frac{2M}{M+1}$ .  $F(N)$  can then be determined by matching coefficients. To be more specific, let us consider the case  $M = 2$  or  $V(x) = x^4$ . To low order

$$R(N) \sim \left(\frac{N}{2}\right)^{-\frac{4}{3}} \left[ 1 - \frac{4}{3N} + \frac{1}{9N^2} + \dots \right] ,$$

and

$$F(N) \sim E \left(\frac{N}{2}\right)^{-\frac{1}{3}} - \frac{E^2}{30} \left(\frac{N}{2}\right)^{-\frac{5}{3}} + O(N^{-7/3}) .$$

It is straightforward to carry this procedure out to higher orders.

Defining

$$F(N) \equiv \sum_{\ell=1}^K F_{\ell} \left(\frac{2}{N}\right)^{\frac{\ell}{3}} \quad (16)$$

The first few values of  $F_{\ell}$  are found to be

$$F_1 = E, \quad F_5 = -E^2/30, \quad F_7 = -55E/252, \quad F_8 = E^2/18, \\ F_{11} = 293 E^2/44 \cdot 3^4 \text{ and } F_{12} = -2E^3/3^4 . \quad (17)$$



The omitted  $F'_l$ 's are zero.

Note: The above series is accurate at fixed E for N large. In dealing with higher excited states it is convenient to rearrange the ratios of Eq. (15) in the form (c = 4 and -2).

$$e^{F(N) - F(N+C)} = W_0(\hat{E})^{C/2} \left[ 1 + \frac{C}{N} W_1(\hat{E}) - \frac{C^2 \hat{E}}{3N} \frac{W'_0}{W_0} + o\left(\frac{1}{N^2}\right) \right] \quad (18)$$

where  $\hat{E} \equiv E(2/N)^{4/3}$  and  $W'_0 = dW_0/d\hat{E}$ . Substituting into Eq. (15), one finds that  $W_0$  and  $W_1$  satisfy

$$W_0^3 - \hat{E} W_0 = 1$$

and

$$W_1 = \frac{4\hat{E}^2}{3} W_0 \left[ (3 + 2\hat{E} W_0)(3W_0^2 - \hat{E}) \right]^{-1}.$$

This expansion should be good when  $\hat{E}$  is fixed and N becomes large.

A simple procedure to solve the quartic oscillator eigenvalue problem is as follows. To determine both the even and odd moments we need six input moments  $Q_{N_\infty}^{N_\infty}$ ,  $Q_{N_\infty+1}^{N_\infty+1}$ , ...,  $Q_{N_\infty+5}^{N_\infty+5}$ , where  $N_\infty$  is even. Since the normalization does not matter, define the five-dimensional vector:

$$\begin{aligned} \vec{V}(N) &= \left\{ \frac{Q_{N+1}}{Q_N}, \frac{Q_{N+2}}{Q_N}, \dots, \frac{Q_{N+5}}{Q_N} \right\} \\ &= \left\{ V^1(N), V^2(N), \dots, V^5(N) \right\} \end{aligned} \quad (19)$$

One may compute  $\vec{V}(N_\infty - 2)$  by using the recursion relations Eq. (12) and by assuming a trial value of E. This procedure is repeated until  $\vec{V}(0)$  is reached. The virial theorem then must be satisfied at the proper E (this is equivalent to the ordinary boundary condition at the origin, or in this language that the term  $N(N-1)(N+1)Q^{N-2}$  is zero as  $N \rightarrow 0+$ ). This

sequence is repeated until the  $E$  satisfying the virial condition is found. Once  $E$  is fixed,  $Q^1, \dots, Q^5$  are then directly known since  $Q^0 = 1$ . There are in general a large number of values of  $E$  satisfying the virial condition (depending on  $N_\infty$  and the starting values of  $\bar{V}$ ). These are the energy eigenvalues.

Numerical Results. Let us numerically examine the convergence properties of this method. Fixing  $K = 5$ , the values of  $E$  and  $Q^2$  for selected values of  $N$  are given in Table I.<sup>13</sup> For completeness, in Table II the values of  $Q^N$  for small  $N$  are given for the first three levels.

The computation of  $E$  and the  $Q^N$  is extremely rapid. For a fixed trial value of  $E$ , the five initial values of the vector  $V(N_\infty)$  must be computed and then  $N_\infty$  recursive steps are performed to calculate down to  $N = 0$ . This is repeated for several values of  $E$  until the appropriate root of the equation  $E - 3Q^4(E) = 0$  is determined. A sample graph of this equation is given in Fig. 1.

One amusing feature of the numerical results is that the values of  $E$  oscillate as a function of  $N_\infty$  with a wave length of 6 (see Fig. 2). Two of the output  $E$  values for  $N_\infty, N_\infty + 2$ , and  $N_\infty + 4$  are found to be larger than the exact  $E$  value while the third one is roughly twice as far below. The average of these three  $E$  values is actually several significant figures closer to the exact value than any single one. We do not completely understand this feature but it clearly depends on the detailed structure of the potential, the recursion relations, and the asymptotic estimates.

To compute the Taylor expansion of the wave function for the quartic oscillator, one may use Eq. (9) and (10). For even or odd eigenstates,

one knows from Eq. (9) that

$$\psi_e(0) = \sqrt{\frac{2Q^3}{E}}$$

$$\psi_o(0) = \sqrt{2Q^3}$$

This is sufficient information to completely determine the wave function from Eq. (10). The first few terms of the Taylor expansion are

$$\begin{aligned} \psi_e(X) &= \psi_e(0) \left[ 1 - \frac{EX^2}{2!} + \frac{E^2X^4}{4!} + \frac{24 - E^3}{6!} X^6 + \frac{E^4 - 384E}{8!} X^8 + \dots \right] \\ \psi_o(X) &= \psi_o'(0) \left[ X - \frac{EX^3}{3!} + \frac{E^2X^5}{5!} + \frac{120 - E^3}{7!} X^7 + \frac{E^4 - 960E}{9!} X^9 + \dots \right] \end{aligned} \quad (20)$$

#### V. THE POTENTIAL $V = x^4 + dx^2$

The moment relations for this potential has form

$$E = \frac{N+3}{N+1} \frac{Q^{N+4}}{Q^N} - \frac{N(N-1)}{4} \frac{Q^{N-2}}{Q^N} + \frac{d(N+2)}{(N+1)} \frac{Q^{N+2}}{Q^N} \quad (21)$$

For large  $N$ , it is easy to see that the first two terms on the right are dominant, and the  $d$  term is larger than the constant  $E$ . Following the previous section, define

$$Q_i^N = q^N e^{-F(N) - D(N)} \quad (22)$$

where  $q^N$  and  $F(N)$  are given by Eq. (13) and (17). Then  $D(N)$  is found to be

$$D(N) = d \left( \frac{N}{2} \right)^{\frac{1}{3}} + \sum_{\ell=1}^K D_{\ell} \left( \frac{2}{N} \right)^{\frac{\ell}{3}}, \quad (23)$$

where

$$\begin{aligned}
 D_1 &= \frac{1}{6} d^2 & D_4 &= \frac{1}{36} d^2 \\
 D_2 &= \frac{1}{6} d & D_5 &= \frac{1}{5} d - \frac{1}{45} E d^2 - \frac{1}{4 \cdot 9^4} d^4 \\
 D_3 &= 0 & & \vdots \\
 & & & \vdots \\
 & & & \vdots
 \end{aligned} \tag{24}$$

One can also scale the series analogous to Eq. (18) and the approximate scaling variable is  $d(2/N)^{2/3} \equiv \hat{d}$ .

A simplified form for  $Q^N$  that is correct in the limit of large  $N$  is

$$Q^N = \left(\frac{N}{2}\right)^{\frac{N}{3} - \frac{5}{6}} \exp \left\{ -\frac{N}{3} - d \left(\frac{N}{2}\right)^{\frac{1}{3}} - \left(E + \frac{d^2}{6}\right) \left(\frac{N}{2}\right)^{-\frac{1}{3}} + \dots \right\} \tag{25}$$

The behavior of the solution of (21) for fixed (but large  $N$ ) and  $d \rightarrow \infty$  is easily found by scaling. Define  $E = d^{1/2} e$ , introduce

$$P^N \equiv d^{N/4} Q^N \tag{26}$$

and the moment recursion relation (21) becomes

$$e - \frac{N+2}{N+1} \frac{P^{N+2}}{P^N} + \frac{N(N-1)}{4} \frac{P^{N-2}}{P^N} = \frac{(N+3)}{(N+1)} \frac{P^{N+4}}{P^N} d^{-\frac{3}{2}} \approx 0 \tag{27}$$

as  $d \rightarrow \infty$ . The solution for  $P^N$  for the lowest state is exactly that of a simple harmonic oscillator.

$$P^N = \frac{\Gamma\left(\frac{N+1}{2}\right)}{\Gamma(1/2)} \tag{28}$$

and  $e = 1$ .

The neglect of the right-hand side of (27) is justified provided that

$$N \ll N_0 = 2 d^{\frac{3}{4}} - 3 \quad (29)$$

Thus only the moments for  $N \ll N_0$  are controlled by the harmonic term in the potential; the anharmonic term controls the  $N \gg N_0$  moments.

The effect of the  $dx^2$  term on the moments is also simple to understand. As  $d$  increases, the wave function must decrease faster as  $|x|$  increases. Hence the wave function for small  $x$  rises and the large  $N$  moments decrease (also the energy obviously rises at the same time). For negative  $d$ , on the other hand, the potential widens (eventually becoming a double well) and the large  $N$  moments must increase.

Some sample values of the ground state  $E(d)$  and  $Q^2(d)$  computed with  $K = 5$  and  $N_\infty = 200$ , are

$$\begin{array}{ll} E(1/2) = 1.23335 & Q^2(1/2) = 0.33103 \\ E(0) = 1.06036 & Q^2(0) = 0.36202 \\ E(-1/2) = 0.87002 & Q^2(-1/2) = 0.40089 \end{array}$$

The first three states for  $d = 1$  have energies

$$\begin{array}{l} E_0(1) = 1.39235 \\ E_1(1) = 4.64881 \\ E_2(1) = 8.65506 \end{array}$$

The first and last values are within the rigorous limits given by Bazley and Fox<sup>14</sup> who discuss only the symmetric states.

In Fig. 3, the values of  $E_0(d)$  and  $E_1(d)$  are given for  $d$  in the range  $-1$  to  $1$ . For large negative  $d$ , the levels approach pairwise degeneracy whereas for large positive  $d$  they must approach a spacing of  $2\sqrt{d}$ .

## VI. TRANSITION MOMENTS

Let us now assume that the (diagonal) moment problem has been solved for two different states as described in the earlier sections. It will now be shown that all the transition moments are computable by a similar procedure. Defining the transition moment between the states  $i$  and  $j$  as (such that  $T^N$  exists for all  $N$  for all possible parities)

$$T^N \equiv 2 \int_0^{\infty} dx x^N \psi_i(x) \psi_j(x) \quad (30)$$

and the choice

$$g(x) = \frac{x^{N+2}}{(N+2)} \quad (31)$$

allows Eq. (2) to be written in the form

$$E = \frac{N+M+1}{N+1} \frac{T^{N+2M}}{T^N} - \frac{N(N-1)}{4} \frac{T^{N-2}}{T^N} - \frac{e^2}{(N+2)(N+1)} \frac{T^{N+2}}{T^N}, \quad (32)$$

where  $2E = E_i + E_j$  and  $2e = E_i - E_j$ .

As before, the asymptotic behavior of  $T^N$  must be determined. One easily finds that

$$T^N = t_0 Q^N(E) e^{-G(N)}, \quad (33)$$

and for the special case  $M = 2$ ,

$$G(N) = \frac{e^2}{20} \left(\frac{2}{N}\right)^{\frac{5}{3}} + \dots \quad (34)$$

Starting at large  $N$ , the  $T^N$  at successively lower values of  $N$  can be computed from (32). Thus they are completely determined at this stage of the calculation except for one overall normalization constant.

The absolute normalization of  $T^N$  can now be fixed by considering sufficiently low values of  $N$ . We must, however, discuss separately the even-even, even-odd, and odd-odd transitions. In the first case, E-E, we have

$$T^N = 2 \int_0^{\infty} dx x^N \psi_i(x) \psi_j(x) = 2 \int_0^{\infty} dx \rho_T(x) , \quad (35)$$

where  $\rho_T(0) \neq 0$ . An integration by parts yields the result

$$\lim_{N \rightarrow 2} (N-1) T^{N-2} = 2\rho_T(0) = 2\psi_i(0)\psi_j(0) , \quad (36)$$

where the relative phase between  $\psi_i$  and  $\psi_j$  is of course arbitrary. Letting  $N \rightarrow 1$  in Eq. (32) produces the condition

$$(M+2)T^{2M+1} - 2ET^1 - \frac{1}{3}e^2T^3 = \rho_T(0) \quad (37)$$

which allows the  $T$ 's to be normalized in this case, since  $\psi_i(0)$  and  $\psi_j(0)$  are given by Eq. (9).

For the E-0 transition,  $T^N$  is written as

$$T^N = 2 \int_0^{\infty} dx x^N \psi_i(x) \psi_j(x) = 2 \int_0^{\infty} dx x^{N+1} \hat{\rho}_T(x) \quad (38)$$

where a factor of  $x$  has been extracted from the odd wave function and hence  $\hat{\rho}_T(0) \neq 0$ . It follows that

$$\lim_{N \rightarrow 0} N T^{N-2} = 2\hat{\rho}_T(0) = 2\psi_i(0)\psi_j'(0)$$

and thus

$$-2(M+1)T^{2M} + 2ET^0 + e^2T^2 = \hat{\rho}_T(0) , \quad (39)$$

where  $\psi_i(0)$  and  $\psi_j'(0)$  are evaluated by using Eq. (8).

Finally, for the 0-0 transition,  $T^N$  is written as

$$T^N = 2 \int_0^{\infty} dx x^{N+2} \bar{\rho}_T(x) .$$

The limit as  $N \rightarrow -1$  of Eq. (32) yields the condition

$$MT^{2M-1} - e^{2T} = \bar{\rho}_T(0) = \psi_i'(0)\psi_j'(0) . \quad (40)$$

Thus it is possible to absolutely normalize the transition moments in terms of the normalization of the individual wave function at the origin.

Applying this method to lowest E - 0 transition, we find for the quartic oscillator  $M = 2$  that

$$\langle 0 | X | 1 \rangle = 0.600805 . \quad (41)$$

Using Eq. (32), one finds ( $N = -1$ )

$$\langle 0 | X^3 | 1 \rangle = \frac{1}{2} \langle 0 | X | 1 \rangle e^2 .$$

Higher moments are determined<sup>12</sup> by successive application of Eq. (32).

## VII. CONCLUSION

The moment method described here seems to possess many practical advantages. Among these are the simplicity of the numerical analysis and the fact that one deals directly with quantities of physical interest, the diagonal and transition moments (rather than a point-by-point description of the wave function which must then be integrated). The moments are computed with essentially the same fractional accuracy as the energy eigenvalue. This is in contrast to, for example, variational methods



which compute the energy quite efficiently but have a much larger (square root of the fractional energy error) uncertainty in the moments. In addition, there is no explicit diagonalization of large matrices required in our method.

An alternative use of the moment approach is in discussions of perturbation theory. For example, the divergence<sup>3,4</sup> of the power series expansion of a quartic perturbation of a harmonic oscillation is easily seen by examining the asymptotic moments. Similarly, if a quartic oscillation is perturbed by a quadratic term, the fractional first order change in the moments is easily seen to grow as  $\sqrt[3]{N}$ . This immediately suggests several possible alternatives to perturbation theory in which the exact recursion relations are used together with perturbation theory to increase the radius of convergence of the expansion.<sup>4</sup>

In summary, the moment approach is simple yet efficient for numerical analysis of power law potentials, and may provide an interesting basis for the discussion of more general mathematical properties. In addition, it treats the Schrödinger problem in terms of moments. This is in direct analogy with the treatment of field theory in terms of Wightman functions.

REFERENCES

1. A. M. Jaffe, Commun. Math. Phys. 1, 127 (1965).
2. C. M. Bender, T. T. Wu, Phys. Ref. 184, 1231 (1969); Phys. Rev. D 7, 1620 (1973).
3. J. J. Loeffel, A. Martin, B. Simon and A. S. Wightman, Phys. Letters 30B, 656 (1969).
4. B. Simon, Ann. Phys. 58, 76 (1970).
5. S. Graffi, V. Grecci and B. Simon, Phys. Letters 32B, 631 (1970).
6. F. W. Halpern, J. Math. Phys. 14, 219 (1973). F. W. Halpern, T. W. Yonkman, J. Math. Phys. 15, 1718 (1974).
7. C. M. Bender, K. Olaussen and P. S. Wang, Phys. Rev. D 16, 1740 (1977).
8. F. T. Hioe, D. MacMillan and E. W. Montroll, J. Math. Phys. 17, 1320 (1976).
9. C. Schwartz, Ann. Phys. 32, 277 (1965). K. Banerjee, Lett. Math. Phys. 1, 323 (1976).
10. R. J. Swenson, S. H. Danforth, J. Chem. Phys. 57, 1734 (1972).
11. J. Killingbeck, Phys. Letters 65A, 87 (1978).
12. K. Banerjee, Phys. Letters 63A, 223 (1977).
13. Using this method with  $k = 12$  and  $N_{\infty} = 900,000$  yields  $E = 1.060362090484182899647046017$  and  $Q^2 = 0.362022648788676845644761000$ .  
The first of these verifies the energy value given in Ref. 7.
14. N. W. Bazley, D. W. Fox, Phys. Rev. 124, 483 (1961).

TABLE I  
CONVERGENCE OF METHOD

$N_{\infty}$	E	$Q^2$	$ \psi(0) ^2 = \frac{2Q^3}{E}$
4	1.051533050	.367921250	.642837408
16	1.060734005	.362508956	.629372638
64	1.060356106	.362034406	.628762340
256	1.060361528	.362022473	.628751219
1024	1.060362084	.362022647	.628751368
4096	1.060362090	.362022648	.628751369
16384	1.060362090	.362022648	.628751369

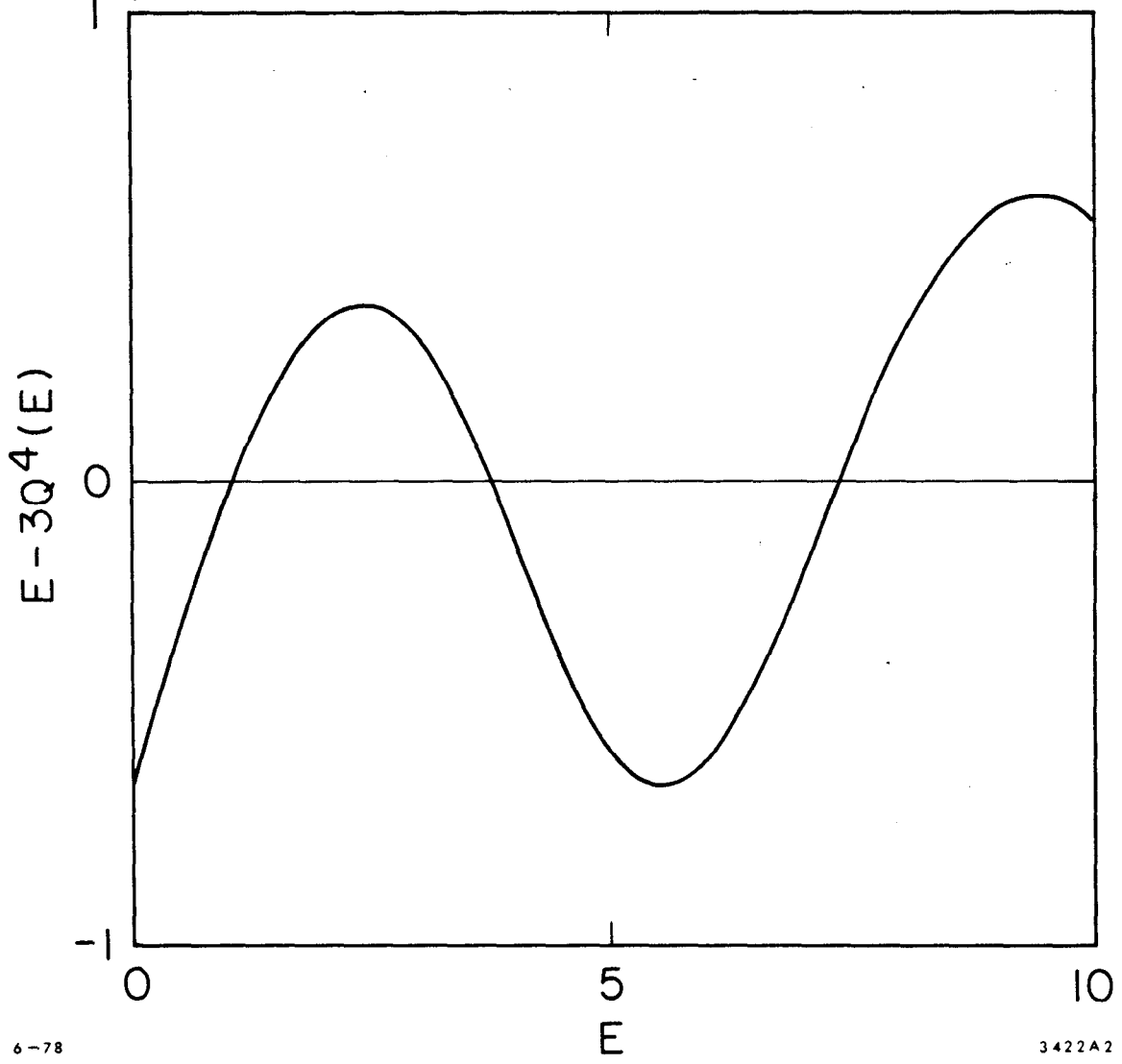
TABLE II

MOMENTS FOR FIRST THREE LEVELS OF  $H = P^2 + X^4$

	Ground	First	Second
E	1.0603620905	3.79967303	7.455698
Q <sup>1</sup>	0.4875770267	0.88301025	0.974638
Q <sup>2</sup>	0.3620226488	0.90160590	1.244714
Q <sup>3</sup>	0.3333520582	1.02458533	1.716708
Q <sup>4</sup>	0.3534540302	1.26655768	2.485233
Q <sup>5</sup>	0.4156919400	1.67757512	3.748430

FIGURE CAPTIONS

1. A graph of the virial function  $E-3Q^4(E)$  whose zeros determine the energy eigenvalues.
2. A display of the convergence properties of the method. Notice the overall convergence and the cycles of three phenomena.
3. A graph of the first two energy values of  $H = P^2 + x^4 + dx^2$  as a function of  $d$ .



6-78

3422A2

Fig. 1

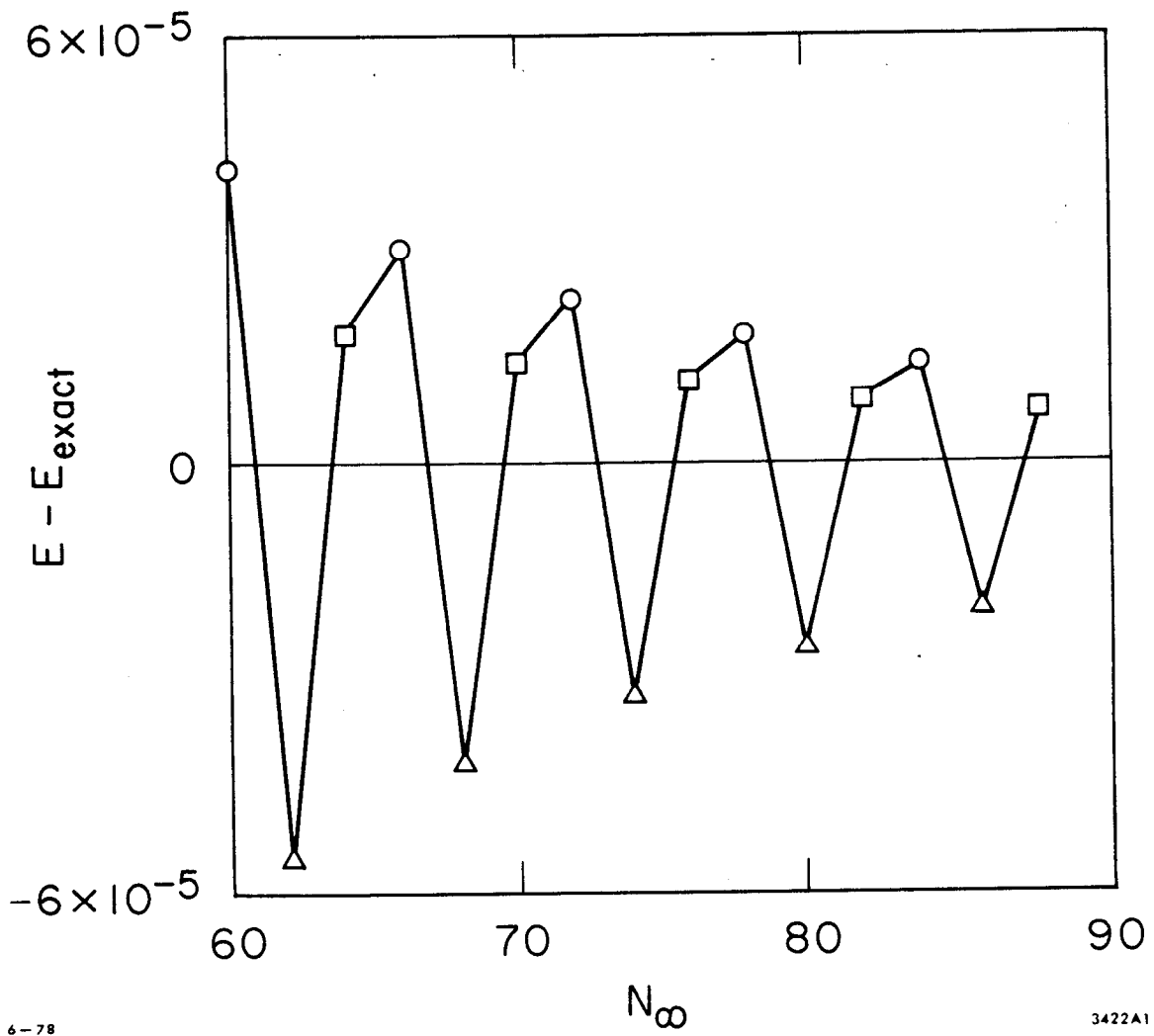


Fig. 2

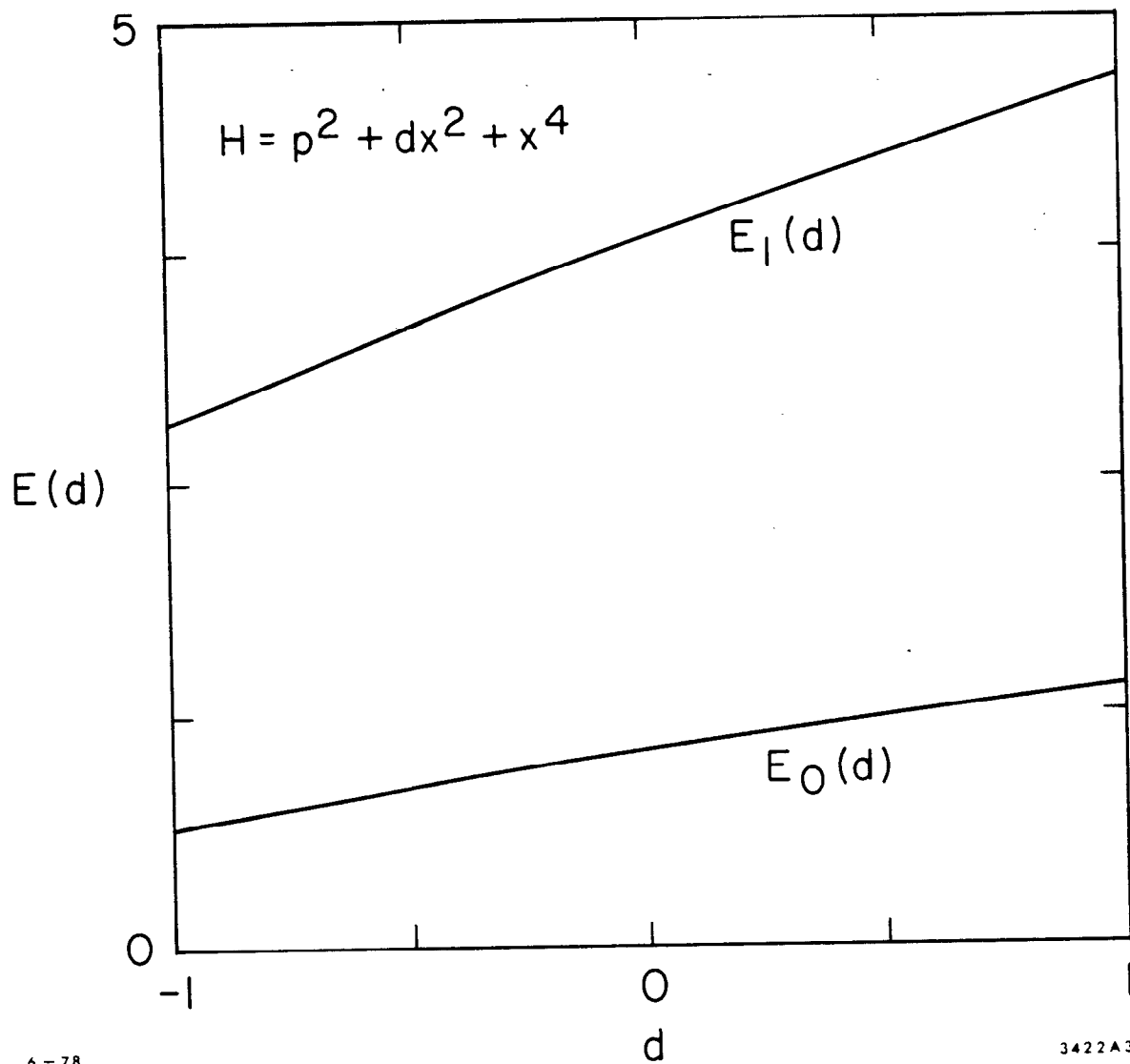


Fig. 3