MOMENT METHOD FOR EIGENVALUES AND EXPECTATION VALUES*

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ABSTRACT

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.

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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 Section 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 Section 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 Schroedinger 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, $\vec{x} = (x_1, \ldots, x_N)$. To this end we introduce the moments

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

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

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

Then

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

and

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

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

$$ES_{n_1\ldots n_N} = \langle \varphi | \left[(\nabla \cdot g) - \vec{g} \cdot \vec{g} + V \right.$$

$$+ \sum_{i=1}^{N} (2g_i(x) n_i x_i^{-1} - n_i(n_i-1)x_i^{-2}) \left] x_1^{n_1} \ldots x_N^{n_N} | \psi \rangle \quad . \tag{6}$$

If both V and g are polynomials in the x_i, then Eq. (6) is a recursion relation among the $S_{n_1, \ldots n_N}$. 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

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

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

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

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

A particularly simple choice for the trial state is

$$g(x) = bx$$

$$\varphi(x) = \exp[-\tfrac{1}{2} bx^2] \quad , \tag{9}$$

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

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

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 $n \geq M \ggg 1$. 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

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

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

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

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 side 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 non-zero S_n can be written in the form

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

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 Schroedinger equation to get an equation for χ:

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

For large positive x we find

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

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

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

The only saddle point relevant to our integral is the one as

$x \approx n^{1/3} - b/3$ which gives[4]

$$S_n = n^{\frac{n}{3}} e^{-\frac{n}{3}} \exp\left[-\frac{1}{2}bn^{2/3} + (f^2 + \frac{2}{3}b^2)n^{1/3} + O(n^{-1/3})\right] \quad (17)$$

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

$$S_n^{\pm} = e^{\pm\frac{2\pi in}{3}} n^{\frac{n}{3}} e^{-\frac{n}{3}} \exp\left[-\frac{1}{2}bn^{2/3}e^{\pm\frac{4\pi in}{3}}\right.$$

$$+ n^{1/3}e^{\pm\frac{2\pi in}{3}}(f^2 + \frac{1}{3}b^2 e^{\pm\frac{2\pi in}{3}} - \frac{1}{6}b^2 e^{\pm\frac{2\pi in}{3}}$$

$$\left. + O(n^{-1/3})\right] \qquad (18)$$

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 $\exp(-\frac{3}{4}bM^{2/3})$ 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 one 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 asymptotic form of the S_n.

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

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

Equation (10) can be rewritten in the form

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

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

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

and

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

The R_n have the asymptotic expansion

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

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 Section III.

In the proceeding 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

$$g(x) = x|x| + bx$$

$$\varphi(x) = \exp\left[-\frac{1}{3}|x|^3 - \frac{1}{2}bx^2\right] \ .$$

(22)

We define the moments for even parity eigenstates to be

$$S_n = \langle\varphi||x|^n|\psi\rangle = 2\int_0^\infty dx \ \varphi(x)\psi(x)x^n$$

(23)

and for odd parity states to be

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

(24)

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

$$2bS_{n+3} + (2f^2+b^2)S_{n+2} - 2(n+1)S_{n+1}$$

(25)

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

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

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

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

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

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,

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

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

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

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

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

$$g(x) = x|x|(x^2+2f^2b)$$

$$\varphi(x) = \exp\left[-\tfrac{1}{5}|x|^5 - \tfrac{2}{3}f^2b|x|^3\right] \quad . \tag{30}$$

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

$$4f^2(b+1)S_{n+6} - 2f^4(3-2b^2)S_{n+4} - 2(n+2)S_{n+3}$$

$$+ 4f^6S_{n+2} - 4f^2b(n+1)S_{n+1} + (E-f^8)S_n + n(n-1)S_{n-2} = 0 \tag{31}$$

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 the asymptotic expansion

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

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

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

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

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

It is convenient to introduce the variables

$$p_{1,2} = 2^{-1/2}(p_x \pm p_y)$$

$$x_{1,2} = 2^{-1/2}(x \pm y) \qquad (35)$$

and rewrite the Hamiltonian in the form

$$H = p_1^2 + p_2^2 + \frac{1}{2}(x_1^2 - 2f^2)^2 + \frac{1}{2}(x_2^2 - 2(f^2-\Delta))^2$$

$$+ 3x_1^2 x_2^2 - 2(f^2-\Delta)^2 \ . \qquad (36)$$

Clearly the energy eigenstates $\psi(x_1,x_2)$ will be either even or odd under the separate symmetry operations $x_1 \rightarrow -x_1$ and $x_2 \rightarrow -x_2$. 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

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

or $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad$ (37)

$$\varphi(x_1, x_2) = \exp\left[-\frac{1}{2} b_1 x_1^2 - \frac{1}{2} b_2 x_2^2\right] \ ,$$

then the moments

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

will be non-zero 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

$$\frac{1}{2}(S_{n_1+4,n_2} + 6S_{n_1+2,n_2+2} + S_{n_1,n_2+4})$$

$$- (2f^2 + b_1^2) S_{n_1+2,n_2} - (2f^2 - 2\Delta + b_2^2) S_{n_1,n_2+2}$$

$$\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad (39)$$

$$+ [(2n_1+1)b_1 + (2n_2+1)b_2 + 2f^4] S_{n_1,n_2}$$

$$- n_1(n_1-1) S_{n_1-2,n_2} - n_2(n_2-1) S_{n_1,n_2-2} = E S_{n_1,n_2}$$

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 $n_1 + n_2 \leq M-4$,

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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

$$[\tfrac{1}{2} R^1_{n_1+2,n_2} + \tfrac{3}{2} R^2_{n_1+2,n_2} - 2f^2 - b_1^2] S_{n_1+2,n_2}$$

$$+ [\tfrac{1}{2} R^2_{n_1,n_2+2} + \tfrac{3}{2} R^1_{n_1,n_2+2} - 2f^2 + 2\Delta - b_2^2] S_{n_1,n_2+2}$$

$$+ [b_1(2n_1+1) + b_2(2n_2+1) + 2f^4] S_{n_1,n_2} \tag{40}$$

$$- n_1(n_1-1) S_{n_1-2,n_2} - n_2(n_2-1) S_{n_1,n_2-2} = E S_{n_1,n_2} \quad,$$

where

$$R^1_{n_1,n_2} = \tilde{S}_{n_1+2,n_2} / \tilde{S}_{n_1,n_2}$$

$$\tag{41}$$

$$R^2_{n_1 n_2} = \tilde{S}_{n_1,n_2+2} / \tilde{S}_{n_1,n_2}$$

Similarly for $n_1 + n_2 = M$ we have

$$[b_1(2n_1+1) + b_2(2n_2+1) + 2f^4 - (2f^2 + b_1^2) R^1_{n_1,n_2}$$

$$- (2f^2 - \Delta + b_2^2) R^2_{n_1,n_2} + \tfrac{1}{2} R^1_{n_1,n_2} R^1_{n_1+2,n_2} + \tfrac{1}{2} R^2_{n_1,n_2} R^2_{n_1,n_2+2}$$

$$+ \tfrac{3}{2} R^1_{n_1 n_2} R^2_{n_1+2,n_2} + \tfrac{3}{2} R^2_{n_1 n_2} R^1_{n_1,n_2+2}] S_{n_1 n_2} \tag{42}$$

$$- n_1(n_1-1) S_{n_1-2,n_2} - n_2(n_2-1) S_{n_1,n_2-2} = E S_{n_1,n_2} \quad.$$

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 $S_{n_1 n_2}$. 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

$$\widetilde{H}S = ES \quad , \tag{43}$$

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 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 $\widetilde{S}_{n_1, n_2}$ approach the S_{n_1, n_2} rapidly as $n_1 + n_2$ increases. The first step in obtaining the $\widetilde{S}_{n_1, n_2}$ is to notice that

$$\psi(x,y) \approx \exp\left[-\frac{1}{3}(x^3 + y^3) + (f^2 - \frac{1}{2}\Delta)(x+y)\right.$$

$$\left. + \Delta(xy(x-y)^{-1})\ln(x/y)\right] \tag{44}$$

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

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$n_1 \geq n_2$ 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

$$H = H_0 - 2\Delta xy \qquad (45)$$

and Eq. (37) as

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

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

$$
\begin{aligned}
S^0_{n_1,n_2} &= \langle\varphi_0|x^{n_1}x^{n_2}|\psi_0\rangle = \langle\varphi_0|\left(\frac{x+y}{\sqrt{2}}\right)^{n_1}\left(\frac{x-y}{\sqrt{2}}\right)^{n_2}|\psi_0\rangle \\[2mm]
&= 2^{-\frac{1}{2}(n_1+n_2)} \sum_{k_1=0}^{n_1} \sum_{k_2=0}^{n_2} S_{k_1+k_2} S_{n_1+n_2-k_1-k_2}
\end{aligned}
\qquad (47)
$$

$$(-)^{n_2-k_2} n_1! n_2! \ / \ [k_1! k_2! (n_1-k_1)! (n_2-k_2)!] \ ,$$

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 $\exp\left[-1/4(b_1 + b_2)x^2\right]$.

We use the saddle point only to calculate the ratio $\tilde{S}_{n_1 n_2}/S^0_{n_1 n_2}$. Our final result is

$$\tilde{S}_{n_1,n_2} = S^o_{n_1,n_2} \exp[\Delta(n_1-n_2)(8n_1-4n_2)^{-1/6}n_2^{-1/2}$$

$$\cdot \ln[(n_1+(2n_1n_2-n_2^2)^{\frac{1}{2}})(n_1-n_2)^{-\frac{1}{2}}] \tag{48}$$

$$- (b_1-b_2)(n_1-n_2)(4n_1-2n_2)^{-1/3}] \quad .$$

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 Figures 3-5.

III. DISCUSSION

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

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

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 Schroedinger 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.

REFERENCES AND FOOTNOTES

1) J.L. Richardson and R. Blankenbecler, Phys. Rev. $\underline{D19}$, 496 (1979). The techniques used in this paper are related to work by R.J. Swenson and S.H. Danforth, J. Chem. Phys. $\underline{57}$, 1734 (1972); J. Killingbeck, Phys. Lett. $\underline{65A}$, 87 (1978) and K. Banerjee, Phys. Lett. $\underline{63A}$, 223 (1977). For an alternate formulation and earlier references, see C.A. Uzes, Phys. Rev. $\underline{D14}$, 3362 (1976).

2) B. Simon, Ann. Phys. (N.Y.) $\underline{58}$, 76 (1970); S. Graffi, V. Grecchi and B. Simon, Phys. Lett. $\underline{32}$, 631 (1970); C. Bender, K. Olaussen, P. Wang, Phys. Rev. $\underline{D16}$, 1740 (1977). See also W. Caswell, preprint Brown-HET-382 (1979) plus references therein.

3) L.N. Lipatov, Zh. Exp. Theor. Fiz. Pis'ma Red. $\underline{25}$, 116 (1977), (JETP Lett. $\underline{25}$, 104 (1977)); E. Brézin, J.C. LeGuillou, and J. Zinn-Justin, Phys. Rev. $\underline{D15}$, 1544 (1977); G. Parisi, Phys. Lett. $\underline{66B}$, 167 (1977); E. Brézin, G. Parisi, and J. Zinn-Justin, Phys. Rev. $\underline{D16}$, 408 (1977); E. Gildener and A. Patrascioiu, Phys. Rev. $\underline{D16}$, 423 (1977); B. Harrington, Phys. Rev. $\underline{D18}$, 2982 (1978).

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: $M^{2/3} \geqslant f^2$. 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, preprint SLAC-PUB-2317 (April, 1979).

TABLE CAPTIONS

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.

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

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

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.

Table I

$$E_O(f^2=2)$$

R_M	M = 10	M = 20	M = 50	M = 200
R_M(Eq.20)	2.30	2.283	2.2896497	2.2896495
$R_M = M^{2/3}$	2.37	2.280	2.289650	2.2896495
$R_M = 2M^{2/3}$	3.04	2.276	2.289652	2.2896495
$R_M = 0$	2.54	2.31	2.289650	2.2896495

$$E_O(f^2 = 0)$$

R_M(Eq.20)	1.063	1.06037	1.0603621	1.0603621
$R_M = M^{2/3}$	1.064	1.06038	1.0603621	1.0603621
$R_M = 2M^{2/3}$	1.059	1.06035	1.0603621	1.0603621
$R_M = 0$	1.054	1.06030	1.0603621	1.0603621

Table II

f^2	E_0	E_1
5	4.36642329	4.3664531
4	3.8636669	3.8651857
3	3.2518095	3.2932075
2	2.2896495	2.7520771
1	1.1377858	2.7130279
0	1.0603621	3.7996730
-1	2.6778265	6.4098280

Table III

f^2	E_0	E_1
4	6.5175	6.5175
3	5.2753	5.2753
2	3.743	3.800
1	1.1704	3.14
0	1.225826	4.80
-1	3.8412	10.1583

Table IV

$$\Delta = 1.0$$

M	$E_0(f^2 = 0)$	$E_1(f^2 = 0)$
8	2.74	5.3409
10	2.7260	5.3417
12	2.7251	5.3403
14	2.72566	5.340079
16	2.72567	5.340083
18	2.725630	5.340090
20	2.7256350	5.3400936
22	2.7256364	5.3400938
24	2.7256353	5.3400935
	$E_0(f^2 = 2)$	$E_1(f^2 = 2)$
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	5.4936
20	5.3906	5.49455
22	5.39092	5.49446
24	5.39149	5.49429

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

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

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.
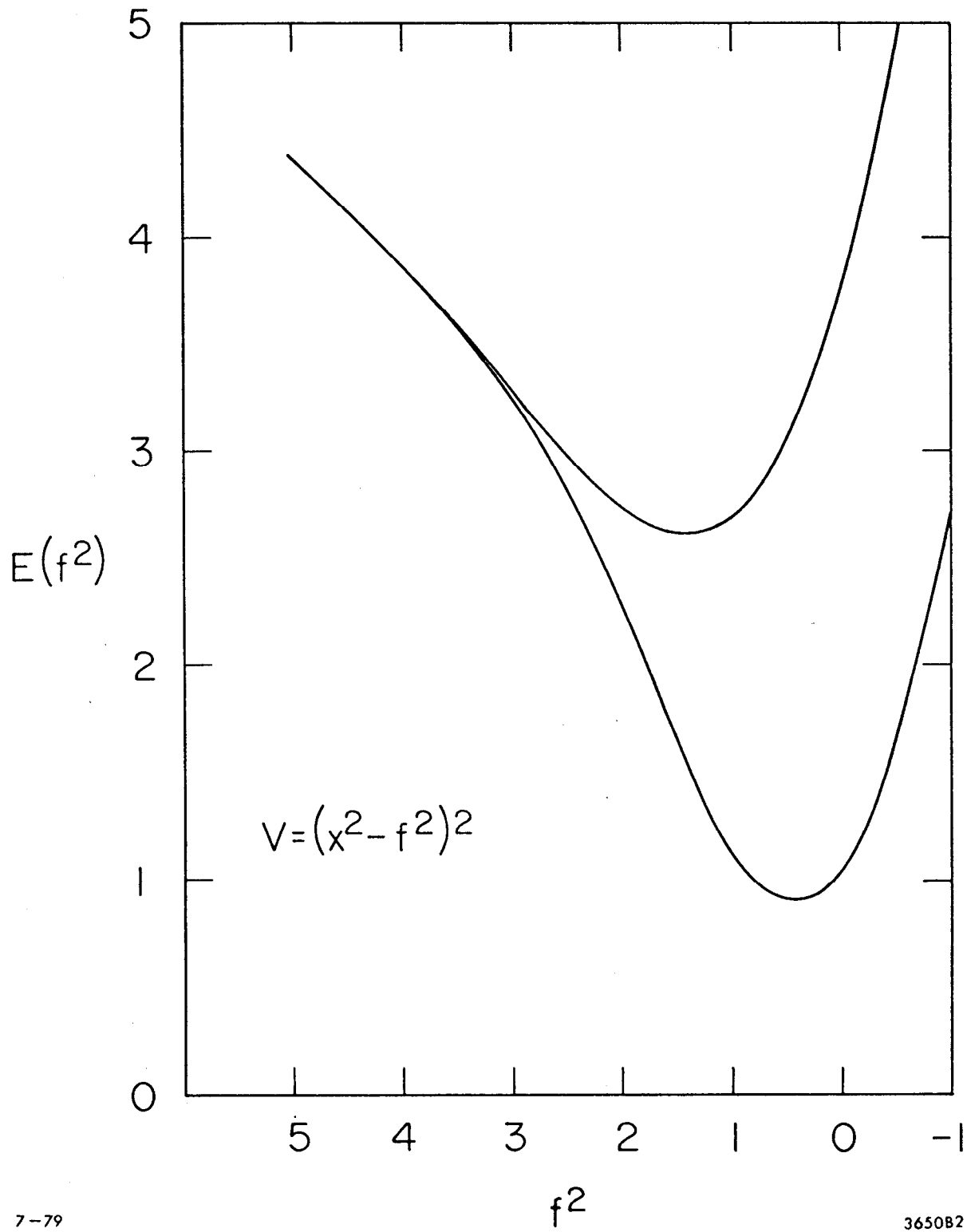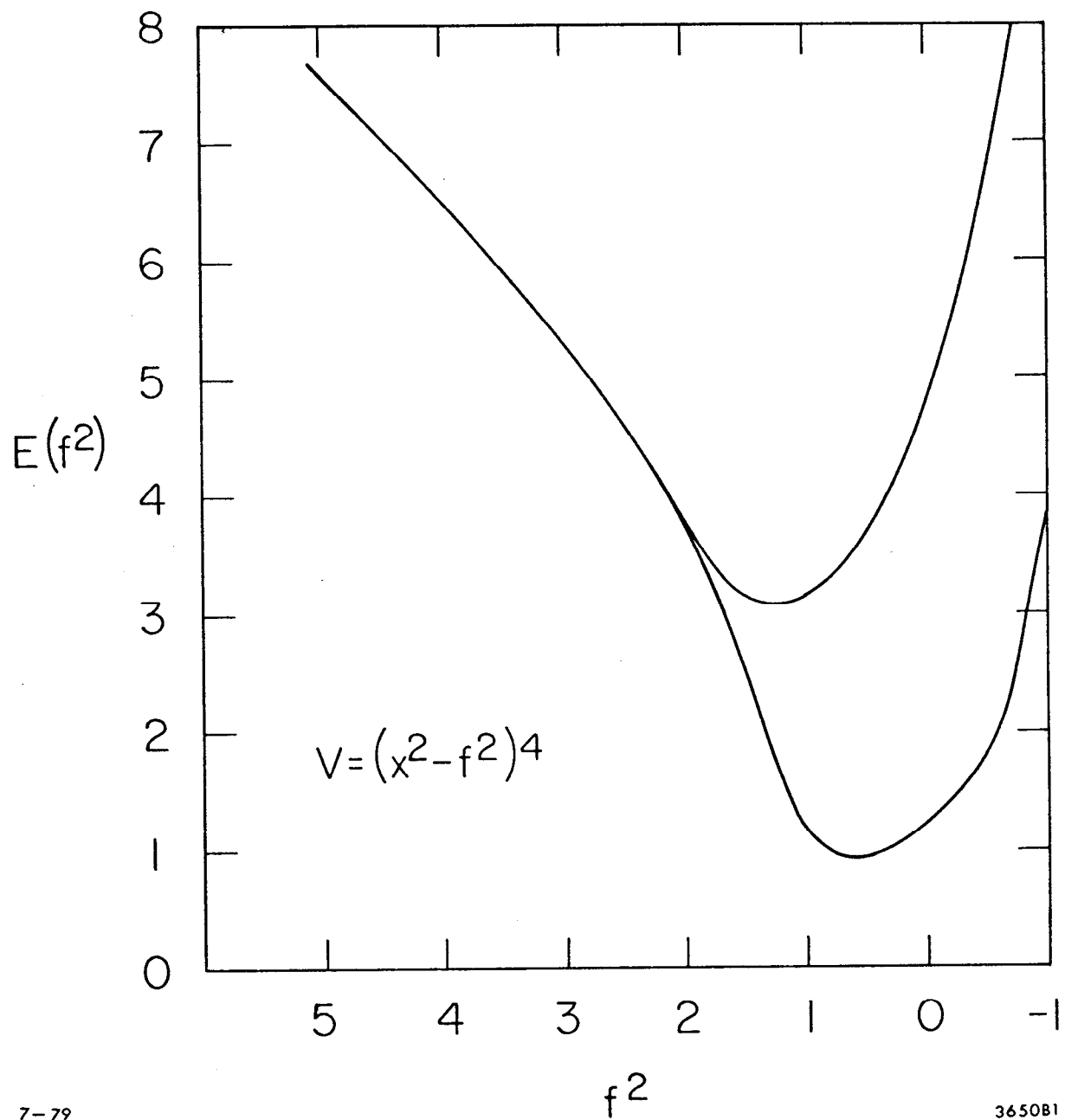
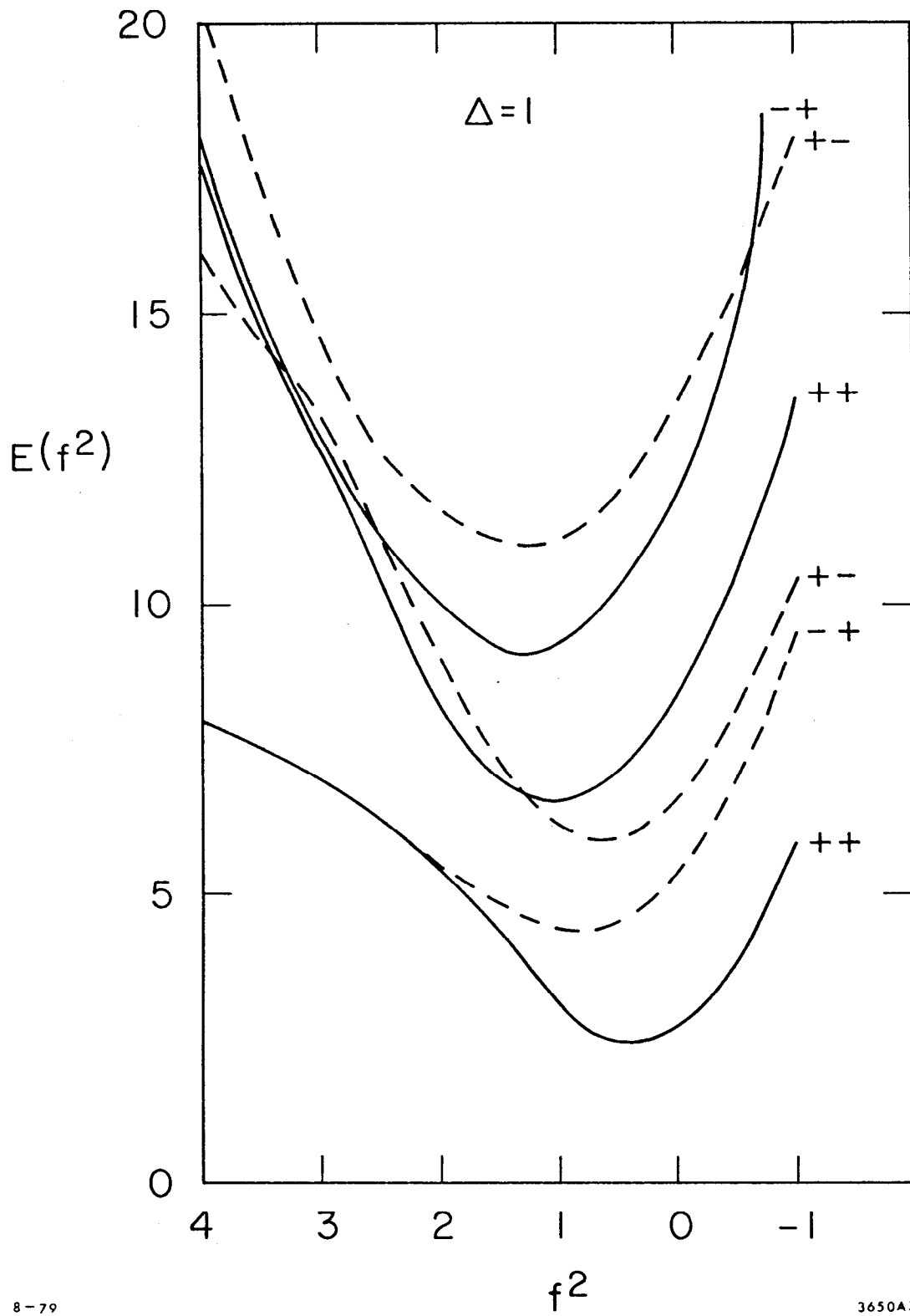$$E(f^2)$$

$$V = (x^2 - f^2)^2$$

$$f^2$$

7-79

3650B2

Fig. 1

$$V = (x^2 - f^2)^4$$

Fig. 2

7-79

3650B1

$\Delta = 1$

$E(f^2)$

Fig. 3

$$V = (x^2 - f^2)^2 + (y^2 - f^2)^2 + \Delta(x-y)^2$$
$$f^2 = 0$$

8-79

365084

Fig. 4

$$V = (x^2 - f^2)^2 + (y^2 - f^2)^2 + \Delta (x - y)^2$$
$$f^2 = 2$$

8−79

3650A5

Fig. 5