Improved Hill determinant method: General approach to the solution of quantum anharmonic oscillators

R. N. Chaudhuri and M. Mondal
Department of Physics, Visva-Bharati University, Santiniketan 731 235, West Bengal, India
(Received 5 April 1990; revised manuscript received 22 August 1990)

The improved Hill determinant method with a variational parameter is applied to the general polynomial quantum anharmonic-oscillator and multiwell-oscillator problems. We calculate the eigenvalues and the expectation values $\langle x^{2m}\rangle$ of the oscillator, which are in good agreement with the exact values obtained by using supersymmetric quantum mechanics.

I. INTRODUCTION

Recently[1] it has been shown in the context of the sextic oscillator that the Hill determinant method[2–9] is improved remarkably if the variational parameter introduced in the Hamiltonian is adjusted properly. It removes the difficulties encountered by various authors[3–5] in connection with the Hill determinant method and also makes the eigenvalues (E) rapidly convergent for a small size of the determinant. Here we apply the same technique to the much more complicated problems of the general quantum anharmonic and multiwell oscillators of type

$$V(x)=\sum_{m=1}^{N} b_{2m}x^{2m} . \tag{1}$$

If a potential term λx^{2m} is added to the Hamiltonian the change in energy according to first-order perturbation theory is

$$\Delta E=\lambda\langle x^{2m}\rangle , \tag{2}$$

where λ is sufficiently small that the first-order perturbation result is quite accurate. We calculate E and ΔE and hence $\langle x^{2m}\rangle$ by application of the Hill determinant method.[7,10] We compare our results of eigenvalues and $\langle x^{2m}\rangle$ obtained by the modified Hill determinant method with those given by supersymmetric quantum mechanics.[11,12] It is found that the agreement is excellent, even for a determinant of small size.

II. GENERAL POLYNOMIAL POTENTIAL

The harmonic term βx^2 is added to and subtracted from the potential (1), and then the Hamiltonian

$$H=-\frac{d^2}{dx^2}+(b_2+\beta)x^2+\sum_{m=2}^{N} b_{2m}x^{2m}-\beta x^2 \tag{3}$$

is expressed in terms of creation and annihilation operators:

$$H=(a^\dagger a+\tfrac{1}{2})\omega+\sum_{m=2}^{N}\frac{b_{2m}}{\omega^m}(a^\dagger+a)^{2m}-\frac{\beta}{\omega}(a^\dagger+a)^2 , \tag{4}$$

where $\omega=2(b_2+\beta)^{1/2}$. We expand $(a^\dagger+a)^{2m}$ and use the following identity:

$$a[(a^\dagger)^n a^m]=n(a^\dagger)^{n-1}a^m+(a^\dagger)^n a^{m+1}, \quad n,m\geq 0 \tag{5}$$

to express the terms in (4) in normal ordering so that the creation operators stand to the left of the annihilation operators.

In order to determine the unknown parameters β or ω we set the coefficients of a^2 and $(a^\dagger)^2$ to zero so that the matrix elements $\langle 2|H|0\rangle=\langle 0|H|2\rangle=0$. This procedure has been used for a long time in nuclear physics[13] to find the most effective Hamiltonian. We use the orthonormal basis vectors

$$|m\rangle=(m!)^{-1/2}(a^\dagger)^m|0\rangle ,$$

having the following properties:

$$a^\dagger|m\rangle=(m+1)^{1/2}|m+1\rangle, \quad a|m\rangle=m^{1/2}|m-1\rangle .$$

We now expand the wave function ψ in terms of the basis vectors $|m\rangle$ as

$$\psi=\sum_{m=0}^{\infty} A_m|m\rangle \tag{6}$$

and use the equation $H\psi=E\psi$, where H is the modified Hamiltonian (4). The coefficients A_m of Eq. (6) satisfy a $(2N+1)$-term recurrence relation of type

$$\sum_{l=0}^{2N} P_k^{(l)}A_{k-2N+2l}=0, \quad k\geq 0$$

$$A_{-1}=A_{-2}=A_{-3}=\cdots=0 \tag{7}$$

where $P_k^{(l)}$ are the functions of E and the coupling constants b_{2m}. The eigenvalue condition of the Hill determinant for large n is

$$\det D_n=0 , \tag{8}$$

with

$$D_n=\begin{vmatrix} P_\nu^{(N)} & P_\nu^{(N+1)} & P_\nu^{(N+2)} & \cdots & P_\nu^{(2N)} & 0 & 0 & \cdots \\ P_{2+\nu}^{(N-1)} & P_{2+\nu}^{(N)} & P_{2+\nu}^{(N+1)} & \cdots & P_{2+\nu}^{(2N-1)} & P_{2+\nu}^{(2N)} & 0 & \cdots \\ \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots & \\ P_{2N+\nu}^{(0)} & P_{2N+\nu}^{(1)} & P_{2N+\nu}^{(2)} & \cdots & P_{2N+\nu}^{(N)} & P_{2N+\nu}^{(N+1)} & P_{2N+\nu}^{(N+2)} & \cdots \\ 0 & P_{2N+2+\nu}^{(0)} & P_{2N+2+\nu}^{(1)} & \cdots & P_{2N+2+\nu}^{(N-1)} & P_{2N+2+\nu}^{(N)} & P_{2N+2+\nu}^{(N+1)} & \cdots \\ \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots & \end{vmatrix}, \tag{9}$$

where $\nu=0$ for even-parity eigenvalues and $\nu=1$ for those of odd parity. The zeros of D_n as a function of the parameter E give the energy eigenvalues of the problem.

Let us consider the example of $N=5$ with the potential

$$V(x)=b_2x^2+b_4x^4+b_6x^6+b_8x^8+b_{10}x^{10} . \tag{10}$$

Now the coefficients $P_k^{(l)}$ are given by

$$P_k^{(0)}=\frac{b_{10}}{\omega^5}[(k-9)(k-8)\cdots(k-1)k]^{1/2} , \tag{11a}$$

$$P_k^{(1)}=\frac{1}{\omega^5}[5b_{10}(2k-7)+b_8\omega][(k-7)(k-6)\cdots k]^{1/2} , \tag{11b}$$

$$P_k^{(2)}=\frac{1}{\omega^5}[45b_{10}(k^2-5k+8)+4b_8\omega(2k-5)+b_6\omega^2][(k-5)(k-4)\cdots k]^{1/2} , \tag{11c}$$

$$\begin{aligned}P_k^{(3)}=\frac{1}{\omega^5}\{&30b_{10}[4(k-4)(k-5)(k-6)+42(k-4)(k-5)+126(k-4)+105]\\&+14b_8\omega[2(k-4)(k-5)+12(k-4)+15]+[15b_6\omega^2+b_4\omega^3+6b_6\omega^2(k-4)]\}[(k-3)(k-2)\cdots k]^{1/2} ,\end{aligned} \tag{11d}$$

$$\begin{aligned}P_k^{(4)}=\frac{k-2}{\omega^5}\{&210b_{10}[(k-3)(k-4)(k-5)+12(k-3)(k-4)+45(k-3)+60]\\&+28b_8\omega[2(k-3)(k-4)+15(k-3)+30]+[15b_6\omega^2(k+1)+4b_4\omega^3]\}[(k-1)k]^{1/2} ,\end{aligned} \tag{11e}$$

$$\begin{aligned}P_k^{(5)}=&\frac{b_{10}}{\omega^5}k(k-1)[252(k-2)(k-3)(k-4)+3150(k-2)(k-3)+12\,600(k-2)+18\,900]\\&+\frac{b_8}{\omega^4}k(k-1)[70(k-2)(k-3)+560(k-2)+1260]+k(k-1)\left[\frac{10b_6}{\omega^3}(5+2k)+\frac{6b_4}{\omega^2}\right]\\&+\frac{945b_{10}}{\omega^5}+\frac{105b_8}{\omega^4}+\frac{15b_6}{\omega^3}+\frac{3b_4}{\omega^2}+\frac{b_2}{\omega}+(k+1/4)\omega-E ,\end{aligned} \tag{11f}$$

$$\begin{aligned}P_k^{(6)}=\Bigg[&\frac{b_{10}}{\omega^5}[210k(k-1)(k-2)(k-3)+2520k(k-1)(k-2)+9450k(k-1)+12\,600k]\\&+\frac{b_8}{\omega^4}[56k(k-1)(k-2)+420k(k-1)+840k]+k\left[\frac{15}{\omega^3}b_6(3+k)+\frac{4}{\omega^2}b_4\right]\Bigg][(k+2)(k+1)]^{1/2} ,\end{aligned} \tag{11g}$$

$$\begin{aligned}P_k^{(7)}=\Bigg[&\frac{b_{10}}{\omega^5}[120k(k-1)(k-2)+1260k(k-1)+3780k+3150]+\frac{b_8}{\omega^4}[28k(k-1)+168k+210]\\&+\left[\frac{3b_6}{\omega^3}(5+2k)+\frac{b_4}{\omega^2}\right]\Bigg][(k+4)(k+3)\cdots(k+1)]^{1/2} ,\end{aligned} \tag{11h}$$

$$P_k^{(8)}=\left[\frac{b_{10}}{\omega^5}[45k(k-1)+360k+630]+\frac{b_8}{\omega^4}(8k+28)+\frac{b_6}{\omega^3}\right][(k+6)(k+5)\cdots(k+1)]^{1/2} , \tag{11i}$$

$$P_k^{(9)}=\left[\frac{b_{10}}{\omega^5}(10k+45)+\frac{b_8}{\omega^4}\right][(k+8)(k+7)\cdots(k+1)]^{1/2} , \tag{11j}$$

$$P_k^{(10)}=\frac{b_{10}}{\omega^5}[(k+10)(k+9)\cdots(k+1)]^{1/2} . \tag{11k}$$

The unknown parameter ω is determined from the positive root of the equation

$$\omega^6-4b_2\omega^4-24b_4\omega^3-180b_6\omega^2 -1680b_8\omega-18\,900b_{10}=0\ . \quad (12)$$

In Table I we present the first four eigenvalues of the potential $b_2x^2+b_4x^4$ for different values of the coupling constant b_4 and the pure x^4 oscillators, as obtained by the modified Hill determinant method, and compare our results with the exact values.[14–18] We have shown in parentheses the roots of the Hill determinant without the variational parameter ($\beta=0$ or $\omega=2$). The modified Hill determinant method produces excellent results for the small size of the determinant. In Fig. 1 the first four eigenvalues of the general $x^2+\lambda x^{2m}$ oscillators are plotted on log scales against λ for $m=3,4,5$. For $m=2$ we have shown the first ten eigenvalues. It appears from the figure that the eigenvalues for any particular m form a family of almost parallel lines on log scales. We also consider the double-well oscillators of type $-x^2+b_{2m}x^{2m}$ with $m=2,3,4,5$ and compare our eigenvalues in Table II with those available in the literature.

III. SUPERSYMMETRIC POTENTIAL

With the function

$$W(x)=\sum_{n=-1}^{N} a_{2n+1}x^{2n+1}\ , \quad (13)$$

we construct the superpotential

$$V_-(x)=W^2(x)-W'(x) =a_{-1}(a_{-1}+1)/x^2+a_1(2a_{-1}-1)+\cdots\ , \quad (14)$$

which has zero energy solution. The corresponding eigenfunction is given by

$$\psi(x)=\exp\left[-\int^x W(x)dx\right] =x^{-a_{-1}}\exp(-a_1x^2/2-a_3x^4/4-\cdots)\ . \quad (15)$$

TABLE I. Comparison of the first four eigenvalues of the potential $b_2x^2+b_4x^4$ obtained by the method of the modified Hill determinant (sizes 5×5, 9×9, and 15×15) with the exact values (Ref. 14 for $b_2=1$ and Ref. 15 for $b_2=0$). The roots of the Hill determinant for $\beta=0$ are given in parentheses for $b_2=1$ and $b_4=100$.

		Modified Hill determinant method			
b_2	b_4	5×5	9×9	15×15	Exact
1	0.1	1.065 286	1.065 286	1.065 286	1.065 286
		3.306 874	3.306 872	3.306 872	3.306 872
		5.747 972	5.747 959	5.747 959	5.747 959
		8.352 807	8.352 678	8.352 678	8.352 678
	1.0	1.392 375	1.392 352	1.392 352	1.392 352
		4.648 859	4.648 813	4.648 813	4.648 813
		8.658 153	8.655 053	8.655 050	8.655 050
		13.168 490	13.156 825	13.156 804	13.156 804
	10.0	2.449 316	2.449 174	2.449 174	2.449 174
		8.599 180	8.599 004	8.599 004	8.599 003
		16.653 640	16.635 966	16.635 922	16.635 921
		25.856 760	25.806 447	25.806 277	25.806 276
	100.0	4.999 800	4.999 419	4.999 418	4.999 418
		(8.084 645)	(5.284 808)	(5.020 073)	
		17.830 643	17.830 194	17.830 193	17.830 192
		(44.731 982)	(22.964 396)	(18.164 436)	
		34.920 733	34.874 124	34.873 985	34.873 984
		(190.147 547)	(72.236 102)	(40.687 879)	
		54.509 913	54.385 763	54.385 292	54.385 292
		(440.514 468)	(165.533 068)	(79.872 450)	
	1000.0	10.640 654	10.639 791	10.639 789	10.639 789
		38.087 843	38.086 836	38.086 834	38.086 833
		74.786 571	74.681 729	74.681 404	74.681 404
		116.879 465	116.604 266	116.603 200	116.603 199
0	1	1.060 450	1.060 362	1.060 362	1.060 362
		3.799 775	3.799 673	3.799 673	3.799 673
		7.466 340	7.455 731	7.455 698	7.455 698
		11.672 588	11.644 854	11.644 746	11.644 746

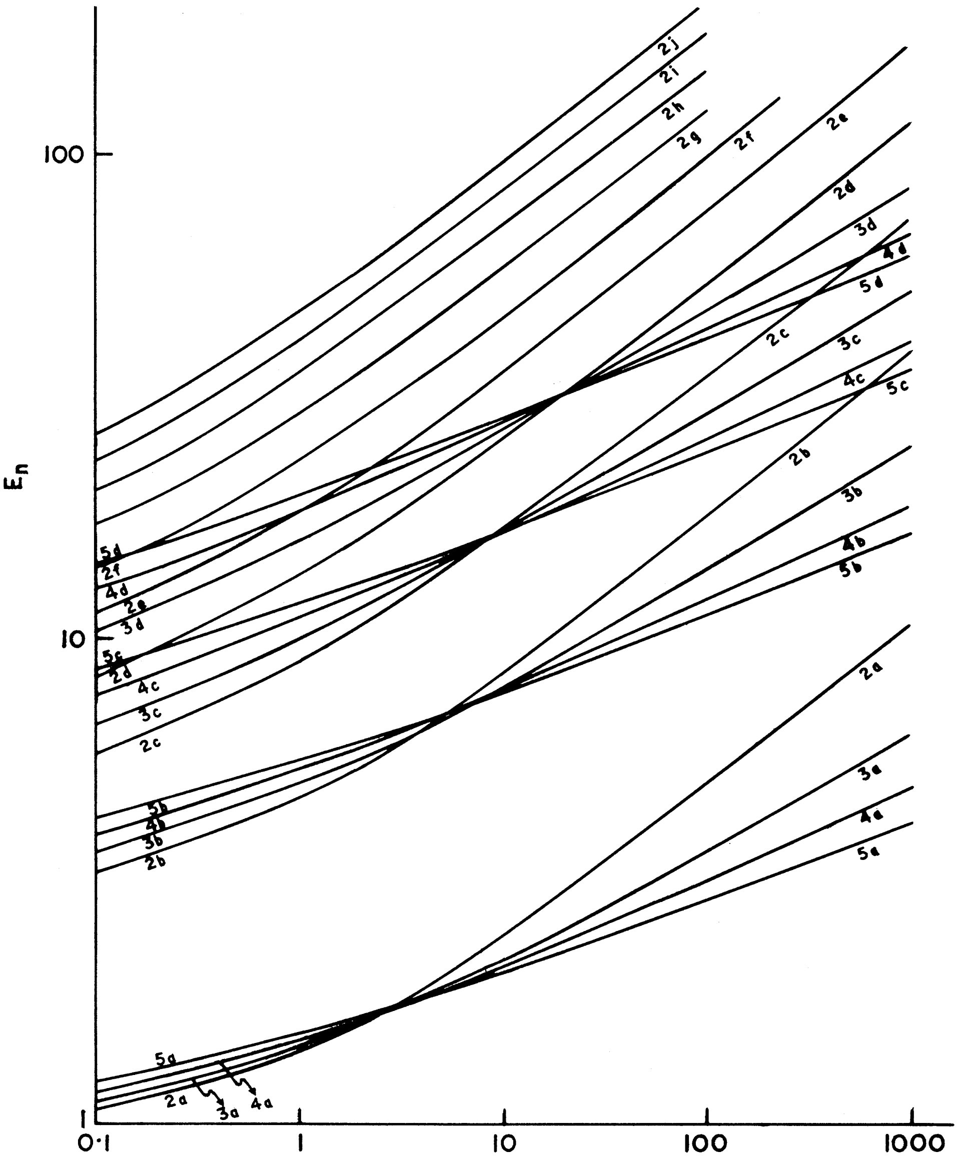

FIG. 1. The eigenvalues E_n of the oscillators $x^2+\lambda x^{2m}$ are plotted against the anharmonic coupling λ for $m=2,3,4,5$. The eigenvalues are designated as $ma, mb, mc, \ldots,$ where the letters $a, b, c, \ldots,$ correspond, respectively, to the first, second, third, . . . , eigenvalues.

If we compare the anharmonic-oscillator potential (1) with the supersymmetric potential $V_-(x)-a_1(2a_{-1}-1)$ we shall obtain the relations satisfied by the parameters a_i. With some choice of a_i we construct the following supersymmetric potentials having exact eigenvalues and eigenfunctions:

$$A(x)=x^2-4x^4+x^6\ ,$$
$$\psi_0(x)=N\exp(x^2-x^4/4)\ , \tag{16}$$
$$E_0=-2\ ;$$

$$B(x)=4x^2-6x^4+x^6\ ,$$
$$\psi_1(x)=Nx\exp(3x^2/2-x^4/4)\ , \tag{17}$$
$$E_1=-9\ ;$$

$$C(x)=\tfrac{105}{64}x^2-\tfrac{43}{8}x^4+x^6-x^8+x^{10}\ ,$$
$$\psi_0(x)=N\exp(-3x^2/16+x^4/8-x^6/6)\ , \tag{18}$$
$$E_0=3/8\ ;$$

$$D(x)=\tfrac{169}{64}x^2-\tfrac{59}{8}x^4+x^6-x^8+x^{10}\ ,$$
$$\psi_1(x)=Nx\exp(-3x^2/16+x^4/8-x^6/6)\ , \tag{19}$$
$$E_1=\tfrac{9}{8}\ .$$

TABLE II. The first four eigenenergies of the double-well oscillator $-x^2+0.1x^{2m}$ with $m=2$, 3, 4, and 5.

m	Modified Hill determinant method 11×11	35×35	40×40	Other methods
2	−1.264 252	−1.265 492	−1.265 492	−1.265 493[a]
	−1.149 333	−1.153 058	−1.153 058	−1.153 059[a]
	0.517 939	0.509 489	0.509 489	0.509 489[a]
	1.559 178	1.543 547	1.543 547	1.543 546[a]
3	−0.043 980	−0.044 241	−0.044 241	−0.044 24[b]
	1.006 662	1.006 304	1.006 304	1.006 30[b]
	3.460 108	3.457 038	3.457 038	3.457 04[b]
	6.476 112	6.467 915	6.467 915	6.467 91[b]
4	0.275 954	0.275 400	0.275 400	0.275[b]
	1.946 439	1.944 248	1.944 248	1.944[b]
	5.271 966	5.265 731	5.265 731	5.266[b]
	9.616 221	9.590 679	9.590 678	9.591[b]
5	0.475 691	0.474 258	0.474 258	
	2.606 891	2.599 296	2.599 294	
	6.636 723	6.620 532	6.620 529	
	12.061 271	11.996 289	11.996 272	

[a]Reference 18.
[b]Reference 17.

TABLE III. The first four eigenenergies of the three- four-, and five-well oscillators: $A(x)=x^2-4x^4+x^6$, $B(x)=4x^2-6x^4+x^6$, $C(x)=\frac{105}{64}x^2-\frac{43}{8}x^4+x^6-x^8+x^{10}$, $D(x)=\frac{169}{64}x^2-\frac{59}{8}x^4+x^6-x^8+x^{10}$, $F(x)=-x^2+2x^4-0.9x^6+0.1x^8$, $G(x)=-x^2+3x^4-2x^6+0.1x^{10}$, $H(x)=2x^2-7.5x^4+5.5x^6-0.877x^8+0.04x^{10}$.

Potential	No. of wells	Modified Hill determinant method 11×11	40×40	45×45	Results of supersymmetric quantum mechanics
$A(x)$	3	−1.919 488	−1.999 994	−1.999 999	−2
		−1.724 171	−1.772 724	−1.772 725	
		2.171 462	2.078 289	2.078 281	
		5.786 607	5.604 040	5.604 034	
$B(x)$	3	−8.029 801	−9.000 978	−9.001 244	
		−8.441 451	−8.998 841	−8.999 758	−9
		1.083 662	0.640 304	0.639 810	
		2.959 678	1.939 005	1.937 489	
$C(x)$	3	0.390 275	0.375 007	0.375 001	0.375
		2.416 880	2.357 409	2.357 404	
		7.073 489	6.988 796	6.988 762	
		14.136 023	13.880 564	13.880 540	
$D(x)$	3	−0.148 789	−0.195 094	−0.195 116	
		1.251 592	1.125 037	1.125 020	1.125
		5.786 613	5.646 238	5.646 163	
		12.768 327	12.384 866	12.384 815	
$F(x)$	4	−0.122 959	−0.223 763	−0.223 928	
		0.269 987	0.083 721	0.083 585	
		1.692 856	1.526 822	1.526 583	
		4.188 792	3.971 516	3.971 308	
$G(x)$	4	−0.025 094	−0.096 127	−0.096 244	
		0.858 132	0.673 217	0.673 090	
		3.311 681	3.111 472	3.111 157	
		7.387 013	7.038 587	7.038 283	
$H(x)$	5	0.808 062	0.807 742	0.807 742	
		3.278 450	3.277 946	3.277 946	
		7.672 342	7.667 481	7.667 481	
		13.591 654	13.578 984	13.578 984	

TABLE IV. Comparison of the expectation values $\langle x^{2m} \rangle$ of the supersymmetric potentials $A(x)$, $B(x)$, $C(x)$, and $D(x)$ obtained by the method of the modified Hill determinant with the exact values.

Potential and eigenstate	Expectation value	Modified Hill determinant method 11×11	40×40	45×45	Exact
$A(x)$, $\psi_0(x)$	$\langle x^2 \rangle$	1.630	1.704	1.704	1.7043
	$\langle x^4 \rangle$	3.681	3.907	3.908	3.9085
	$\langle x^6 \rangle$	9.730	10.349	10.349	10.3735
	$\langle x^8 \rangle$	28.800	30.212	30.212	30.5184
	$\langle x^{10} \rangle$	85.396	93.210	93.210	97.3440
$B(x)$, $\psi_1(x)$	$\langle x^2 \rangle$	3.018	3.178	3.179	3.1796
	$\langle x^4 \rangle$	10.197	11.031	11.035	11.0387
	$\langle x^6 \rangle$	37.684	40.969	40.985	41.0649
	$\langle x^8 \rangle$	149.828	159.855	159.909	161.8299
	$\langle x^{10} \rangle$	616.518	625.121	625.164	670.2814
$C(x)$, $\psi_0(x)$	$\langle x^2 \rangle$	0.368	0.458	0.458	0.4583
	$\langle x^4 \rangle$	0.427	0.438	0.439	0.4385
	$\langle x^6 \rangle$	0.529	0.547	0.547	0.5474
	$\langle x^8 \rangle$	0.770	0.796	0.796	0.7967
	$\langle x^{10} \rangle$	1.252	1.287	1.288	1.2895
$D(x)$, $\psi_1(x)$	$\langle x^2 \rangle$	1.025	0.957	0.957	0.9568
	$\langle x^4 \rangle$	1.131	1.195	1.194	1.1944
	$\langle x^6 \rangle$	1.628	1.638	1.738	1.7384
	$\langle x^8 \rangle$	2.635	2.812	2.812	2.8134
	$\langle x^{10} \rangle$	4.673	4.930	4.930	4.9350

We apply the modified Hill determinant method to these potentials and other complicated potentials of type

$$F(x) = -x^2 + 2x^4 - 0.9x^6 + 0.1x^8 ,$$

$$G(x) = -x^2 + 3x^4 - 2x^6 + 0.1x^{10} ,$$

$$H(x) = 2x^2 - 7.5x^4 + 5.5x^6 - 0.877x^8 + 0.04x^{10} ,$$

with more than two wells in the potential (see Table III). Our calculations agree very well with the exact eigenvalues of the supersymmetric potentials $A(x)$, $B(x)$, $C(x)$, and $D(x)$. We apply Eq. (2) to calculate $\langle x^{2m} \rangle$, and compare our results in Table IV with the exact values obtained by using the exact eigenfunctions of the supersymmetric potentials. The agreement is excellent even for a determinant of small size.

IV. DISCUSSION

We have given here the Hill determinant method with a variational parameter for the general quantum anharmonic oscillators. The method is very simple and accurate. Due to introduction of the variational parameter our calculation converges very quickly to give stable roots for a small size of determinant. It makes a significant improvement over the original method of Biswas *et al.*[2] and yields excellent results for the eigenvalues and the expectation values of the anharmonic oscillators, pure oscillators, and multiwell oscillators.

It has been shown that the shifted $1/N$ expansion scheme is inaccurate and in some cases totally inapplicable for double- and triple-well potentials.[12] Our method works very well even for four- and five-well potentials. The supersymmetric quantum mechanics yields exact eigenvalues for a single state only, for a potential of type (1), with some constraints among the coupling constants. Our method is applicable to any general anharmonic oscillator (1), and it produces excellent results for the low-lying states. Equation (2) gives us the ready estimation of the expectation values $\langle x^{2m} \rangle$ for the general anharmonic oscillator.

[1]R. N. Chaudhuri and M. Mondal, Phys. Rev. A **40**, 6080 (1989), and references cited therein.
[2]S. N. Biswas, K. Datta, R. P. Saxena, P. K. Srivastava, and V. S. Varma, Phys. Rev. D **4**, 3617 (1971); J. Math. Phys. **14**, 1190 (1973).
[3]M. Znojil, Phys. Rev. D **26**, 3750 (1982).
[4]D. Masson, J. Math. Phys. **24**, 2074 (1983).
[5]R. N. Chaudhuri, Phys. Rev. D **31**, 2687 (1985).
[6]M. Tater, J. Phys. A **20**, 2483 (1987).
[7]J. Killingbeck, J. Phys. A **18**, L1025 (1985).
[8]A. Hautot, Phys. Rev. D **33**, 437 (1986).
[9]M. Znojil, Phys. Rev. D **34**, 1224 (1986).
[10]R. N. Chaudhuri, J. Phys. A **21**, 567 (1988).
[11]R. Dutt, A. Khare, and U. P. Sukhatme, Am. J. Phys. **56**, 163 (1988).
[12]R. Adhikari, R. Dutt, and Y. P. Varshni, Phys. Lett. A **141**, 1 (1989).
[13]R. K. Nesbet, Proc. R. Soc. London Ser. A **230**, 312 (1955).
[14]K. Banerjee, Proc. R. Soc. London Ser. A **364**, 265 (1978).
[15]F. M. Fernandez, Q. Ma, and R. H. Tipping, Phys. Rev. A **39**, 1605 (1989).
[16]A. V. Turbiner, J. Phys. A **14**, 1641 (1981).
[17]R. N. Chaudhuri and B. Mukherjee, Pramana **24**, 685 (1985).
[18]K. Banerjee and S. P. Bhatnagar, Phys. Rev. D **18**, 4767 (1978).