PHYSICAL REVIEW A VOLUME 40, NUMBER 10 NOVEMBER 15, 1989

Hill determinant method with a variational parameter

R. N. Chaudhuri and M. Mondal
Department of Physics, Visva-Bharati University, Santiniketan 731 235, West Bengal, India

(Received 10 July 1989)

A very simple variational parameter is introduced in the Hamiltonian of the quantum anharmonic oscillator. A suitable choice of this parameter not only removes the difficulties encountered by various authors in connection with the application of the Hill determinant method, but also makes the eigenvalues rapidly convergent for a small size of the determinant.

I. INTRODUCTION

The problem of the quantum anharmonic oscillator has been the subject of much discussion,[1-11] both from the analytical and the numerical points of view, because of its important applications in quantum field theory and molecular physics.[12,13] The eigenvalues of the anharmonic oscillators of type λx^{2n} have been calculated by Biswas *et al.*[14] with great success using the Hill determinant method. Very accurate eigenvalues have been obtained for the potential $\pm x^2+\lambda x^4$ by the scaled Hill determinant technique.[15] Recently it has been pointed[16-18] out that the method has a limited domain of applicability in the plane of couplings for the sextic oscillator:

$$V(x)=\mu x^2+\lambda x^4+\eta x^6, \quad \eta>0 . \tag{1}$$

Some possible improvements[19] and the procedure for removal[20-22] of the difficulties in the Hill determinant approach have also been discussed.

Although different nonperturbative techniques produce the eigenenergies of the anharmonic oscillators to a high degree of accuracy, people have been using some kind of perturbation theory for a long time. Hsue and Chern[23] have developed an elegant method to determine the accurate energy eigenvalues for the anharmonic oscillator using a coherent-state ansatz. Recently Patnaik[24] has shown that perturbation theory is applicable to the Hamiltonian of Hsue and Chern.[23] Feranchuk and Komarov[25] have solved the anharmonic-oscillator problem using variational plus perturbation procedure.

Killingbeck[20,26] has introduced a variational parameter in the exponential convergence factor of the wave function of the anharmonic oscillator and has shown by the process of computation that the Hill determinant method of Biswas *et al.*[14] is improved remarkably if this parameter is adjusted properly. Killingbeck, however, fails to produce any analytic expression for the correct choice of this parameter. Here we have given an analytic expression for the proper choice of this parameter and have obtained eigenvalues quite accurately with a determinant of small size. With this choice of the parameter no difficulty is encountered in the evaluation of the eigenvalues of the doubly anharmonic oscillator (1) by the Hill determinant method.

The potential (1) is of great interest in scalar field theory[27] and in the calculations of the vibrational spectra of molecules.[28] Flessas and Das[29,30] have discussed the conditions under which the potential (1) admits exact analytic solutions for the ground state. Recently it has been shown[31] that the potential has a supersymmetric character and the exact solutions are obtainable if the coupling constants satisfy certain supersymmetric constraints. Supersymmetric quantum mechanics has also been applied[32] to compute the eigenvalues of the double-well potential x^6-3x^2. Using the supersymmetric Wentzel-Kramers-Brillouin (WKB) approach, an averaging method[33] is given to compute energy eigenvalues of the potential $V(x)=(ax^3+bx)^2$. We have compared our results with those obtained by supersymmetric quantum mechanics and the agreement is excellent even for a determinant of small size.

II. THE $\mu x^2+\lambda x^4+\eta x^6$ OSCILLATOR

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

$$H=-d^2/dx^2+(\mu+\beta)x^2+\lambda x^4+\eta x^6-\beta x^2$$

is expressed in terms of creation and annihilation operators:

$$\begin{aligned}H=&\tfrac{1}{2}\omega+\frac{3\lambda}{\omega^2}+\frac{15\eta}{\omega^3}-\frac{\beta}{\omega}+\left[\omega+\frac{12\lambda}{\omega^2}+\frac{90\eta}{\omega^3}-\frac{2\beta}{\omega}\right]a^\dagger a+\left[\frac{6\lambda}{\omega^2}+\frac{45\eta}{\omega^3}-\frac{\beta}{\omega}\right][(a^\dagger)^2+a^2]\\&+\left[\frac{\lambda}{\omega^2}+\frac{15\eta}{\omega^3}\right][(a^\dagger)^4+a^4]+\frac{\eta}{\omega^3}[(a^\dagger)^6+a^6+6(a^\dagger)^5a+15(a^\dagger)^4a^2+20(a^\dagger)^3a^3+15(a^\dagger)^2a^4+6a^\dagger a^5]\\&+\left[\frac{60\eta}{\omega^3}+\frac{4\lambda}{\omega^2}\right](a^\dagger)^3a+\left[\frac{90\eta}{\omega^3}+\frac{6\lambda}{\omega^2}\right](a^\dagger)^2a^2+\left[\frac{60\eta}{\omega^3}+\frac{4\lambda}{\omega^2}\right]a^\dagger a^3 ,\end{aligned} \tag{2}$$

where $\omega=2(\mu+\beta)^{1/2}$. We set the coefficients of a^2 and $(a^\dagger)^2$ to zero so that the matrix element $\langle 2|H|0\rangle$ vanishes. This procedure has been adopted for a long time in nuclear physics[34] to find the most effective Hamiltonian. This yields

$$\omega^4-4\mu\omega^2-24\lambda\omega-180\eta=0\ , \tag{3}$$

which determines the unknown parameter β or ω.

For the modified Hamiltonian (2) we now apply the method of the Hill determinant and expand the wave function ψ in terms of the orthonormal basis vectors $|m\rangle$ as

$$\psi=\sum_{m=0}^{\infty} A_m|m\rangle \tag{4}$$

and use the equation

$$H\psi=E\psi\ .$$

We have the following recurrence relations satisfied by A_m

$$P_m A_{m-6}+Q_m A_{m-4}+R_m A_{m-2}+S_m A_m+T_m A_{m+2}+U_m A_{m+4}+V_m A_{m+6}=0\ , \tag{5}$$

where

$$P_m=\frac{\eta}{\omega^3}[m(m-1)(m-2)(m-3)(m-4)(m-5)]^{1/2}\ , \tag{6a}$$

$$Q_m=\left[\frac{\lambda}{\omega^2}+\frac{3\eta}{\omega^3}(2m-3)\right]\times[m(m-1)(m-2)(m-3)]^{1/2}\ , \tag{6b}$$

$$R_m=\left[\frac{4\lambda}{\omega^2}+\frac{15\eta}{\omega^3}(m+1)\right](m-2)[m(m-1)]^{1/2}\ , \tag{6c}$$

TABLE I. Comparison of the first four eigenvalues of the potential $\mu x^2+\eta x^6$ obtained by the method of the modified Hill determinant with the exact values (Ref. 6 for $\mu=1$, and Ref. 11 for $\mu=0$). The roots of the Hill determinant for $\beta=0$ are given in parentheses for $\mu=1$ and $\eta=1$ and 100.

			Modified Hill determinant method with determinant of size			
μ	λ	η	7×7	13×13	19×19	Exact
1	0	0.1	1.109 094	1.109 087	1.109 087	1.109 087
			3.596 066	3.596 037	3.596 037	3.596 037
			6.645 441	6.644 393	6.644 392	6.644 392
			10.239 255	10.237 883	10.237 874	10.237 874
		1.0	1.435 670	1.435 625	1.435 625	1.435 625
			(1.438 279)	(1.435 740)	(1.435 633)	
			5.034 082	5.033 398	5.033 396	5.033 396
			(5.060 826)	(5.034 422)	(5.033 425)	
			9.970 292	9.966 662	9.966 622	9.966 622
			(10.049 850)	(9.970 023)	(9.967 019)	
			15.998 792	15.989 556	15.989 442	15.989 441
			(16.925 198)	(16.019 146)	(15.991 167)	
		10.0	2.205 894	2.205 726	2.205 723	2.205 723
			8.117 260	8.114 848	8.114 843	8.114 843
			16.649 180	16.641 368	16.641 219	16.641 218
			27.187 822	27.155 350	27.155 092	27.155 086
		100.0	3.717 369	3.716 981	3.716 975	3.716 975
			(4.954 914)	(3.796 564)	(3.765 139)	
			13.951 456	13.946 219	13.946 207	13.946 207
			(32.722 363)	(15.110 318)	(14.080 685)	
			28.992 638	28.977 618	28.977 297	28.977 294
			(191.228 863)	(47.571 315)	(31.054 365)	
			47.636 546	47.565 486	47.564 998	47.564 985
			(606.760 779)	(133.891 538)	(64.961 674)	
		1000.0	6.493 112	6.492 362	6.492 350	6.492 350
			24.535 245	24.525 339	24.525 317	24.525 316
			51.210 539	51.183 091	51.182 487	51.182 480
			84.311 248	84.176 494	84.175 608	84.175 584
0	0	1	1.144 943	1.144 805	1.144 802	1.144 802
			4.340 415	4.338 603	4.338 599	4.338 599
			9.078 141	9.073 196	9.073 086	9.073 085
			14.960 013	14.935 333	14.935 174	14.935 169

TABLE II. Comparison of the first ten eigenvalues of the potential $V(x)=(ax^3+bx)^2$ for $a=10$ and $b=\sqrt{30}$ obtained by the method of the modified Hill determinant with the average SWKB values (Ref. 33).

Modified Hill determinant method with determinant of size			
13×13	19×19	25×25	Average SWKB
7.3569	7.3569	7.3569	7.3786
24.6462	24.6462	24.6462	24.6861
46.3355	46.3355	46.3355	46.3690
71.3534	71.3534	71.3534	71.3823
99.1872	99.1871	99.1871	99.2128
129.5101	129.5100	129.5100	129.533
162.0921	162.0891	162.0891	162.111
196.7513	196.7473	196.7472	196.767
233.3945	233.3436	233.3436	233.362
271.9515	271.7630	271.7626	271.780

$$S_m=\frac{\omega}{4}+\frac{3\lambda}{\omega^2}+\frac{15\eta}{\omega^3}+\frac{\mu}{\omega}-E+m\omega+\left[\frac{10\eta}{\omega^3}(5+2m)+\frac{6\lambda}{\omega^2}\right]m(m-1)\,, \tag{6d}$$

$$T_m=\left[\frac{4\lambda}{\omega^2}+\frac{15\eta}{\omega^3}(3+m)\right]m[(m+1)(m+2)]^{1/2}\,, \tag{6e}$$

$$U_m=\left[\frac{\lambda}{\omega^2}+\frac{3\eta}{\omega^3}(5+2m)\right]\times[(m+1)(m+2)(m+3)(m+4)]^{1/2}\,, \tag{6f}$$

$$V_m=\frac{\eta}{\omega^3}[(m+1)(m+2)(m+3)\times(m+4)(m+5)(m+6)]^{1/2}\,. \tag{6g}$$

The eigenvalue condition of the Hill determinant for large N is

$$\det D_n=0\,, \tag{7}$$

with

$$D_n=\begin{vmatrix} S_\nu & T_\nu & U_\nu & V_\nu & 0 & \cdots \\ R_{2+\nu} & S_{2+\nu} & T_{2+\nu} & U_{2+\nu} & V_{2+\nu} & \cdots \\ Q_{4+\nu} & R_{4+\nu} & S_{4+\nu} & T_{4+\nu} & U_{4+\nu} & \cdots \\ P_{6+\nu} & Q_{6+\nu} & R_{6+\nu} & S_{6+\nu} & T_{6+\nu} & \cdots \\ 0 & P_{8+\nu} & Q_{8+\nu} & R_{8+\nu} & S_{8+\nu} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \end{vmatrix}\,, \tag{8}$$

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.

TABLE III. The first four eigenenergies of the double-well oscillator $\mu x^2+\lambda x^4+\eta x^6$ with negative μ.

			Modified Hill determinant method with determinant of size			
μ	λ	η	13×13	19×19	25×25	Other methods
−3	0	1	0.000 038	0.000 001	0.000 000	−0.000 001[a]
			1.935 780	1.935 490	1.935 482	1.935 482[a]
			6.299 050	6.298 513	6.298 497	6.298 495[a]
			11.684 397	11.681 072	11.680 976	11.680 971[a]
−2	−2	1	−0.998 401	−0.999 886	−0.999 987	−1[b]
			−0.149 388	−0.153 809	−0.154 093	
			3.635 758	3.630 264	3.629 880	3.629 827[b]
			8.039 318	8.009 965	8.007 742	
−1	0	0.1	−0.044 214	−0.044 241	−0.044 241	
			1.006 501	1.006 309	1.006 304	
			3.457 386	3.457 049	3.457 039	
			6.470 193	6.467 987	6.467 919	

[a]Reference 32.
[b]Reference 20.

III. RESULTS AND DISCUSSION

In Table I we present the first four eigenvalues of the $x^2+\eta x^6$ anharmonic oscillator for different values of η and the pure x^6 sextic oscillator as obtained by the modified Hill determinant method and compare our results with the exact values. For $\mu=1$ and $\eta=1$ and 100, we have given in the parentheses the roots of the Hill determinant without the variational parameter ($\beta=0$ or $\omega=2$). We find that our calculation converges very quickly to give stable roots for small size of the determinant.

Adhikari, Dutt, and Varshni[33] have computed the eigenvalues of the potential $V(x)=(ax^3+bx)^2$ with $a=10$ and $b=\sqrt{30}$ by using the supersymmetric WKB (SWKB) averaging procedure. We present the first ten eigenvalues of this potential in Table II. In comparison with the average SWKB energy eigenvalues our results are much improved. Next we consider the double-well oscillator with negative μ and compare our eigenvalues in Table III with those available in the literature.

Our method is very simple and accurate. It makes a significant improvement over the original Hill determinant method of Biswas *et al.*[14] and yields excellent results for the anharmonic oscillator ($\mu>0$), pure sextic oscillator ($\mu=\lambda=0$), and double-well oscillator ($\mu<0$). It has been shown[18,20] that the method of Singh, Biswas, and Datta[9] fails to produce correct eigenvalues for the potential $-2x^2-2x^4+x^6$. The present treatment with the variational parameter removes this problem. The method presented here is quite general and can be applied to any general anharmonic-oscillator problem.

[1]N. Bazley and D. Fox, Phys. Rev. **124**, 483 (1961).

[2]C. Bender and T. T. Wu, Phys. Rev. **184**, 1231 (1969).

[3]F. T. Hioe, D. MacMillen, and E. W. Montroll, Phys. Rep. **43**, 305 (1978).

[4]F. T. Hioe and E. W. Montroll, J. Math. Phys. **16**, 1945 (1975).

[5]B. Simon, Ann. Phys. (N.Y.) **58**, 76 (1970).

[6]K. Banerjee, Proc. R. Soc. London, Ser. A **364**, 265 (1978).

[7]R. N. Chaudhuri and B. Mukherjee, J. Phys. A **17**, 3327 (1984).

[8]K. Banerjee and S. P. Bhatnagar, Phys. Rev. D **18**, 4767 (1978).

[9]V. Singh, S. N. Biswas, and K. Datta, Phys. Rev. D **18**, 1901 (1978).

[10]H. Taseli and M. Demiralp, J. Phys. A **21**, 3903 (1988).

[11]F. M. Fernández, Q. Ma, and R. H. Tipping, Phys. Rev. A **39**, 1605 (1989).

[12]J. P. Boyd, J. Math. Phys. **19**, 1445 (1978).

[13]Itzykson and J. B. Zuber, *Quantum Field Theory* (McGraw-Hill, New York, 1980).

[14]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).

[15]K. Banerjee and K. Bhattacharjee, Phys. Rev. D **29**, 1111 (1984).

[16]M. Znojil, Phys. Rev. D **26**, 3750 (1982).

[17]D. Masson, J. Math. Phys. **24**, 2074 (1983).

[18]R. N. Chaudhuri, Phys. Rev. D **31**, 2687 (1985).

[19]M. Tater, J. Phys. A **20**, 2483 (1987).

[20]J. Killingbeck, J. Phys. A **18**, L1025 (1985).

[21]A. Hautot, Phys. Rev. D **33**, 437 (1986).

[22]M. Znojil, Phys. Rev. D **34**, 1224 (1986).

[23]C. S. Hsue and J. L. Chern, Phys. Rev. D **29**, 643 (1984).

[24]P. K. Patnaik, Phys. Rev. D **33**, 3145 (1986).

[25]I. D. Feranchuk and L. I. Komarov, Phys. Lett. **88A**, 211 (1982).

[26]J. Killingbeck, Phys. Lett. **84A**, 95 (1981).

[27]C. A. Aragão de Carvalho, Nucl. Phys. **B119**, 401 (1977).

[28]D. G. Lister, J. N. MacDonald, and N. L. Owen, *Internal Rotation and Inversion* (Academic, New York, 1978).

[29]G. P. Flessas, Phys. Lett. **72A**, 289 (1979); **81A**, 17 (1981).

[30]G. P. Flessas and K. P. Das, Phys. Lett. **78A**, 19 (1980).

[31]P. Roy and R. Roychowdhuri, J. Phys. A **20**, 6597 (1987).

[32]L. J. Boya, M. Kmiecik, and A. Bohm, Phys. Rev. D **35**, 1255 (1987).

[33]R. Adhikari, R. Dutt, and Y. P. Varshni, Phys. Lett. **131A**, 217 (1988).

[34]R. K. Nesbet, Proc. R. Soc. London, Ser. A **230**, 312 (1955).