Energy-level calculation through modified Hill determinant approach: for general oscillator

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Received 26 November 1998, accepted 19 April 1999

Abstract A method for calculation of energy levels using the modified Hill determinant approach has been developed. An example of this approach is given for the general oscillator $V(X) = \lambda X^1 + \lambda X^4 + \lambda X^8$. Very accurate convergent energy levels are presented.

Keywords Energy-level calculation, Hill determinant approach, general oscillator

PACS No. 03.65.Ge

1. Introduction

In quantum mechanics, as in classical mechanics, there are relatively few systems of physical interest for which equations of motion yield exact solutions. In practice, since the exactly solvable problems are rare, one must frequently resort to approximations. This has culminated in the development of many useful approximation techniques, some perturbative and some nonperturbative. Among the nonperturbative approximations, one has for example, the Hill determinant [1], the two-step procedure [2], the operator method [3], various $1/N$ expansions for spherically symmetric potentials [4], the rational function approach [5], the multiple-step recursion approach [6], supersymmetric quantum mechanics-based methods [7], and variational approach [8]. Almost all these methods use the anharmonic oscillator Hamiltonian

$$H = P^2 + X^2 + \lambda X^4$$

(1)
as an example, not only because of its important applications in quantum field theory and molecular physics [9] but also because of the work of Bender and Wu [10] who have shown

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that the perturbation expansion for the energy level \( E_n(\lambda) \) is not convergent. The eigenvalues of the anharmonic oscillator of the type \( \lambda X^{2m} \) have been calculated by Biswas et al [1] with great success using the Hill determinant approach. Later on, it was pointed out [11-16] that the method [1] has a limited domain of applicability in the plane of couplings for the sextic oscillator

\[
V(X) = \lambda_1 X^2 + \lambda_2 X^4 + \lambda_3 X^6, \quad \lambda_3 > 0.
\]

It has been shown [13-15] that the method of Singh, et al [17] fails to produce correct eigenvalues for the potential \( V(X) = -2X^2 - 2X^4 + X^6 \). Chaudhuri and Mondal [16] have calculated the first four energy levels of this oscillator by introducing a variational parameter in the Hill determinant approach following the operator method of Feranchuk and Komarov [3]. Killingbeck [15] has calculated energy levels of this oscillator by introducing a variational parameter in the exponential convergence factor of the wave function. Recently, Agarwal and Varma [18] have shown that it is necessary to introduce a modification on the method of Hill determinants by Chaudhuri and Mondal [16] which incorporates the operator method of Feranchuk and Komarov [3]. Further we find that even the low-lying energy levels calculated by Chaudhuri and Mondal [16] are not exactly the same as those reported by Killingbeck [15]. Hence, we feel that there is a need for generalizing the Hill determinant approach for a general oscillator Hamiltonian.

In this communication, we generalize the Hill determinant approach.

2. Hill determinant method

The Hamiltonian under consideration is defined by the relation

\[
H = \mu T + V(q),
\]

where

\[
V(q) = CB(q) + \lambda_1 H_1(q) + \lambda_2 H_2(q) + \lambda_3 H_3(q) + \ldots.
\]

\[
= CB(q) + \sum_{l=1}^{N} \lambda_l H_l(q). \tag{3}
\]

In the above, \( T \) is the kinetic energy, \( CB(q) \) is the unperturbed potential, \( \sum_{l=1}^{N} \lambda_l H_l(q) \) represents the perturbation term and \( \mu \) is a dimensionless constant. The unperturbed Hamiltonian

\[
H_C = \mu \left[ T + \frac{CB(q)}{\mu} \right]. \tag{4}
\]

satisfies the eigenvalue relation

\[
H_C |n >_C = \mu E_n(C) |n >_C , \tag{5}
\]

where \( E_n(C) \) is the \( n \)-th unperturbed energy and \( |n >_C \) is the corresponding \( n \)-th eigenfunction.

Now we shift the parameter \( C \) to a new parameter \( C_1 \) where

\[
C_1 = \frac{C}{\mu} + \sum_{l=1}^{N} \lambda_l \alpha_l \frac{<g | H_l(q) | g>}{<g | B(q) | g>}. \tag{6}
\]
Hence, the new unperturbed Hamiltonian $E_{C_1}$ satisfies the eigenvalue relation.

$$H_{C_1} | n >_{C_1} = \mu \left[ T + C_1 B(q) \right] | n >_{C_1}$$  \hspace{1cm} (7)

The function $| n >_{C_1}$ can be obtained directly from the unperturbed function $| n >_C$ by replacing $C$ by $C_1$. In the above, $| g >$ represents the groundstate wave function of $H_{C_1}$. It is seen that in eq. (6) $C_1$ is also a function of $C$. Further, the contribution of $C_1$ is determined in terms of diagonal term of $H_q(q)$ without considering the non-diagonal contribution of $H_q(q)$. Hence, the contribution of non-diagonal part of $H_q(q)$ can be included through the parameter $\alpha_j$. Therefore, we propose to determine $\alpha_j$ using the non-diagonal matrix elements of $H_q(q)$ through the parameter $C$ as [19]

$$\sum_{m \in C} \left[ \frac{< g | H_q(q) | m > - \alpha_j < g | H_q(q) | g >}{< g | B(q) | g >} - \frac{< g | B(q) | m >}{< g | B(q) | g >} \right] = 0,$$  \hspace{1cm} (8)

where suffix 'C' stands for unperturbed state in eq.(4). Further in eq.(8) the value of $m$ to be considered for which the matrix elements $< g | H_q(q) | m >$ and $< g | B(q) | m >$ yield nonzero value. Hence, the original Hamiltonian in eq. (2) is rewritten as

$$H = H_{C_1} + H_N + H_N,$$  \hspace{1cm} (9)

where $H_N$ and $H_N$ are the diagonal and the nondiagonal parts of

$$H_2 = \sum \lambda_i H_i(q) - \alpha_j \frac{< g | H_q(q) | g >}{< g | B(q) | g >}$$.  \hspace{1cm} (10)

Now, we use orthonormal basis vector $| m >_{C_1}$ to express the wave function $\Psi$ as

$$\Psi = \sum_{m=0} \lambda_m | m >_{C_1}$$  \hspace{1cm} (11)

and solve the eigenvalue equation

$$H \Psi = E \Psi.$$  \hspace{1cm} (12)

3. Application

In order to make the procedure accessible to the reader, we apply it to the general oscillator characterized by the Hamiltonian

$$H = \mu p^2 + \lambda_1 X^2 + \lambda_2 X^4 + \lambda_3 X^6$$  \hspace{1cm} (13)

with ($\lambda_i > 0$). The expression for $H_w$ for the above Hamiltonian is

$$H_w = \mu \left( p^2 + W^2 X^2 \right).$$  \hspace{1cm} (14)
where

\[
W^2 = \frac{\lambda_1 + \alpha_1}{\mu} \frac{<01\lambda_2X^410>_W + \alpha_2}{<01\mu X^210>_W} + \alpha_2 <01\mu X^210>_W.
\]  

(15)

The value of \(\alpha_1\) is determined by the condition

\[
\begin{bmatrix}
<01X^4l2> - \alpha_1 <01X^410> - \alpha_2 <01X^2l2>
\end{bmatrix} = 0
\]

(16)

on substituting \(l = 1\) in eq. (8) and is found to be 2. Similarly by putting \(l = 2\) in eq. (8), the value of \(\alpha_2\) is found to be 3. Hence, the parameter \(W\) satisfies the following quartic equation

\[
4W^2\mu - 4\lambda_1W^2 - 12\lambda_2W - 45\lambda_3 = 0.
\]

(17)

The expression for \(H_2\) is

\[
H_2 = \lambda_2 \left[ X^4 - \frac{3}{W} X^2 \right] + \lambda_3 \left[ X^6 - \frac{45}{4W^2} X^2 \right].
\]

(18)

Using eqs. (11, 12), one obtains the following recurrence relation that is satisfied by \(A_m\),

\[
P_m A_{m-6} + Q_m A_{m-4} + R_m A_{m-2} + S_m A_m + T_m A_{m+2} + U_m A_{m+4} + V_m A_{m+6} = 0.
\]

(19)

where

\[
P_m = \frac{\lambda_1}{8W^3} \left[ m(m-1)(m-2)(m-3)(m-4)(m-5) \right]^{1/2},
\]

(19a)

\[
Q_m = \left[ \frac{3\lambda_1(2m-3)}{8W^3} + \frac{\lambda_2}{4W^2} \right] \left[ m(m-1)(m-2)(m-3) \right]^{1/2}.
\]

(19b)

\[
R_m = \left[ \frac{15\lambda_1(m+1)}{8W^3} + \frac{\lambda_2}{2W} \right] \left[ (m-2) \right] \left[ m(m-1) \right]^{1/2}.
\]

(19c)

\[
S_m = mW\mu + \frac{\lambda_1m}{W} + \frac{6\lambda_2}{4W^2}(m^2 + m) + \frac{\lambda_3}{8W^3}(20m^3 + 30m^2 + 40m)
\]

\[
+ \frac{W\mu}{2} + \frac{3\lambda_1}{2W} + \frac{15\lambda_3}{8W^3} - E.
\]

(19d)

\[
T_m = R_{m+2}.
\]

(19e)

\[
U_m = Q_{m+4}.
\]

(19f)

\[
V_m = P_{m+6}.
\]

(19g)
The eigenvalue condition of the Hill determinant in the limit of large $N$ is $\det D_N = 0$. With

$$D_N = \begin{pmatrix}
S_n & T_n & U_n & V_n & 0 & \cdots \\
R_{n+2} & S_{n+2} & T_{n+2} & U_{n+2} & V_{n+2} & \cdots \\
Q_{n+4} & R_{n+4} & S_{n+4} & T_{n+4} & U_{n+4} & \cdots \\
P_{n+6} & Q_{n+6} & R_{n+6} & S_{n+6} & T_{n+6} & \cdots \\
& & & & & \\
& & & & & \\
& & & & & \\
& & & & & \\
& & & & & \\
& & & & & \\
& & & & & \\
& & & & &
\end{pmatrix} = 0,$$

(20)

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

4. Comparison with some exact results

For any arbitrary values of $\lambda_1$, $\lambda_2$, and $\lambda_3$, it is impossible to find exact solution of the Hamiltonian in Eq. (13). However, for some specific values of $\lambda_1$, $\lambda_2$ with $\lambda_2 = 0$, one can solve it exactly. We

Table 1. Comparison with exact result

<table>
<thead>
<tr>
<th>First two even levels</th>
<th>$\lambda_1$</th>
<th>$\lambda_2$</th>
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<td>1</td>
<td>3</td>
<td>0</td>
<td>1 935</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>3</td>
<td>0</td>
<td>1 1680</td>
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<td>1</td>
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<td>4</td>
<td>1 836</td>
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<td>8 159</td>
</tr>
<tr>
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<td>0</td>
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<td>0 440</td>
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<td>2</td>
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<td>7 231</td>
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<td>-1</td>
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<td>5 374</td>
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<td>-1 153</td>
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<td>-5</td>
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<td>2</td>
<td>4 478</td>
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<td>-1 915</td>
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<td>-11</td>
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<td>2</td>
<td>0 000</td>
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</tbody>
</table>
have compared the first two even states with the exact results of Tater and Turbiner [14] and find that in all the cases, present computed value yields good agreement (see Table 1).

5. Comparison between self-consistent and variational parameter calculation

In the previous examples, we find that the present self-consistent parameter $C_1$ when used in eq. (11) has yielded results that are in good agreement with the previous one. Let us consider another exactly solvable non-linear oscillator of the form [20-22]

$$H = P^2 + X^2 + X^2 <X^2>.$$  

(21)

Using present self-consistent method, we find that the parameter $W$ satisfies the cubic equation

$$W^3 - W - 0.5 = 0$$  

(22)

and the ground state energy is

$$E_n = W = 1.191487,$$  

(23)

which remains the same as the exact one [20]. However, when variational principle is used, the parameter $W$ satisfies the cubic equation

$$W^3 - W - 1 = 0$$  

(24)

and the ground state energy is found to be $E_n$ (variational) = 1.176560. Hence, we find that the variational based calculation has failed in reproducing the correct ground state energy of the non-linear oscillator eq. (21).

6. Discussion

Apart from the comparison with the exactly solvable results in Table 1, we also present the first five (even and odd) convergent energy levels of the anharmonic oscillator $V(X) = \frac{X^2}{2} + \frac{X^4}{4} (\mu = \frac{1}{2}, \lambda_1 = \frac{1}{2}, \lambda_2 = 1, \lambda_3 = 0)$ in Table 2 and compare the same with the 20th-order perturbation calculation by Caswell [23]. In this case, we have calculated the results

<table>
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<th>Levels</th>
<th>Present (even)</th>
<th>Previous [23]</th>
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<tbody>
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<td>0.803 770 651 234 27</td>
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<tr>
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<td>5.179 291 687 639 4</td>
<td>5.179 291 681 3</td>
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<td>4</td>
<td>10.963 583 094 127</td>
<td>10.963 583 096</td>
</tr>
<tr>
<td>6</td>
<td>17.634 049 116 138</td>
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<tr>
<td>8</td>
<td>24.994 936 409 502</td>
<td>24.994 936 412</td>
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<table>
<thead>
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<th>Levels</th>
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</tr>
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<td>3</td>
<td>7.942 403 984 391 0</td>
<td>7.942 404 391</td>
</tr>
<tr>
<td>5</td>
<td>14.203 139 104 529</td>
<td>14.203 139 102</td>
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<td>21.236 435 486 758</td>
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<tr>
<td>9</td>
<td>28.897 251 119 223</td>
<td>28.897 251 12</td>
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</table>

Table 2. The first five (even and odd) energy levels of the oscillator $V(X) = \frac{X^2}{2} + \frac{X^4}{4} (\mu = \frac{1}{2}, \lambda_1 = \frac{1}{2}, \lambda_2 = 1, \lambda_3 = 0)$.
for $N = 40$ and find that the results do not change even if $N$ is increased up to $N = 400$. Present 12 decimal results are taken from the determinant size ($80 \times 80$).

In the above case, the cubic equation has exact solution, i.e., $W = 2$. However, for anharmonic oscillator $V(X) = X^2 + X^4 (\mu = 1, \lambda_1 = \lambda_2 = 1, \lambda_3 = 0)$, we find cubic equation $W^3 - W - 3 = 0$ has a single positive root. Using $W = 1.6716998816$, we are able to reproduce values tabulated previously [24]. Similarly, for the quartic oscillator $V(X) = X^4$ using the value of $W = 1.4422495703074$, we are able to reproduce previous values [24]. In Table 3, we quote first five even and odd parity levels. Present results are from the size $N = 80$.

### Table 3. First five even and odd energy levels of the $V(X) = X^2 + X^4$ and $V(X) = X^4$

(See Banerjee et al. [24] for comparison)

<table>
<thead>
<tr>
<th>Levels</th>
<th>Present</th>
<th>Previous</th>
<th>$W = 1.6716998816$</th>
<th>Present</th>
<th>Previous</th>
<th>$W = 1.4422495703074$</th>
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<td>009 505</td>
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</table>

In Table 4, we present the first ten convergent energy levels of the sextic double well oscillator $V(X) = -X^2 + 0.1X^6 (\mu = 1, \lambda_1 = 1, \lambda_2 = 0, \lambda_3 = 0.1)$ and compare with that of Chaudhuri and Mondal [16]. In this case, we have started from $V = 49$ and increased up to $V = 490$. Here also we find very good convergence.

### Table 4. The first five (even and odd) energy levels of the Sextic-double-well-oscillator $V(X) = -X^2 + 0.1X^6 (\mu = 1, \lambda_1 = 1, \lambda_2 = 0, \lambda_3 = 0.1)$

<table>
<thead>
<tr>
<th>Levels</th>
<th>Present (even)</th>
<th>Previous [16]</th>
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<td>2</td>
<td>3.457 038 385</td>
<td>91 3.457 019</td>
</tr>
<tr>
<td>4</td>
<td>10.063 083 061</td>
<td>2 1.006 303</td>
</tr>
<tr>
<td>6</td>
<td>18.549 407 539</td>
<td>9 1.006 304</td>
</tr>
<tr>
<td>8</td>
<td>28.637 155 094</td>
<td>8 1.006 304</td>
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<table>
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<th>Levels</th>
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<th>Previous [16]</th>
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<td>1.006 303 806</td>
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<tr>
<td>9</td>
<td>34.206 055 345</td>
<td>2 34.206 055</td>
</tr>
</tbody>
</table>
In Table 5, we present the first seven convergent energy levels of the $V(X) = -2X^2 - 2X^4 + X^6$ ($\mu = 1, \lambda_1 = -2, \lambda_2 = -2, \lambda_3 = 1$) sextic-double-well-oscillator and compare results with the previous results [15, 16]. Like the previous cases, we have started from $N = 63$ and increased up to $N = 490$.

<table>
<thead>
<tr>
<th>Levels</th>
<th>Present (even)</th>
<th>Previous [16]</th>
<th>Previous [15]</th>
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Further, we have included only few energy levels as we do not find more results for comparison. In all cases, while computing eigenvalues, we use the appropriate value of $W$ satisfying the limiting condition [19] $W \rightarrow \sqrt{\lambda_1}$, when $\lambda_2 \rightarrow 0, \lambda_3 \rightarrow 0$.

In this approach for the oscillator Hamiltonian, we find that the value of $W$ used here is in contradiction with the Hill determinant approach of Biswas et al [1] where the value of $W$ is taken as 1 i.e. $W = 1$. Further for the value of $W = 1$, the strength of the diagonal matrix element $\langle n | H | n \rangle$ as well as the non-diagonal matrix element $\langle n | H | m \rangle$ is never reduced to minimum. Perhaps this is the reason why the determinant size in the Hill determinant approach of Biswas et al [1] is very large. The larger the strength of the matrix element, the larger is the size of the determinate needed to yield accurate energy levels [8]. Using wave functions $| m \rangle >_{C_1}$, the strength of matrix element $\langle n | H | m \rangle >_{C_1}$ or $\langle n | H | n \rangle >_{C_1}$ (for $\mu = 1/2$ or $\lambda = 1/2$ or 1, $\lambda_2 = 1, \lambda_3 = 0$) in the large $n$ limit, goes as $n^2/W^2$ whereas in the previous Hill determinant approach [1], it goes as $n^2$. For potential of the type $V(X) = X^2 + X^4 < X >$ where $m$ is an even number, the present method yields the correct ground state where as variational parameter fails to yield correct ground state.

In addition to this, using the present value of $W$ from eq. (17), we find that matrix element $\langle 0 | H | 2 \rangle >_{C_1}$ turns out to be zero for the oscillator Hamiltonian i.e. $\langle 0 | H | 2 \rangle >_{C_1} = 0$. This has been made possible due to the value of $\alpha_1$. Without the value of $\alpha_1$, the condition $\langle 0 | H | 12 \rangle >_{C_1} = 0$ is never achieved for the oscillator Hamiltonian. It is worth mentioning that the condition $\langle 0 | H | 2 \rangle > = 0$ has been widely used in nuclear physics [25] to find out the most effective Hamiltonian. However for other Hamiltonians, the condition $\langle g | H | m \rangle > = \langle 11 | H | 2 \rangle > = 0$ ($g \neq m$) should not be used to yield effective Hamiltonians. For example, consider the charmonium model potential [26] $V(r) = -1/2 + 50$. The ground state energy using $\alpha_1$ from eq (8) is $\langle 11 | H | 1 \rangle >_{C_1} = -0.42707$ in the zeroth order approximation [27]. However, if the condition $\langle 11 | H | 2 \rangle > = 0$ alone is used instead of eq.(8), then the ground state energy becomes...
Energy-level calculation through modified Hill determinant etc

\[ \langle 1 | H | 1 \rangle = -0.42645. \] The exact ground state energy [26] for this Hamiltonian is \(-0.42811\). Hence, in finding out the effective Hamiltonian for energy calculation, the role of \(\alpha_i\) is absolutely indispensable. It is interesting to note that the present self-consistent parameter which is non-variational in nature, remains the same as variational parameter for oscillator of the type \(V(X) = \lambda_1 X^2 + \lambda_2 X^4 + \lambda_3 X^6\). However, for oscillator of the type \(V(X) = X^2 + X^2 < X^2 >\), present self-consistent parameter is different from that of the variational parameter.

Lastly, the present method is simple and accurate. It can be applied to all oscillator potentials uniformly without any modification unlike other approximation [16, 18]. Apart from oscillator potentials, we find this approximation can also be used for non-oscillator potentials discussed elsewhere [19, 27].

Acknowledgment

Author (B.R) is grateful to the University Grants Commission, New Delhi India for financial support. Author (H. M) gratefully acknowledges the KFUPM support.

References