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On the Hill determinant method

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Abstract. The conditions of applicability of the Hill determinant method to the potentials $V(r) = v_1 r + v_2 r^2$ and $V(x) = x^2 + \lambda x^2/(1 + gx^2)$ are investigated. It is shown that the procedure leads to the actual eigenvalues in the former case provided the ansatz is properly chosen, but it completely fails to yield the right answer in the latter one.

1. Introduction

Non-perturbative techniques have been successfully applied to the calculation of the eigenvalues of anharmonic oscillators and central-field models [1, 2]. Among them, the Hill determinant method (HDM) seems to be preferred by most authors [3-6] because of its simplicity. However, it has been proved that in some cases the HDM may be divergent or even yield unphysical eigenvalues.

Flessas and Anagnostatos [7] argued that the vanishing of the Hill determinant is insufficient to assure the physical behaviour of the wavefunction. Hautot [8] showed that the HDM actually applies to the anharmonic oscillator $x^2 + \lambda x^4$ as suggested by previous accurate numerical calculations [1, 3].

Upon investigating the anharmonic oscillator $ax^2 + bx^4 + cx^6$ Chaudhuri [9] proved that the roots of the Hill determinant differed from the actual eigenvalues when the Schrödinger equation was transformed into a three-term recurrence relation. More recently Killingbeck [10] showed that supersymmetric pairs of potentials have common true and false eigenvalues and developed a criterion, based on the expectation values of x^2, for distinguishing between them. An improved procedure was put forward by Tater [11] but it is not as simple as the standard HDM. The same potential was also investigated by Hautot [12] who found the conditions of applicability of the HDM by studying the asymptotic form of the solutions of the HDM difference equations and the eigenfunctions obtained from them. He concluded that the HDM does not always assure the square-integrability of the eigenfunction.

The rotating oscillator was also under dispute. Masson [13] reviewed the problem and pointed out that some authors had obtained wrong eigenvalues through the HDM or an equivalent approach based on continued fractions. Killingbeck [14] showed how to remove the difficulty numerically but he did not give a rigorous mathematical justification.

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The applicability of the standard HDM to rational potentials such as $x^2+\lambda x^2/(1+gx^2)$ has not been discussed. Hautot [4] obtained the eigenvalues by expanding the wavefunction in the harmonic oscillator basic set. Exact solutions for particular choices of λ and g values were given by Whitehead [15] and Chaudhuri [16] but they did not consider the general case.

The purpose of the present paper is to investigate the applicability of the HDM to the last two problems which are discussed in sections 2 and 3, respectively. Further comments are found in section 4.

2. The rotating oscillator

The rotating displaced oscillator is one of the simplest approaches to a rotating vibrating diatomic molecule. The radial part of the Schrödinger equation can be written (units are chosen so that $\hbar=1$):

$$\{-D^2+l(l+1)/r^2+(r-1)^2/4\alpha^2\}\psi=(n+\tfrac{1}{2})\psi/\alpha \tag{1}$$

where $D=\mathrm{d}/\mathrm{d}r$, $\psi(0)=\psi(\infty)=0$, $l=0,1,\ldots,$ is the angular momentum quantum number, and α is a model parameter.

It is convenient to consider the more general problem:

$$\{-D^2+l(l+1)/r^2+v_1r+v_2r^2\}=E\psi. \tag{2}$$

The choice $v_1=-2v_2=-1/2\alpha^2$, $E=(n+\frac{1}{2})/\alpha-1/4\alpha^2$ leads to (1).

Equation (2) has two linearly independent solutions ψ_{conv} and ψ_{div} which behave asymptotically as

$$\begin{aligned}\psi_{\mathrm{conv}}&\sim\exp(-v_1r/2v_2^{1/2}-v_2^{1/2}r^2/2)\\ \psi_{\mathrm{div}}&\sim\exp(v_1r/2v_2^{1/2}+v_2^{1/2}r^2/2)\end{aligned} \tag{3}$$

when $r\to\infty$.

On introducing the ansatz

$$\psi=r^{l+1}\exp(-a_1r-a_2r^2/2)\sum_{j=0}^{\infty}C_jr^j \tag{4}$$

into (2) it is found that the coefficients C_j satisfy the following five-term recurrence relation:

$$\begin{aligned}(j+2)(j+2l+3)C_{j+2}-(2j+2l+4)a_1C_{j+1}+[a_1^2+E-(2j+2l+3)]C_j\\ +(2a_1a_2-v_1)C_{j-1}+(a_2^2-v_2)C_{j-2}=0\end{aligned} \tag{5}$$

where $j=-1,0,1,\ldots,$ and $C_j=0$ if $j<0$.

The HDM consists of choosing those E values for which the determinant of this set of linear homogeneous equations truncated up to C_N vanishes. This criterion proves to be equivalent to the boundary condition $C_{N+1}=0$.

If $a_1=v_1/2v_2^{1/2}$ and $a_2=v_2^{1/2}$, (5) becomes a three-term recurrence relation which is amenable to continued fraction or tridiagonal matrix eigenvalue techniques. However, the procedures related to the HDM are useless when $v_1<0$.

Killingbeck [14] chose $a_2=v_2^{1/2}$ and $a_1=Ra_2$ for the rotating oscillator ($v_1=-2v_2$) and proceeded to calculate the HDM eigenvalues for several R values. The method yielded the actual eigenvalues when $R>1.5$ and those of the partner potential (which has the sign of v_2 reversed) when $R<1.5$. This fact explains the failure of the procedures based on the three-term recurrence relation ($R=-1$).

Killingbeck's [14] results can be easily proved in a rigorous way. To this end we set $a_2 = v_2^{1/2}$ and $a_1 = Rv_1/2v_2^{1/2}$. Therefore when $R = -1$ we have a three-term recurrence relation and it is shown below that:

(a) if $v_1 > 0$ the HDM coefficients C_j lead to a function $\Phi = C_0 + C_1 r + \ldots + C_n r^n + \ldots$ bounded on the whole real axis so that $\psi \sim \psi_{\text{conv}}$ (cf (3) and (4)) at infinity.

(b) If $v_1 < 0$ then $\psi \sim \psi_{\text{div}}$ and the HDM is unsuitable.

The theory of linear difference equations [4, 17, 18] tells us that any hth-order linear homogeneous recurrence has h independent solutions $C_j^{(1)}, C_j^{(2)}, \ldots, C_j^{(h)}$ that are asymptotically well contrasted, i.e. $|C_j^{(1)}| \geqslant |C_j^{(2)}| \geqslant \ldots \geqslant |C_j^{(h)}|$ for large enough j. $C_j^{(1)}$, $C_j^{(h)}$ and $C_j^{(i)}$ $(1 < i < h)$ are termed dominant, subdominant and intermediate, respectively. It is well known that $C_j^{(1)}$ and $C_j^{(h)}$ are stable when using the forward and backward (i.e. Miller's algorithm) recurrences, respectively [18, 19]. The other solutions can be selected by means of the extended Miller's algorithm due to Oliver [20]. Besides, Hautot [8, 12] showed that setting the Hill determinant equal to zero amounts to searching for $C_j^{(2)}$. The asymptotic form of $C_j^{(2)}$ determines that of Φ. In order to obtain the latter one we proceed as discussed by Hautot [12]. Stirling's formula and the saddle-point method lead to

$$\sum_{j=0}^{\infty} C_j r^j = \sum_{j=0}^{\infty} \exp[f(j, r)] \sim \int_0^{\infty} \exp[f(j, r)]\, \mathrm{d}j \sim \exp[f(j^*, r)] \tag{6}$$

where $f(j, r) = \ln C_j + j \ln r$ and j^* is a root of $\partial f/\partial j = 0$.

For the particular case discussed in (a) and (b) one has $h = 2$ and the solutions are found to be asymptotic to

$$\begin{aligned} Z_j^{(1)} &= (2a_2)^{j/2}\Gamma(j)^{-1/2} j^{-a_1^2/4a_2} \exp[2a_1(j/2a_2)^{1/2}] \\ Z_j^{(2)} &= (-2a_2)\Gamma(j)^{-1/2} j^{-a_1^2/4a_2} \exp[-2a_1(j/2a_2)^{1/2}]. \end{aligned} \tag{7}$$

It follows immediately that $C_j^{(1)} \sim Z_j^{(1)}$ or $C_j^{(1)} \sim Z_j^{(2)}$ provided $v_1 > 0$ or $v_1 < 0$, respectively. Since $\Phi[Z_j^{(1)}] \sim \exp(2a_1 r + a_2 r^2)$ it is concluded that $\Phi[Z_j^{(2)}]$ has to be bounded. Therefore the standard HDM will lead to a bounded eigenfunction only when $v_1 > 0$, because in this case $C_j^{(2)} \sim Z_j^{(2)}$.

When $R \neq -1$ we have a four-term recurrence relation (third-order difference equation). The three linear independent solutions are asymptotic to

$$\begin{aligned} Z_j^{(1)} &= (2a_2)^{j/2}\Gamma(j)^{-1/2} j^{-(a_1-a_2)^2/16a_2} \exp[(a_1 - a_2)(2a_2)^{-1/2} j^{1/2}] \\ Z_j^{(2)} &= (-1)^j (2a_2)^{j/2}\Gamma(j)^{-1/2} j^{-(a_1-a_2)^2/16a_2} \exp[(a_2 - a_1)(2a_2)^{-1/2} j^{1/2}] \\ Z_j^{(3)} &= (a_1 + a_2)^j \Gamma(j)^{-1}. \end{aligned} \tag{8}$$

If $R > 1$ then $a_1 > a_2$ and $|Z_j^{(1)}| > |Z_j^{(2)}|$. It follows that $C_j^{(2)} \sim Z_j^{(2)}$ with the initial conditions $C_j^{(2)} = 0$ if $j < 0$. On arguing as before it is found that $C_j^{(2)}$ leads to ψ_{conv} and therefore the HDM yields the actual eigenvalues for all v_1 and v_2 values. If, on the other hand, $R < 1$, then the HDM selects ψ_{div} and the actual eigenvalues are not obtained. It is certainly difficult to explain how the eigenvalues of the partner potential occur when negative R values are used. However, the present argument clearly shows why Killingbeck [14] obtained the 'physical' eigenvalues when $R > 1.5$. Besides, when $1.5 > R > 1$ the R values are close to the critical value and the convergence is expected to be slow, in agreement with Killingbeck's results [14].

3. Rational potential

The Schrödinger equation

$$-\psi''(x)+[x^2+\lambda x^2/(1+gx^2)]\psi(x)=E\psi(x) \tag{9}$$

where $-\infty<x<\infty$, has been studied by many authors using variational techniques [21, 22], perturbation theory [23] and the perturbed operator method [24]. Exact solutions can be found for particular values of λ and g [15, 16, 25-27].

When the wavefunction is written as a linear combination of harmonic oscillator eigenfunctions the HDM proves to yield the actual eigenvalues [4]. If, on the other hand, the wavefunction is written

$$\psi(x)=P(t)\,\mathrm{e}^{-t/2} \qquad P(t)=\sum_{j=0}^{\infty} C_j t^j \qquad t=x^2 \tag{10}$$

the following three-term recurrence relation is obtained [15, 16]:

$$2(j+1)(2j+1)C_{j+1}+[E-1+j(4gj-2g-4)]C_j+[Eg-\lambda-g+4g(j-1)]C_{j-1}=0$$
$$j=0, 1, \ldots . \tag{11}$$

Whitehead *et al* [15] pointed out that the coefficients C_j obtained from (11) satisfy $C_{j+1}/C_j\to 0$ as $j\to\infty$. This is certainly not the case because, according to the Poincaré-Penon theorem [18, 28], there are two solutions, namely $C_j^{(1)}$ and $C_j^{(2)}$, leading to $C_{j+1}^{(1)}/C_j^{(1)}\to -g$ and $C_{j+1}^{(2)}/C_j^{(2)}\to 0$ as $j\to\infty$. The asymptotic behaviour of $C_j^{(1)}$ originates in the singular point of the potential at $x=\pm ig$. Furthermore, a straightforward calculation shows that $C_j^{(1)}$ and $C_j^{(2)}$ are asymptotic to

$$Z_j^{(1)}=(-g)^j j^{-2}\exp[-(1+\lambda/4g+g/2)/gj]$$
$$Z_j^{(2)}=j^{(\lambda-g-Eg)/4g}\Gamma(j)^{-1}\exp[(\lambda-g-Eg)/32g^2 j] \tag{12}$$

respectively.

Therefore, on proceeding as before one concludes that the non-dominant solution $C_j^{(2)}$ selected by the HDM leads to $P(t)\sim \mathrm{e}^t$ (up to unimportant factors). In other words the HDM fails to give a well behaved wavefunction except in those cases where $P(t)$ has a finite number of terms [15, 16, 25-27].

One may try to improve the HDM by choosing the more general ansatz

$$\psi=P(t)\,\mathrm{e}^{-\beta t/2} \tag{13}$$

that gives rise to the four-term recurrence relation:

$$-(2j+1)(2j+2)C_{j+1}+[\beta(4j+1)-E-2gj(2j-1)]C_j$$
$$+[g\beta(4j-3)-\beta^2+\lambda+1-Eg]C_{j-1}+g(1-\beta^2)C_{j-2}=0. \tag{14}$$

If $\beta>0$ the three solutions $C_j^{(1)}$, $C_j^{(2)}$ and $C_j^{(3)}$ are found to be asymptotic to (up to unimportant factors)

$$Z_j^{(1)}=(-g)^j j^{-2}$$
$$Z_j^{(2)}=(\beta+1)^j/2^j\Gamma(j) \tag{15}$$
$$Z_j^{(3)}=(\beta-1)^j/2^j\Gamma(j)$$

respectively. Therefore, the HDM does not yield a well behaved eigenfunction because $C_j^{(2)}$ leads to $P(t)\sim\exp[(\beta+1)t/2]$ for large t values. A similar conclusion can be drawn for $\beta<0$, showing that the standard HDM cannot be improved in this case by means of the adjustable parameter β. As said before, if P is written as a linear combination of Hermite polynomials the HDM yields the actual eigenvalues [4].

4. Further comments and conclusions

It has been shown that the HDM applies to the rotating oscillator provided the ansatz is properly chosen and that such a method is useless in treating certain rational potentials. It has not been difficult to give rigorous proofs because in both cases the HDM gives rise to finite-order difference equations.

Other problems cannot be treated so easily. For instance, in order to apply the HDM to the rotational-vibrational motion of diatomic molecules one has to expand the internuclear potential in Taylor series around the potential minimum and the resulting difference equation has an infinite number of terms [6]. In such a case the applicability of the HDM may be determined by numerical investigation.

In closing it is worth mentioning that the HDM does not provide bounds to the energy levels. Upper bounds to them can be obtained by the closely related zero-coefficient method, which is a particular form of solving the Rayleigh-Ritz secular equations [29]. General powerful methods for obtaining bounds to the properties of a quantum mechanical system are available. Among them we mention the inner projection method [30] and Padé approximants of the generalised Brillouin-Wigner perturbation theory [31].

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