False eigenvalues of the Hill determinant method

1988 J. Phys. A: Math. Gen. 21 567

(http://iopscience.iop.org/0305-4470/21/2/035)

J. Phys. A: Math. Gen. 21 (1988) 567-568. Printed in the UK

COMMENT

False eigenvalues of the Hill determinant method

R N Chaudhuri

Department of Physics, Visva-Bharati University, Santiniketan 731235, West Bengal, India

Received 22 July 1987

Abstract. It is shown analytically that the false eigenenergies of a potential obtained by the method of Hill determinants are the physical energies of a different potential.

Recently, Killingbeck (1986) has observed numerically a relationship between the false eigenvalues, as obtained by the Ginsberg-Killingbeck (Ginsberg 1982, Killingbeck 1986) version of the Hill determinant method, for the potential $-r^{-1}+r+r^2$ and the true energies for the potential $r^{-1}-r+r^2$. In the present comment we have demonstrated analytically that the following is a general rule. Given a potential $V(r)=a/r+br+cr^2$ when $c>0$, those eigenvalues identified as false by Killingbeck's method are in fact true eigenvalues of the associated potential $V''(r)=-a/r-br+cr^2$.

For the perturbed Coulomb potential

$$V(r)=a/r+br+cr^2 \qquad c>0. \tag{1}$$

Killingbeck has shown numerically that the false eigenvalues reveal themselves by having negative values for the expectation values of r and r^{-1} obtained by the technique developed by him (Killingbeck 1985). If a potential term λr^n is added to the Hamiltonian the change in energy according to the first-order perturbation theory is

$$\delta E=\lambda\langle r^n\rangle \tag{2}$$

where λ is quite small. Killingbeck (1986) has applied this equation to compute $\langle r\rangle$ and $\langle r^{-1}\rangle$ for the potential (1) and obtained the negative results for some values of the parameters. (For a more detailed explanation of the $\langle r^n\rangle$ computations the reader is referred to equation (5) of Killingbeck (1986).) We explain here why the Hill determinant method yields such unphysical results.

By applying the simple power-series ansatz

$$\psi(r)=r^{l+1}\exp(-\beta r^2-\alpha r)\sum_{n=0}^{\infty}A_n r^n \tag{3}$$

to the radial Schrödinger equation

$$-D^2\psi+[V(r)+l(l+1)/r^2]\psi=E\psi \tag{4}$$

the differential equation (4) is transformed to the difference equation

$$b_nA_{n+1}+a_nA_n+c_nA_{n-1}+d_nA_{n-2}=0 \qquad n\geqslant 0 \tag{5}$$

with

$$b_n=(n+1)(n+2l+2)$$
$$a_n=-2\alpha(n+l+1)-a$$
$$c_n=-2\beta(2n+2l+1)+\alpha^2+E$$
$$d_n=4\alpha\beta-b$$
$$\beta=\tfrac{1}{2}\sqrt{c}>0 \qquad A_{-1}=A_{-2}=0.$$

The eigenvalue condition of the Hill determinant for large N is

$$\det Q_N = 0 \tag{6}$$

$$Q_N = \begin{pmatrix} a_0 & b_0 & 0 & 0 & \dots & & \\ c_1 & a_1 & b_1 & 0 & \dots & & \\ d_2 & c_2 & a_2 & b_2 & \dots & & \\ \vdots & & & & & & \\ 0 & \dots & & 0 & d_{N-1} & c_{N-1} & a_{N-1} \end{pmatrix}. \tag{7}$$

It may be noted that

$$A_N = (-1)^N A_0 \det Q_N/(b_0 b_1 \dots b_{N-1}) \tag{8}$$

which shows that the vanishing of $\det Q_N$ ensures the vanishing of A_N. Killingbeck (1986) has computed the eigenvalues from the zeros of A_N in terms of the parameter E for some large N and obtained the physical eigenenergies for the potential (1) with a sufficiently large positive α. As soon as the sign of α is reversed and made negative the unphysical eigenvalues are produced in this method. When we change $\alpha \to -\alpha$ in equation (7) we get the determinant Q'_N which is completely different from $\det Q_N$ and therefore we get different eigenvalues from the zeros of the two determinants. However, in (7) if we do not change the sign of α, but change the signs of a and b, i.e. $\alpha \to \alpha$, $a \to -a$ and $b \to -b$ we get the determinant Q''_N with the following property:

$$\det Q''_N = (-1)^N \det Q'_N. \tag{9}$$

Thus the false eigenvalues of the potential $a/r + br + cr^2$ obtained from $\det Q'_N = 0$ are the physical eigenvalues of the potential $-a/r - br + cr^2$ obtained from $\det Q''_N = 0$. Killingbeck (1986) discovered this finding by the process of computation. Here we establish the result analytically.

Killingbeck (1986) has applied equation (2) for computation of $\langle r^n \rangle$ from $\det Q'_N = 0$ which gives negative values of $\langle r \rangle$ and $\langle r^{-1} \rangle$. It may be noted that the zeros of $\det Q''_N$ are identically the same as those of $\det Q'_N$ leading to the same value of δE, but the sign of λ in equation (2) is reversed. Thus the false eigenvalues of the table 1 of the paper of Killingbeck (1986) should be reinterpreted accordingly. If x and y are the expectation values of r and r^{-1} as obtained from (2) for the potential $-r^{-1} + r + r^2$ in case of false eigenvalues derived from the equation $\det Q'_N = 0$, the false energies agree with the true energies for the potential $r^{-1} - r + r^2$ and the expectation values of r and r^{-1} for the potential $r^{-1} - r + r^2$ according to equation (2) are $-x$ and $-y$ giving positive sign to the expectation values when x and y are negative.

References

Ginsberg C A 1982 *Phys. Rev. Lett.* **48** 839
Killingbeck J 1985 *J. Phys. A: Math. Gen.* **18** L1025
—— 1986 *J. Phys. A: Math. Gen.* **19** 2903