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COMMENT

**On the Hill determinant method**

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**Abstract.** Explicit examples are given of the false eigenvalues of the Hill determinant method, the existence of which had been suspected by workers using analytic methods. A simple criterion is discovered for distinguishing between false and physical eigenvalues.

**1. Introduction**

In recent years several workers have suggested on mathematical grounds that the Hill determinant method can give false (i.e. unphysical) eigenvalues for a Schrödinger equation which involves perturbed oscillator or perturbed Coulomb potentials. In particular, Flessas (1982) suggested that the Hill determinant approach of Datta and Mukherjee (1980) could give false eigenvalues for a radial Schrödinger equation of the form

$$-D^2\psi + \sum_{-2}^2 V(m)r^m\psi = E\psi. \tag{1}$$

Until recently, an explicit example of such a false eigenvalue had not been published. Chaudhuri (1985) established analytically for a special perturbed oscillator problem that the Hill determinant eigenvalues must differ from those of the associated Schrödinger equation. Killingbeck (1986) finally gave explicit examples of false eigenvalues and showed that they share several of the properties of the physical eigenvalues. In the present comment we give the first examples of false eigenvalues for a perturbed Coulomb potential and show that it is possible to generate at will either physical or false eigenvalues. The false eigenvalues reveal themselves by having a negative value for the expectation values  $\langle r \rangle$  and  $\langle r^{-1} \rangle$ , when the expectation values are defined by the standard equation

$$\langle r^n \rangle = \partial E / \partial V(n) \tag{2}$$

and the  $V(n)$  are the potential coefficients in the Schrödinger equation (1).

Since equation (2) plays a key role in the calculation, we should first clarify its connection with the traditional formula for an expectation value.  $\langle r^n \rangle$  would usually be obtained as an integral involving the product  $\psi^2 r^n$ , with  $\psi$  a normalised wavefunction. However, first-order perturbation theory shows that adding a small extra perturbing potential  $\lambda r^n$  to the Hamiltonian will produce an energy change  $\lambda \langle r^n \rangle$ . Thus  $\langle r^n \rangle$  can alternatively be regarded as a response coefficient and can be obtained by monitoring how the energy eigenvalue changes as the coefficient of  $r^n$  increases. It is this point of view which leads to equation (2) and it has the advantage that it can be applied directly in energy calculations (by varying the potential slightly) without actually

forming a normalised wavefunction and calculating integrals. For a proper bound state the integral definition and the response coefficient definition of  $\langle r^n \rangle$  give the same number. However, from the integral definition it is clear that  $\langle r^n \rangle$  must be positive for a physical state, whereas (as we see in what follows) application of the response coefficient view can lead to negative values. These cannot correspond to a proper physical state. In terms of the energy, a negative  $\langle r^n \rangle$  indicates an eigenvalue which *falls* if the coefficient of  $r^n$  in the potential increases, whereas it is clear that for the correct physical states the eigenvalues must *increase* as more of the positive definite operator  $r^n$  is added to the potential. Thus a negative value for  $\langle r^n \rangle$ , as defined by equation (2), reveals an energy eigenvalue which 'goes the wrong way' as the potential strength is increased.

## 2. Method of calculation

We proceed by inserting into equation (1) the ansatz

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

for states of angular momentum  $l$ . For such states the coefficient  $V(-2)$  in the Schrödinger equation (1) is assigned the value  $l(l+1)$ . After a little algebra we obtain the recurrence relation

$$\begin{aligned} & [(n+1)(n+2) - l(l+1)]A(n+2) \\ &= [V(-1) + 2\alpha(n+1)]A(n+1) + [(4n+2)\beta - \alpha^2 - E]A(n) \\ &+ [V(1) - 4\alpha\beta]A(n-1) + [V(2) - 4\beta^2]A(n-2). \end{aligned} \quad (4)$$

To use (4) the initial value  $A(l+1) = 1$  is used, with all preceding  $A(n)$  zero. The relation (4) is then used to compute  $A(N)$  for some large  $N$  (typically 50) and for a trial  $E$  value.  $E$  is then varied and the eigenvalues  $E_n$  are the  $E$  values which make  $A(N)$  zero. The idea of the method is that the  $E_n$  should tend to limiting values (indeed, the eigenvalues of the Schrödinger equation (1)) as  $N$  increases. Ginsburg (1982) has used this approach to obtain eigenvalues and Killingbeck (1985a) showed that it is equivalent to the usual (but more tedious) one which evaluates Hill determinants of increasing size. He also extended the method to permit the direct evaluation of expectation values. To calculate  $\langle r^n \rangle$  by this method we differentiate the recurrence relation (4) with respect to  $E$  and  $V(n)$  and then use equation (2) in conjunction with the equation

$$\frac{\partial E}{\partial V(n)} = -\frac{\partial A(N)}{\partial V(n)} \left( \frac{\partial A(N)}{\partial E} \right)^{-1}. \quad (5)$$

All of the recurrence relations involved use the same coefficients, which simplifies the computations. The details of the computation have been described in two previous works (Killingbeck 1985a, b) and we concentrate here on the distinction between physical and false eigenvalues.

## 3. Physical and false eigenvalues

To simplify the calculation we choose  $\beta$  such that  $4\beta^2 = V(2)$ , with  $\beta > 0$ , which removes one term from the recurrence relation (4). We assume  $V(2)$  to be non-negative

to ensure the existence of proper bound states. It would be possible to choose  $\alpha$  to render (4) a three-term recurrence relation, corresponding to a tridiagonal matrix eigenvalue problem. This choice was in fact made by Datta and Mukherjee (1980), but we have discovered that by leaving  $\alpha$  variable we can produce either physical or false eigenvalues. For a sufficiently large positive  $\alpha$  the eigenvalues are the correct Schrödinger equation ones. As  $\alpha$  is decreased a region of very slow convergence is reached, below which the false eigenvalues are produced. When the calculation converges it produces either the physical or the false eigenvalues, not any varying intermediate values (i.e. it jumps from one mode of operation to the other). Table 1 shows some typical results, which illustrate the negative values of  $\langle r \rangle$  and  $\langle r^{-1} \rangle$  which we found to be invariably associated with the false eigenvalues. For the case of the oscillator potential  $V = r^2$  we found that the false and physical energies agreed, with the false  $\langle r \rangle$  and  $\langle r^{-1} \rangle$  values being exactly the negatives of the physical values. This special case suggests that there might be a functional relationship between the false and physical numbers, but so far we have not been able to discover it. (We should note that in the case of perturbed oscillator problems Znojil (1986) has shown that our computed false energies can be regarded as physical energies for a different potential.) However, this comment shows that (for a fixed potential) the false energies, which until recently were only theoretically conjectured, can be generated and also distinguished from the physical energies. Indeed, it turns out that it is the recently developed technique of expectation value calculation (Killingbeck 1985a) which enables the distinction to be made.

Table 1. Specimen results for the potential  $-r^{-1} + r + r^2$ .

$\alpha, l$	$E$	$\langle r \rangle$	$\langle r^{-1} \rangle$
5, 0	2.750 000 0	0.926 727 79	1.426 727 8
	7.621 433 7	1.549 650 9	1.054 078 3
-5, 0	2.750 000 0	-1.382 043 4	-0.882 043 39
	6.105 909 7	-1.861 464 3	-0.819 485 64
5, 1	5.621 433 7	1.345 281 4	0.849 708 83
	10.180 899	1.822 100 8	0.735 570 90
-5, 1	4.105 909 7	-1.699 964 6	-0.657 985 85
	7.615 295 3	-2.112 118 4	-0.617 103 66
5, 2	8.100 743 9	1.659 873 5	0.657 591 17
	12.547 301	2.062 574 6	0.598 200 53
-5, 2	5.683 783 2	-1.979 952 2	-0.545 754 25
	9.273 235 1	-2.342 381	-0.518 378 48

*Note added.* We have discovered, by computation and by analysis of (4), that the false energies (with  $\alpha = -5$ ) in table 1 agree with the true energies (with  $\alpha = 5$ ) for the different potential  $r^{-1} - r + r^2$ .

## References

- Chaudhuri R N 1985 *Phys. Rev. D* **31** 2687  
 Datta D P and Mukherjee S 1980 *J. Phys. A: Math. Gen.* **13** 3161  
 Flessas G P 1982 *J. Phys. A: Math. Gen.* **15** L1

- Ginsburg C A 1982 *Phys. Rev. Lett.* **48** 839  
Killingbeck J 1985a *J. Phys. A: Math. Gen.* **18** L1025  
— 1985b *J. Phys. A: Math. Gen.* **18** 245  
— 1986 *Phys. Lett.* A in press  
Znojil M 1986 *Phys. Lett.* A in press