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COMMENT

Moment approach for mixed parity potentials

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Abstract. A moment approach to the calculation of energy levels for mixed parity potentials is described and is tested by means of a formula from the theory of odd parity perturbations.

1. Introduction

The use of so-called moment or inner product methods for the calculation of the eigenvalues of the perturbed oscillator Schrödinger equation

$$H\psi = -D^2\psi + \sum V_M x^M \psi = E\psi \quad (1)$$

(with $M = 2, 4, 6$) has been described by several authors (Blankenbecler *et al* 1980, Killingbeck *et al* 1985, Handy and Bessis 1985). In this comment we show that one such method can be extended to work for potentials of mixed parity and then use it in conjunction with a formula of perturbation theory which we derive from an argument involving translational invariance. Section 2 describes the moment method, § 3 presents the relevant perturbation theory and § 4 gives some illustrative numerical results.

2. Use of the recurrence relations

The methods of calculation used by the authors cited above start from the equation

$$\langle \phi | x^N H | \psi \rangle = E \langle \phi | x^N | \psi \rangle \quad (2)$$

obtained by taking the inner product of the Schrödinger equation (1) with the product $x^N \phi$, where the reference function

$$\phi = \exp(-\beta x^2/2) \quad (3)$$

contains an adjustable parameter β . Using the H of (1) to work out the left-hand side of (2) gives the recurrence relation

$$N(N-1)S_{N-2} = [(2N+1)\beta - E]S_N - \beta^2 S_{N+2} + \sum V_M S_{N+M} \quad (4)$$

where the S_N , sometimes called moments, are defined by

$$S_N = \langle \phi | x^N | \psi \rangle \quad (5)$$

for some fixed (but arbitrary) normalisation of ϕ and ψ .

When the indices M in (1) are all even integers, then the eigenfunctions ψ have a well defined parity. In that case (Killingbeck 1987) the even parity energies are found by setting

$$S_Q = 1 \quad S_N = 0 \quad (N > Q) \quad (6)$$

(for a sufficiently large even integer Q) and picking a trial E value. The S_N for even N down to $N=0$ are then evaluated using (4) and the function

$$F_0(E) = (\beta - E)S_0 - \beta^2 S_2 + \sum V_M S_M \tag{7}$$

is rendered zero by varying E . Odd parity levels are found by using an odd integer Q in the initial condition (6) and by varying E to render zero the function

$$F_1(E) = (3\beta - E)S_1 - \beta^2 S_3 + \sum V_M S_{M+1}. \tag{8}$$

We observe that in calculating each energy level we actually make *both* $F_0(E)$ and $F_1(E)$ zero, with one equation being fulfilled trivially. To find the energy levels for mixed parity potentials we *again* make both functions zero, but now have a non-trivial problem, since the odd parity terms in the potential couple together the S_N with even and odd N . Equation (4) gives us the value of S_0, S_1 , etc to insert in (7) and (8), provided that we have the right starting values at large N . We found that the appropriate procedure is to use the conditions

$$S_Q = 1 \quad S_{Q-1} = R \quad S_N = 0 \quad (N > Q) \tag{9}$$

and to vary *both* R and E to render both $F_0(E)$ and $F_1(E)$ zero. To solve the two-variable problem the most simple approach is to find first an energy level with the odd parity terms omitted (so that R is zero). For example, to find an even parity level we vary E to make $F_0(E)$ zero, holding R at zero, with Q a sufficiently large even integer. Then, with the odd parity terms turned on, we still vary E (with R fixed) to make $F_0(E)$ zero, but also vary R (with E fixed) to make $F_1(E)$ zero. This sequential process, which modifies one variable at a time, converges quickly when the odd parity terms do not displace the initial energy by much. (This point is discussed further in § 3.)

3. A special perturbation formula

In general, when an even parity potential V gives rise to an energy level E_0 , the effect of adding an odd parity potential λF to V is to perturb the energy level in a way described by the perturbation series

$$E(\lambda) = E_0 + \lambda^2 E_2 + \lambda^4 E_4 + \dots \tag{10}$$

in which only even powers of λ appear (Byers Brown 1972). The effective strength of the odd parity perturbation is thus of order λ^2 , which helps to explain why the computational procedure described in this work is successful.

For the Schrödinger equation in one dimension, with boundary conditions $\psi(\pm\infty) = 0$, we have the obvious principle that a translational shift of the potential should not affect the bound state energies. However, from the viewpoint of perturbation theory a change of the potential from $V(x)$ to $V(x + \delta)$ changes the potential to

$$V(x + \delta) = V(x) + \delta V'(x) + \frac{1}{2} \delta^2 V''(x) + \dots \tag{11}$$

and so should change the energy to

$$E(\delta) = E_0 + \delta E_1(V, V') + \delta^2 [\frac{1}{2} E_1(V, V'') + E_2(V, V')] + \dots \tag{12}$$

where $E_n(V, F)$ denotes the n th order energy perturbation coefficient for a perturbation λF added to the potential V . Since the energy is actually unchanged we obtain from (12) the results

$$E_1(V, V') = \langle \psi | V' | \psi \rangle = 0 \tag{13}$$

$$E_2(V, V') = -\frac{1}{2} E_1(V, V'') = -\frac{1}{2} \langle \psi | V'' | \psi \rangle \tag{14}$$

where ψ is any bound state eigenfunction associated with the potential V . Equation (13) is the usual result that the mean force is zero. From the less familiar equation (14) we can produce results such as $E_2(x^2, x) = -\frac{1}{4}$ and $E_2(x^4, x^3) = -\frac{3}{8}\langle\psi|x^2|\psi\rangle$, which can be used to provide tests of the numerical method described in § 2.

4. Specimen results

We give some results obtained by applying the method of § 2 to calculate the quantities on both sides of the equation

$$E_2(x^4, x^3) = -\frac{3}{8}\langle\psi|x^2|\psi\rangle. \tag{15}$$

To calculate a quantity such as $\langle x^2 \rangle$ an approach based on energies can be used (Killingbeck 1985) by applying the prescription

$$2\varepsilon\langle x^2 \rangle = E(x^4 + \varepsilon x^2) - E(x^4 - \varepsilon x^2) \tag{16}$$

in the limit $\varepsilon \rightarrow 0$. The computation actually uses two or three small ε values and the Richardson extrapolation. To calculate $E_2(x^4, x^3)$ involves taking a one-sided derivative using the equation

$$\varepsilon^2 E_2(x^4, x^3) = E(x^4 + \varepsilon x^3) - E(x^4) \tag{17}$$

(for $\varepsilon \rightarrow 0$). Applying (16) and (17) to verify (15) thus provides a reasonably severe test of the accuracy of the energy values produced by the modified moment technique described earlier. Readers wishing to implement the methods of this work should note that computer underflow and overflow problems can be minimised by using the quantities $F^N S_N$ instead of S_N , with F some simple scaling factor. The required modification in the algebra is straightforward.

Table 1 shows some energy results for the four lowest states associated with the potential x^4 . The value of the parameter Q was set at 50 for the states with mainly even parity and at 51 for the states with mainly odd parity. Adding 10 to Q did not change the energies. The roots of the functions F_0 and F_1 were located quickly by using the numerical Newton's method (Killingbeck 1985) which locates the roots of a function $f(x)$ by using the iterative formula

$$x' = x + hf(x)[f(x) - f(x + h)]^{-1} \tag{18}$$

with $h = 10^{-3}$. A single ε value of 10^{-2} in (16) was found to be adequate to find $\langle x^2 \rangle$ to five digits for the states considered.

Table 1. Lowest four energy levels for the case $V_1 = 0$ and various values of $V = (V_2, V_3, V_4)$. $\beta = 5$ throughout.

V				
(0, 0, 1)	1.060 3621	3.799 6730	7.455 6980	11.644 746
(0, 0.1, 1)	1.059 0028	3.796 2900	7.451 0284	11.638 902
(0, 0.2, 1)	1.054 9051	3.786 1172	7.436 9980	11.621 348
(0.01, 0, 1)	1.063 9789	3.808 6833	7.468 1404	11.660 320
(-0.01, 0, 1)	1.056 7384	3.790 6512	7.443 2461	11.629 162

The use of the results in the table in conjunction with formulae (16) and (17) shows that the theoretical relation (15) is obeyed and provides the following numerical values for the quantity $|E_2(x^4, x^3)|$ associated with the four lowest states:

0.135 76 0.338 10 0.466 77 0.584 21.

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