The perturbed two-dimensional oscillator

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Abstract. A renormalised version of inner product theory is used to give accurate energies for six states of a perturbed two-dimensional oscillator and to obtain the Rayleigh-Schrödinger energy perturbation series.

1. Introduction

The inner product method of eigenvalue calculation investigated by Blankenbecler *et al* (1980) was recently extended by Killingbeck *et al* (1985) and applied to several one-dimensional problems. In the latter work it was stated that the perturbation theory based on the inner product approach is valid only for ground states. We have since established that the method can be modified quite easily to apply to excited states and to problems in more than one dimension. This paper is intended to point out the flexibility of the inner product perturbation theory, which gives it an advantage over the hypervirial method (Killingbeck 1981) and the method of Bender and Wu (1969). The particular example which we consider is that of the Schrödinger equation with a Hamiltonian of the perturbed oscillator form $-\nabla^2 + x^2 + y^2 + V(x, y)$, with

$$V(x, y) = \lambda[A(x^4 + y^4) + Bx^2y^2]. \tag{1.1}$$

The potential is non-separable but shows a high symmetry; this cuts down the amount of computation required, although the more general anisotropic case can also be treated by the method. Since the energy perturbation series is expected to be divergent, we start by introducing a renormalisation parameter β (Killingbeck 1981) and write the potential in the form

$$\mu^2(x^2 + y^2) + \lambda[V(x, y) - \beta(x^2 + y^2)]. \tag{1.2}$$

We set $\mu^2 = 1 + \lambda\beta$, so that the total potential is invariant but the portion of it used as the perturbation varies with β. The use of a variable β is helpful in improving convergence in the hypervirial approach and would also improve convergence in those techniques which involve matrix diagonalisation (Hioe *et al* 1978, Pullen and Edmonds 1981). The present approach does not require the matrix elements of $V(x, y)$ in any basis, but is based on a recurrence relation which can be handled by a simple computer program. We should emphasise again a point made previously (Killingbeck 1981); direct use of the β parameter is computationally preferable to the alternative route (Caswell 1979) of first obtaining the traditional ($\beta = 0$) series and then transforming it. The divergence of the series means that the latter approach often needs double precision arithmetic to get single precision results.

2. The recurrence relation and its use

The inner product approach uses a reference function

$$\phi = x^{P_1} y^{P_2} \exp[-(\mu/2)(x^2 + y^2)] \tag{2.1}$$

with μ having the same numerical value as in (1.2) and with the x and y parity indices P_1 and P_2 equal to 0 (even) or 1 (odd). The inner products

$$S(M, N) = \langle \phi | x^{2M} y^{2N} | \psi \rangle \tag{2.2}$$

play a key role in the method. Here ψ is a solution of the Schrödinger equation $-\nabla^2 \psi + V\psi = E\psi$, with V written as in equation (1.2). The first step is to work out the quantity

$$ES(M, N) = \langle \psi | Hx^{2M} y^{2N} | \phi \rangle \tag{2.3}$$

by acting with the Hamiltonian $H = -\nabla^2 + V$ on the triple product to the right of it. The resulting collection of terms produces a recurrence relation between the $S(M, N)$ which we do not write down here, since it is visible in (2.6) below. The second step is to substitute the perturbation expansions

$$S(M, N) = \sum S(M, N, K)\lambda^K, \tag{2.4}$$

$$E = \sum E(K)\lambda^K, \tag{2.5}$$

into the $S(M, N)$ recurrence relation. The result is the new recurrence relation

$$\sum_1^K E(P)S(M, N, K - P) = AS(M + 2, N, K - 1) + AS(M, N + 2, K - 1)$$

$$+ BS(M + 1, N + 1, K - 1) - \beta S(M + 1, N, K - 1)$$

$$- \beta S(M, N + 1, K - 1) + 4\mu[M + N - S_1 - S_2]S(M, N, K)$$

$$- 2M(2M + 2P_1 - 1)S(M - 1, N, K)$$

$$- 2N(2N + 2P_2 - 1)S(M, N - 1, K). \tag{2.6}$$

In writing (2.6) we have moved one term $E(0) S(M, N, K)$ from the sum over P to the right of the equation and have adopted the convention that the unperturbed energy is expressed in the form

$$E(0) = \mu(2 + 2P_1 + 2P_2 + 4S_1 + 4S_2). \tag{2.7}$$

Choosing the x and y parity indices P_1 and P_2 (0 or 1) and the x and y state numbers S_1 and S_2 (0, 1, 2, ...) then specifies which particular state is being treated. If $P_1 = P_2$ we can further specify an x-y interchange symmetry index P_3 (0 or 1) such that

$$S(N, M, K) = (-1)^{P_3} S(M, N, K). \tag{2.8}$$

The initial condition imposed on the $S(N, M, K)$ if $P_1 = P_2$ is

$$S(S_1, S_2, 0) = (-1)^{P_3} S(S_2, S_1, 0) = 1 \tag{2.9}$$

and the recurrence relation (2.6) is then used as follows. If the energy sum up to $E(Q)\lambda^Q$ is required, then the indices have the ranges set out below if $P_1 = P_2$ (with the convention $S_1 \leq S_2$ on the state labels):

$$K = 0, 1, 2, \ldots, Q,$$
$$(\text{fixed } K) \ N = 0, 1, 2, \ldots, S_2 + 2Q - 2K, \tag{2.10}$$
$$(\text{fixed } K, N) \ M = 0, 1, \ldots, N - P_3.$$

The indices are scanned in the order given above and the relation (2.6) is used to work out $S(M, N, K)$ in terms of other elements which are already known. $S(N, M, K)$ is then filled in from the symmetry relation (2.8). For the special cases in which $M = S_1$ and $N = S_2$ the relation (2.6) is used differently. The sum on the left-hand side becomes $E(K)$, because of the intermediate normalisation convention $S(S_1, S_2) = 1$ which we impose on the algorithm. This gives the value of the energy coefficient $E(K)$ in terms of already calculated elements of the S array. The sum of the energy perturbation series can then be calculated term by term, and β is varied to give the best possible semi-convergence of the sequence of partial sums.

3. Results and checking calculations

The algorithm outlined in § 4 was implemented on a Sinclair Spectrum microcomputer and several checks were devised to verify that it was giving correct energy eigenvalues. A few relevant energies are available in the literature (Hioe *et al* 1978, Ari and Demiralp 1985). We obtained agreement with them, but found it better to devise more general checks. First, we set up a simplified version of the method for the one-dimensional perturbed oscillator and confirmed that varying the parameters P_1 and S_1 correctly gave the perturbation series for several excited states, with the hypervirial method (Killingbeck 1981) as the reference standard. Second, for the special cases ($A = 1, B = 0$) and ($A = 1, B = 2$) we checked the energies obtained using (2.6) against results for the potential $r^2 + \lambda r^4$ in one dimension ($A = 1, B = 0$) and two dimensions ($A = 1, B = 2$). The test energies were obtained very easily from a power series method of the kind described by Killingbeck (1985a). Table 1 shows the results of the calibratory calculation at $\lambda = 0.1$. The states are labelled by giving the x and y oscillator quantum numbers $(0, 1, 2, \dots)$ and the parity label e(even) or o(odd) for the x-y interchange symmetry. The first two columns of table 1 show how the numerical results give the correct degeneracies required by the high symmetry of the potential.

Table 1. Energies at $\lambda = 0.1$ (order 10 throughout). (The results in the first two columns were checked by the series method.)

State	$A = 1, B = 0$ ($\beta = 10$)	$A = 1, B = 2$ ($\beta = 10$)	$A = 0, B = 1$ ($\beta = 3$)
$(0, 0, e)$	2.130 5710	2.168 5972 ($m = 0$)	2.024 1383
$(0, 2, e)$	6.813 2448	7.039 7076 ($m = 0$)	6.159 2858
$(0, 2, o)$	6.813 2448	6.908 3321 ($m = \pm 2$)	6.071 6400
$(1, 1, e)$	6.613 7440	6.908 3321 ($m = \pm 2$)	6.208 2008
$(1, 3, e)$	11.659 550	12.415 256 ($m = \pm 2$)	10.588 282
$(1, 3, o)$	11.659 550	12.084 472 ($m = \pm 4$)	10.343 900

For the case of the perturbing potential $\lambda x^2 y^2$ (i.e. $A = 0, B = 1$) table 2 shows some of the $E(K)$ coefficients for three states. The three series are all alternating ones, but have $E(K)$ values with different orders of magnitude. Table 3 compares the ground state energies obtained by three methods.

(a) The present inner product perturbation calculation.

(b) The adiabatic approximation. The energies are those for the effective Hamiltonian $-D^2 + x^2 + [(1 + \lambda x^2)]^{1/2}$, since the ground state energy of the potential $y^2 + \lambda x^2 y^2$

Table 2. Energy coefficients at $\beta = 0$.

K	(0, 0, e)	(0, 2, e)	(0, 2, o)
0	2	6	6
1	0.25	1.75	0.75
2	−0.093 75	−1.875	−0.375
3	0.085 937 5	3.824 218 8	0.457 031 25
4	−0.118 774 41	−10.355 713	−0.816 650 39
5	0.213 490 8	33.578 262	1.846 176 1
6	−0.466 409 58	−124.042 91	−4.947 429
7	1.192 660 3	507.602 07	15.174 457
8	−3.485 569 2	−2 260.761 2	−52.143 241
9	11.451 354	10 834.694	197.915 20
10	−41.775.356	−55 439.400	−821.447 78

Table 3. Ground state energy estimates ($V = \lambda x^2 y^2$).

λ	Adiabatic	Perturbation	Axial
0.1	2.023 8954	2.024 1383	2.024 3369
0.2	2.045 9819	2.046 7957	2.047 4847
0.3	2.066 6736	2.068 2421	2.069 6098
0.4	2.086 2276	2.088 6677	2.090 8404
0.5	2.104 8347	2.108 2138	2.111 2784
0.6	2.122 6257	2.126 9899	2.131 0065

with x frozen is given by the square root term. A finite difference method was used to calculate the eigenvalues.

(c) An axial approximation, analogous to the spherical approximation used for the quadratic Zeeman effect (Killingbeck 1979). In two dimensions the identity

$$8x^2y^2 = r^4 + (6x^2y^2 - x^4 - y^4) \tag{3.1}$$

involves two terms. The first is a tensor operator with $m = 0$ (axial symmetry); the second is a sum of tensor operators with $m = \pm 4$, and will only affect the $m = 0$ ground

Table 4. Some energy values at order 40. $V = \lambda x^2 y^2$.

λ, β	State	Semi-converged energy (with Aitken extrapolation)
0.1, 2	(0, 0, e)	2.024 138 321 415 612 724 5
0.1, 2	(0, 2, e)	6.159 285 750 751 598
0.1, 2	(0, 2, o)	6.071 640 017 418 102 530
0.5, 2	(0, 0, e)	2.108 213 779 70
0.5, 3	(0, 2, e)	6.623 323 980 2
0.5, 2	(0, 2, o)	6.313 168 654
1, 3	(0, 0, e)	2.195 918 085
1, 3	(0, 2, e)	7.031 272 34
1, 3	(0, 2, o)	6.557 803 33

state energy in second and higher orders of perturbation theory. The axial approximation represents the potential $r^2 + \lambda x^2 y^2$ by $r^2 + \frac{1}{8}\lambda r^4$, which can be treated by power series methods (Killingbeck 1985a). The results of table 3 confirm what would be expected on mathematical grounds, namely that the energies from methods (b) and (c) straddle the true energy. By taking energy differences (Killingbeck 1985a, b) it is possible to evaluate $\langle x^2 y^2 \rangle$ at $\lambda = 0.5$. The values obtained (0.1818, 0.1914, 0.2007) show the same ordering as the energy values. Table 4 shows a few energies calculated to higher accuracy.

4. State labels and degeneracy

The state indices S_1 and S_2 of § 2 were chosen to simplify the recurrence relation (2.6); we can indicate how they are related to the indices used in table 1 by looking at the examples $(0, 2, e)$ and $(0, 2, o)$. We have $P_1 = P_2 = 0$ (even parity) and also $S_1 = 0$ (ground x state) and $S_2 = 1$ (first excited y state); these values give the correct $E(0)$ in (2.7). Further, the unperturbed function will have $S(0, 0) = 0$ because of the orthogonality properties of harmonic oscillator functions, but will have $S(0, 1) \neq 0$. To make $S(0, 1)$ equal 1 we set $S(0, 1, 0) = 1$ and $S(0, 1, K) = 0$ for $K > 0$, with $P_3 = \pm 1$ in the algorithm to give the e or o state. The later $S(M, N, K)$ are then proportional to $S(0, 1, 0)$ and so give $E(K)$ coefficients which are independent of the fixed $S(0, 1)$ value. The $S(M, N, 0)$ with $M < S_1$ and $N < S_2$ are zero, but those with $M \geq S_1$ and $N \geq S_2$ are not. The six states of table 1 can all be treated with these simple initial conditions, as can the state $(0, 1)$ of mixed parity, for which all the $S(M, N, K)$ have to be evaluated using (6), since $S(N, M, K)$ and $S(M, N, K)$ are not simply related. For higher states degeneracy problems arise. For example $(1, 2)$ and $(3, 0)$ are initially degenerate and linked by the potential, so the appropriate zeroth-order ratio of $S(0, 1, 0)$ and $S(1, 0, 0)$ has to be used in the initial conditions. However, with $S_1 + S_2 = 1$, $M = 1$, $N = 1$, $P_1 = 1$, $P_2 = 0$, $K = 0$ in (2.6) we find $S(1, 0, 0)$ in terms of $S(0, 1, 0)$ and can still set $S(0, 1, 0) = 1$ by convention. The states with $P_1 \neq P_2$ stick together in pairs, whereas the states with $P_1 = P_2$ show interesting splitting effects as A and B vary. The preliminary results reported here clearly illustrate the value of combining the renormalisation (variable β) technique with the inner product perturbation approach; the extensions of the method to treat the Henon–Heiles perturbation $\lambda(xy^2 - \frac{1}{3}x^3)$ and the three-dimensional perturbed oscillator are now under investigation.

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