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The perturbed three-dimensional oscillator

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Abstract. A renormalized version of inner product and hypervirial theories is used to calculate the energy eigenvalues for four states of a perturbed three-dimensional oscillator and to obtain the Rayleigh-Schrödinger energy perturbation series.

1. Introduction

The inner product method has been used by Killingbeck (1986) and Witwit (1991) and applies to the two-dimensional oscillator. We have since established that the method can be modified and extended quite easily to apply to problems in three dimensions. This paper is intended to point out the flexibility of the inner product perturbation theory, which gives it an advantage over the hypervirial method.

The particular example we consider is that of the Schrödinger equation with a Hamiltonian of the perturbed oscillator form

$$H = -\nabla^2 + x^2 + y^2 + z^2 + V_J(x, y, z) \qquad J = 1, 2 \tag{1}$$

where

$$V_{J=1}(x, y, z) = \lambda[a_{11}x^4 + a_{22}y^4 + a_{33}z^4 + 2a_{12}x^2y^2 + 2a_{13}x^2z^2 + 2a_{23}y^2z^2] \tag{2}$$

and

$$V_{J=2}(x, y, z) = \lambda[a_{11}x^6 + a_{22}y^6 + a_{33}z^6 + 6a_{123}x^2y^2z^2 + 3a_{13}x^4z^2 + 3a_{12}x^4y^2 + 3a_{23}y^4z^2 + 3a_{12}y^4x^2 + 3a_{13}z^4x^2 + 3a_{23}z^4y^2]. \tag{3}$$

The potentials (2) and (3) are non-separable but show a high symmetry; this cuts down the amount of computation required. The energy perturbation series is expected to be divergent, so we start by introducing a renormalization parameter (β), and write the potential in (1) in renormalized form

$$V_r^J(x, y, z) = \mu^2[x^2 + y^2 + z^2] + [V_J(x, y, z) - \lambda\beta(x^2 + y^2 + z^2)] \tag{4}$$

where

$$\mu^2 = 1 + \lambda\beta. \tag{5}$$

Setting $\beta = 0$ in the perturbation calculation gives the traditional Rayleigh-Schrödinger series for the problem and ensures that the form of the potential in (4) reduces to the original one in (1). The use of the renormalization parameter β is helpful in improving convergence in this technique as well as in the hypervirial approach. It is important to point out that the effect of varying the parameter β is to allow us to

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obtain results of high accuracy as we will see later. Many techniques have been used to obtain the energy eigenvalues for the two-dimensional potential $V(x, y)$. The work of Hioe *et al* (1978) involved matrix diagonalization. They were able to calculate energy eigenvalues for different values of λ and for various quantum numbers. Blankenbecler *et al* (1980) used the inner product method to calculate the energy eigenvalues for the two-dimensional oscillator. Ari and Demiralp (1985) computed the eigenvalues of a two-dimensional oscillator by using perturbation theory and Padé approximants. Witwit (1990) used the inner product method and renormalized series method to calculate accurate energies for six states, $E_{0,0}$, $E_{1,1}$, $E_{0,2}$, $E_{2,0}$, $E_{1,3}$ and $E_{3,1}$ for different values of (a_{11}, a_{22}, a_{12}) and perturbation parameter λ.

But the abundance of studies of the two-dimensional oscillator is not matched in the case of three-dimensional problems, for which there are few reported results in the literature. The work of Witwit (1991) has used the renormalized series method and power series method to calculate the energy eigenvalues for a three-dimensional oscillator for perturbation $(\lambda r^4, \lambda r^6, \lambda r^8)$ and also investigated all spherically symmetric states in any dimension $(N = 1, 2, 3, \ldots, 1000)$. We also computed the energy eigenvalues for potentials Nr^4 and $N^{-1}r^4$ and obtained results of high accuracy.

In the present work we present some extended numerical calculations using the inner product technique for three dimensions. We computed the eigenvalues for different values of the potential parameters $(a_{11}, a_{22}, a_{33}, a_{12}, a_{23}, a_{13}, a_{123})$ and for four eigenstates $(E_{n_1,n_2,n_3}, n_1, n_2, n_3 = 0, 1, 2, 3)$, over a wide range of perturbation parameter values, $0.01 \leqslant \lambda \leqslant 10^6$.

The renormalized series method in the present work is used for the special case $a_{11} = a_{22} = a_{33} = a_{12} = a_{13} = a_{23} = 1$, to calculate the energy eigenvalues for the perturbed oscillator potential in three dimensions. In rectangular coordinates the Schrödinger equation for the renormalized potential $V_r^J(x, y, z)$ can be written

$$\left[-\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial y^2}\right)+V_r^J(x, y, z)\right]\Psi(x, y, z) = E\Psi(x, y, z). \tag{6}$$

The energy eigenvalues of the unperturbed oscillator is given by

$$E_{n_1,n_2,n_3} = [2n_1+2n_2+2n_3+3] \qquad n_1, n_2, n_3 = 0, 1, 2, \ldots. \tag{7}$$

In each state the energy levels depend on the triplet quantum numbers (n_1, n_2, n_3). The energy levels are degenerate, because of the sum

$$n_1+n_2+n_3 = n. \tag{8}$$

2. The recurrence relation for the inner product and its use

To find the recurrence relations which allow us to calculate the eigenvalues for the Schrödinger equation (6) we use the reference function:

$$\Phi(x, y, z) = (x^{P_1}y^{P_2}y^{P_3})\exp\left[-\frac{\mu}{2}(x^2+y^2+z^2)\right] \tag{9}$$

where p_1, p_2 and p_3 are parity indices, with values 0 for even parity and 1 for odd parity. The methods of calculation used by the authors cited above Blankenbecler *et al* (1980, Killingbeck (1986), Witwit (1991) start from the equation

$$EA(M, N, L) = \langle\Psi|Hx^{2M}y^{2N}z^{2L}|\Phi\rangle \tag{10}$$

obtained by taking the inner product of the Schrödinger equation (6) with the reference function (9), where the $A(M, N, L)$, sometimes called moments, are defined by

$$A(M, N, L) = \langle \Phi | x^{2M} y^{2N} z^{2L} | \Psi \rangle. \tag{11}$$

Then, substituting the perturbation expansions

$$A(M, N, L) = \sum_{K} A(M, N, L, K)\lambda^{K} \tag{12}$$

$$E = \sum_{I} E(I)\lambda^{I} \tag{13}$$

into the $A(M, N, L)$ recurrence relation given by equation (10) leads to a recurrence relations for the coefficients; for the renormalized potential $V_r^{J=1}(x, y, z)$ given by (4) the relation can be written as

$$\begin{aligned}
&\sum_{1}^{k} E(I)A(M, N, L, K-I) \\
&\quad = a_{11}A(M+2, N, L, K-1) + a_{22}A(M, N+2, L, K-1) \\
&\quad + a_{33}A(M, N, L+2, K-1) + 2a_{12}A(M+1, N+1, L, K-1) \\
&\quad + 2a_{13}A(M+1, N, L+1, K-1) + 2a_{23}A(M, N+1, L+1, K-1) \\
&\quad - \beta A(M+1, N, L, K-1) - \beta A(M, N+1, L, K-1) \\
&\quad - \beta A(M, N, L+1, K-1) \\
&\quad + 4\mu[M+N+L-S_1-S_2-S_3]A(M, N, L, K) \\
&\quad - 2M[2M+2P_1-1]A(M-1, N, L, K) \\
&\quad - 2N[2N+2P_2-1]A(M, N-1, L, K) \\
&\quad - 2L[2L+2P_3-1]A(M, N, L-1, K)
\end{aligned} \tag{14}$$

and for the renormalized potential $V_r^{J=2}(x, y, z)$, the relation can be written as

$$\begin{aligned}
&\sum_{1}^{k} E(I)A(M, N, L, K-1) \\
&\quad = a_{11}A(M+3, N, L, K-1) + a_{22}A(M, N+3, L, K-1) \\
&\quad + a_{33}A(M, N, L+2, K-1) + 6a_{123}A(M+1, N+1, L+1, K-1) \\
&\quad + 3a_{12}A(M+2, N+1, L, K-1) + 3a_{13}A(M+2, N, L+1, K-1) \\
&\quad + 3a_{12}A(M+1, N+2, L, K-1) + 3a_{23}A(M, N+2, L+1, K-1) \\
&\quad + 3a_{13}A(M+1, N, L+2, K-1) + 3a_{23}A(M, N+1, L+2, K-1) \\
&\quad - \beta A(M+1, N, L, K-1) - \beta A(M, N+1, L, K-1) \\
&\quad - \beta A(M, N, L+1, K-1) + 4\mu[M+N+L-S_1-S_2-S_3]A(M, N, L, K) \\
&\quad - 2M[2M+2P_1-1]A(M-1, N, L, K) \\
&\quad - 2N[2N+2P_2-1]A(M, N-1, L, K) \\
&\quad - 2L[2L+2P_3-1]A(M, N, L-1, K).
\end{aligned} \tag{15}$$

In writing the relations (14) and (15) we have moved one term $E(0)A(M, N, L, K)$ from the sum over I to the right of the equation, and have expressed the unperturbed energy in the form

$$E(0) = \mu[3+2P_1+2P_2+2P_3+4S_1+4S_2+4S_3]. \tag{16}$$

The unperturbed energy, given by (16), must have the same value of (7). The parity indices for x, y and z are P_1, P_2 and P_3 (0 or 1). The x, y and z state numbers S_1, S_2 and S_3 (0, 1, 2), specify which particular state is being treated. When $P_1 = P_2 = P_3$, we can further specify an x-y-z interchange symmetry index P_4 (0 or 1) such that

$$A(M, N, L, K) = (-1)^{P_4}A(N, M, L, K) = (-1)^{P_4}A(N, L, M, K) = \ldots. \tag{17}$$

The initial condition imposed on the $A(M, N, L, K)$ if $P_1 = P_2 = P_3$ is

$$\begin{aligned} A(S_1, S_2, S_3, 0) &= (-1)^{P_4}A(S_2, S_1, S_3, 0) \\ &= (-1)^{P_4}A(S_3, S_2, S_1, 0) = 1. \end{aligned} \tag{18}$$

In the present work we wish to point out that, although the results displayed are restricted to even-parity states ($P_4 = 0$), the method can be used for odd-parity states ($P_4 = 1$). The recurrence relations (14) and (15) are 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 $P_1 = P_2 = P_3$, with the convention $S_1 \leqslant S_2 \leqslant S_3$ on the state labels:

	$K = 0, 1, 2, \ldots, Q$
(fixed K)	$L = 0, 1, 2, \ldots, S_2+2Q-2K$
(fixed K, L)	$N = 0, 1, \ldots, L-P_3$
(fixed K, L, N)	$M = 0, 1, \ldots, N-P_3$.

The indices are scanned in the order given above and the relations (14) and (15) are used to work out $A(M, N, L, K)$ in terms of lower order elements which are already known. Then we can get $A(N, M, L, K)$, $A(L, N, M, K)$, $A(N, L, M, K), \ldots$, from the symmetry relation (17). $E(K)$ is found from the equation for the special case $M = S_1$, $N = S_2$, $L = S_3$, and the sum on the left-hand side becomes $E(K)$, because of the intermediate normalization convention $A(S_1, S_2, S_3, 0) = 1$ which we impose on the algorithm.

3. The recurrence relation for the renormalized series approach

The renormalized series method has been found to work very well in previous work and produced highly accurate results for the problems investigated by Witwit (1989). As indicated previously the renormalized series can be used to compute the energy eigenvalues for the Schrödinger equation (6) in some cases. When the relationship $a_{11} = a_{22} = a_{33} = a_{12} = a_{23} = a_{13} = 1$ holds, the equation (6) has a spherical symmetry. The energy levels are then most appropriately characterized by the quantum numbers (n_r, l) rather than (n_1, n_2, n_3). Letting $x = r\cos\theta\sin\phi$, $y = r\sin\theta\sin\phi$ and $z = r\cos\theta$, such that $r^2 = x^2+y^2+z^2$, the radial part of the eigenvalue equation (6) is

$$\left(-\frac{d^2}{dr^2}+v(r)\right)\Psi(r) = E\Psi(r) \tag{19}$$

where

$$v(r) = l(l+1)r^{-2} + r^2 + \lambda r^{2I} \qquad 2I = 4, 6. \tag{20}$$

We can write $v(r)$ in other form by using the renormalization parameter β

$$V(r) = \mu r^2 + l(l+1)r^{-2} + \lambda[r^{2I} - \beta r^2] \qquad \mu = 1 + \lambda\beta \tag{21}$$

where l is the angular momentum; on the other hand, in spherical polar coordinates, the energies of the unperturbed levels are

$$E(0) = [2n+3]\sqrt{\mu}. \tag{22}$$

As in (7) we find again the degeneracy of the same multiplicities, where n is the principal quantum number, which can be expressed as

$$n = 2n_r + l \equiv n_1 + n_2 + n_3. \tag{23}$$

Here n_r is called the radial quantum number; n is seen to be even or odd according to whether l is even or odd.

If we use the perturbation expansions

$$E = \sum E(I)\lambda^I \tag{24}$$

$$\langle x^N \rangle = \sum A(N, M)\lambda^M \tag{25}$$

in the hypervirial relation given by Killingbeck (1985) in the form

$$2E(N+1)\langle x^N \rangle = \sum V_I(2N+2+I)\langle x^{N+I} \rangle - \frac{N}{2}(N^2-1)\langle x^{N-2} \rangle \tag{26}$$

and apply the Hellmann–Feynman theorem in the form

$$\frac{\partial E}{\partial \lambda} = \left\langle \frac{\partial V}{\partial \lambda} \right\rangle \tag{27}$$

to the potential given by (21), we get the following recurrence relation after some algebra

$$\begin{aligned}(2N+2)\sum_0^M E(I)A(N, M-I) &= 2N[(l(l+1)) - \tfrac{1}{4}(N^2-1)]A(N-2, M) \\ &+ (2N+4)[\mu A(N+2, M) - \beta A(N+2, M-1)] \\ &+ (2N+2+2I)A(N+2I, M-1)\end{aligned} \tag{28}$$

$$(M+1)E(M+1) = A(2I, M) - \beta A(2, M). \tag{29}$$

From the recurrence relations (28) and (29), we can find the energy coefficients with the help of the $E(0)$ value and the condition $B(0, 0 = 1$. The expression $(2n_r + l + 1)$ show that a degeneracy exists between energy levels to the degree that all allowable combinations of n_r and l consistent with the same values of the l and n_r yield the same energy levels.

4. Results and discussion

In this section we investigate and discuss the results of the numerical calculations for three-dimensional systems. We used two methods to produce our results for this problem: the renormalized series method and the inner product method; also we checked some of our results by using a power series method which has been used widely by Witwit (1989). We extended our numerical calculations for higher values of perturbation parameter λ in order to get a clear picture about the applicability of our methods to investigate this type of perturbation. It is important to point out that it is well known in perturbation theory that the accuracy of the energy eigenvalues decreases as λ increases. This situation occurs in all problems involving eigenvalues in perturbation theory. But in this case it is apparent from our listed results in tables 1–5† that the accuracy is in general insensitive to the values of the perturbation parameter λ; for instance in table 2, the accuracy of energy eigenvalue for $E_{0,0,0}$ at $\lambda = 5$ is four digits but at $\lambda = 5000$ it is three digits. We have not observed any fundamental difference in behaviour between the accuracy of the other eigenvalues such as $E_{1,1,1}$, $E_{0,0,2}$ and $E_{0,2,3}$.

It is important to point out that the renormalization parameter (β) has played the important role of enabling convergence of our calculations. We can see from the results that the accuracy depends on the value of the renormalized parameter (β). The best β values in this calculation have been obtained by numerical search, so our calculation reveals the importance of finding the best values of the renormalization parameter. Table 6 shows some specimen results for two eigenstates $E_{0,0,0}$ and $E_{1,1,1}$ at $\lambda = 0.1$ for different values of the renormalization parameter; it is clear how the accuracy varies with the values of β; for example, the accuracy is very poor at $\beta = 0$ but the accuracy changes with various β values. The first difficulty we face is to guess the best values of β. We continue to change the renormalized parameter until energy eigenvalues of the best required accuracy are obtained. The values of energy in tables 1–4 are for the case $a_{11} = a_{22} = a_{33} = a_{12} = a_{23} = a_{13} = 1$; we show some energies for states (n_1, n_2, $n_2 = 0$, 1, 2, 3) and for $0.1 \leqslant \lambda \leqslant 10^6$. The two approaches work very well for the three-dimensional oscillator, and the results obtained by these methods are in good agreement with each other. We observe that the two approaches yield a good number of accurate digits for the eigenvalues at low values of λ. For higher values of the perturbation parameter λ the renormalized series method gives more digits than the inner product method. In the absence of other reported results (to the best of our knowledge), we have used the non-perturbative method (power series) to check some of our results for higher values of the perturbation parameter λ for the case of a spherical symmetric potential ($a_{nm} = 1$, $n, m = 1, 2, 3$) in which the potential reduces to a one-dimensional potential.

One main difference between the two perturbative techniques is that the hypervirial method can only work for the case of a symmetric potential $a_{11} = a_{22} = a_{33} = a_{12} = a_{23} = a_{13} = 1$ in which the potential reduces to a one-dimensional potential. The inner product method deals with more general parameter values but still requires $a_{11} = a_{22} = a_{33}$, since the equations used exploit this symmetry to reduce computation. Also we face a problem in dealing with the inner product method because the elements of $B(N, M, L, K)$ require high memory and thus we only managed to obtain energies

† Tables 1–6 have been deposited in the British Library Supplementary Publication scheme, document no. SUP70043.

series up to 18 terms; we reduce the effect of this restriction by choosing the best values of the renormalization parameter β in order to obtain the best convergence results with this limited range of terms, and this took a long time to do our calculations. In tables 2 and 5 we obtained energy values for the case $a_{nn} = 0$ and $a_{nm} = 1$ ($n, m = 1, 2, 3$), with in the wide range $0.01 \leqslant \lambda \leqslant 5000$; the inner product method gave good and accurate results even for the higher values of λ and we worked hard to obtain these results with good accuracy. Sometimes we ran our program many times, with different values of β, to get the best accuracy. In table 3 the results we presented for the case $a_{nn} = 1$, $a_{nm} = -1$, for $0.01 \leqslant \lambda \leqslant 0.5$, converged very well for small values of λ but the convergence deteriorated for $\lambda > 0.5$ and high state number.

Summarizing our results we can say the following.

We succeeded in finding the energy eigenvalues for states $E_{0,0,0}$, $E_{1,1,1}$, $E_{0,0,2}$, $E_{0,2,3}$ with good accuracy even for high values of λ ($0.1 \leqslant \lambda \leqslant 10^6$), and for different values of the potential parameters ($a_{n,m} = 1, -1, 0$); ($a_{n,n} = 1, 0$). The set of tables 1-5 cover a wide range of values of (λ). It is clear from our calculations that the accuracy of potential 2, in general, is better than the accuracy of potential 3, and we also faced the same situation in the one- and three-dimensional cases for perturbation λx^4, λx^6, λx^8, λr^4, λr^6, λr^8. It is important to point out, as the power index of the perturbation increases the convergence of the perturbation series begin to decrease even with small values of λ (see tables 2.3 and 3.7 of Witwit 1989).

We avoided the phenomenon of bogus convergence by computing the energy eigenvalues for different values of the renormalization parameter β, and we also used another technique, the power series method. We believe that some of the accuracy of our results may be improved with a better choice of β, and in this respect we did our best to achieve this choice.

We wish to note that the results yielded by the inner product were improved by using the Aitken extrapolation; it seems that this extrapolation improves the convergence of the perturbation series and gives accuracy to extra digits. We also wish to draw attention to our calculations in three dimensions which may be regarded as a guide to future numerical calculations. As far as we know, we are the first to investigate numerically the energy eigenvalues for a wide range of potential parameters in three dimensions.

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