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COMMENT

The rotating oscillator

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Abstract. Methods recently devised for anharmonic oscillator calculations are used to investigate a longstanding problem for the rotating displaced oscillator.

The rotating displaced oscillator problem, with the Schrödinger equation

$$-D^2\psi+\frac{l(l+1)}{r^2}\psi+\frac{(r-1)^2}{4\alpha^2}\psi=\left(\frac{\lambda+\frac{1}{2}}{\alpha}\right)\psi \tag{1}$$

and with $\psi(0)=\psi(\infty)=0$ has been the subject of some dispute in the literature. Masson (1983a) reviewed the history of the problem, pointing out that some previous workers (Flessas 1979, Singh *et al* 1972) had reached erroneous conclusions about the eigenvalues λ of equation (1). In this comment we point out that all the workers concerned (including Masson) have used a formalism based on a three-term recurrence relation. This is what causes the problems, as recent work on the anharmonic oscillator has shown (Killingbeck 1986).

To simplify the formulae we still set $\psi(0)=\psi(\infty)=0$ but treat the more general Schrödinger equation

$$-D^2\psi+l(l+1)r^{-2}\psi+V_1r\psi+V_2r^2\psi=E\psi. \tag{2}$$

To convert (2) to (1) requires the special choices

$$V_1=-2V_2=\frac{-1}{2\alpha^2}\qquad E=\frac{\lambda+\frac{1}{2}}{\alpha}-\frac{1}{4\alpha^2}. \tag{3}$$

Using the ansatz

$$\psi=r^{l+1}\exp(-\alpha r-\tfrac{1}{2}\beta r^2)\sum_0^\infty A(n)r^n \tag{4}$$

in (2) leads to the recurrence relation

$$\begin{aligned}(n+2)(n+2l+3)A(n+2)&=(2n+2l+4)\alpha A(n+1)+[(2n+2l+3)-\alpha^2-E]A(n)\\&\quad+(V_1-2\alpha\beta)A(n+1)+(V_2-\beta^2)A(n-2).\end{aligned} \tag{5}$$

What previous workers have done is equivalent to choosing α and β so as to remove the last two terms on the right-hand side of the recurrence relation (Singh *et al* 1978, 1982, Flessas 1979, Masson 1983a). This choice seems obvious. It leaves only a three-term recurrence relation, which is amenable to continued fraction techniques or

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to tridiagonal matrix eigenvalue techniques, and it also gives the wavefunction the correct asymptotic form at large r values. However, recent microcomputer experiments (Killingbeck 1986) show that for anharmonic oscillator problems the use of three-term recurrence relations can lead to false eigenvalues. The results reported here show that this is also true for the rotating displaced oscillator problem. Thus it is not surprising that Flessas (1979) and Singh *et al* (1978, 1982) reached erroneous conclusions, while Masson (1983a) only managed to obtain information about the eigenvalues after a lengthy analysis which involved analytic continuation and the use of a modified type of approximant for continued fractions.

Our computational approach is very simple. For the case $V_1 = -2V_2$ with $V_2 > 0$ we set

$$\beta = \sqrt{V_2} \qquad \alpha = RV_1/2\beta = -R\beta. \tag{6}$$

The choice $R = -1$ corresponds to that made by the previous works cited. We set $n = -1$ in (5), with $A(0) = 1$ and all other $A(n)$ initially zero. Repeated application of (5) then gives $A(1)$, $A(2)$, etc, for any proposed trial energy E and for a given R value. Varying E until $A(N)$ is zero for some large integer N (typically around 50) yields a set of eigenvalues. As N is increased these eigenvalues quickly tend to limiting values, so that we obtain a set of eigenvalues which (for a given potential) depend on R. Speedy algorithms for carrying out such computations on a microcomputer were described by Killingbeck (1985), who also showed how to obtain expectation values directly along with the energies. Killingbeck (1985) showed that the simple procedure described above is equivalent to the Hill determinant method, which is traditionally presented in a more complicated form.

Table 1 shows some typical results, for the case $V_2 = 25$, $V_2 = -50$ and at $R = 3$. These results remain independent of R down to $R \sim 1.5$, where the convergence (as $N \to \infty$) becomes very slow. For smaller R, including the value $R = -1$, the energy eigenvalues are again R independent but are different from the values at $R > 1.5$. The same kind of analysis which was recently devised for anharmonic oscillator problems (Killingbeck 1986, Znojil 1986) shows that the energy values at $R = -1$, although incorrect for the potential in equation (2), are correct energies for the partner potential which has the sign of V_1 reversed. This suggests that previous workers who made the implicit choice $R = -1$ were unwittingly drawing conclusions about this partner potential rather than the true potential.

Table 1. Results for the case $V_2 = 25$, $V_1 = -50$, with $R = 3$†.

l	E	$\langle r \rangle$	δ
0	−19.925 057	1.013 1863	0.3078
0	−9.416 9704	1.077 8002	0.5164
0	1.982 004	1.196 5864	0.6346
1	−17.461 758	1.108 5977	0.2910
1	−5.744 0818	1.204 9186	0.4906
1	6.752 8312	1.319 6155	0.6108
2	−13.743 654	1.207 0577	0.2806
2	−1.152 7636	1.309 8194	0.4754
2	12.065 527	1.418 9721	0.5969

† The E_0 values are −20.00, −17.69 and −13.98.

The virial theorem

$$2E = 3V_1\langle r\rangle + 4V_2\langle r^2\rangle \tag{7}$$

allows $\langle r^2\rangle$ to be calculated when E and $\langle r\rangle$ are known, so that the RMS width δ of the wavefunction can be calculated from the formula $\delta^2 = \langle r^2\rangle - \langle r\rangle^2$. δ is shown in table 1 and the results show that for $V_2 = 25$ the ground-state wavefunction is fairly well localised around the minimum of the potential. A fair estimate of the ground-state energy should thus be obtainable from the harmonic oscillator approximation:

$$E_0 = V(r_0) + (\tfrac{1}{2}V''(r_0))^{1/2} \tag{8}$$

where r_0 is the r value at which the potential $V(r)$ in equation (2) has a minimum (recalling that we set $V_1 = -V_2$). Table 1 gives the E_0 values as calculated numerically using (8).

The numerical approach described in this comment will clearly work for arbitrary values of V_1 and V_2 (with $V_2 > 0$), although we have used it here to throw light on a problem in the theory of the rotating oscillator (with $V_1 = -V_2$). As a practical means of computing energy levels for the rotating oscillator our method is computationally simple and speedy; although Masson (1983b) showed that a perturbation approach using the $V_1 r$ term in the potential as a perturbation should be formally possible, it seems that the calculation of the energy perturbation series is difficult; the hypervirial perturbation approach (Killingbeck 1985a, b, c) leads to equations which do not appear to be solvable. The problem appears to be due to the boundary condition at $r = 0$; for a one-dimensional oscillator with the perturbation λx and boundaries at $x = \pm\infty$ the hypervirial method works satisfactorily.

The choice $V_2 = 25$ in (2) corresponds to the choice $\alpha = 0.1$ in (1). Froman *et al* (1980) gave some eigenvalues for (1) at $l = 0$ and 1, $\alpha = 0.1$, calculated by a finite difference method. When the conversion formula (3) is used our energies agree with theirs to the few digits which they quote. For the case $l = 0$, shifting the origin to $r = 1$ in equation (1) apparently yields a simple harmonic oscillator problem with the traditional spectrum. However, the unorthodox asymmetric boundary conditions $\psi(-1) = \psi(+\infty) = 0$ are required and this changes the eigenvalues, as noted by Froman *et al* (1980). For example, the shift from -20 to $-19.925\,057$ shown in table 1 is due to this effect. When V_1 is zero in equation (2) the associated three-dimensional problem becomes separable in cartesian coordinates and yields energy levels with a high degeneracy which can be explained in terms of the SU_3 dynamical symmetry group (Killingbeck 1975). However, for $V_1 = 0$ exact analytic solutions are not possible and an approach using cartesian coordinates becomes very complicated. Even for a two-dimensional oscillator with the perturbing potential $A(x^4 + y^4) + Bx^2y^2$ explicitly written in terms of cartesian coordinates it is easier to use a radial equation approach to obtain accurate eigenvalues for the special case $B = 2A$ (Killingbeck and Jones 1986).

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