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1991 J. Phys. A: Math. Gen. 24 1351

(http://iopscience.iop.org/0305-4470/24/6/025)

J. Phys. A: Math. Gen. 24 (1991) 1351–1353. Printed in the UK

COMMENT

Analytical bound eigenstates and eigenvalues of a truncated Coulomb potential

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Received 9 October 1990

Abstract. We obtain exact eigenfunctions and eigenvalues of the Schrödinger equation with the potential $V(r) = -Ze^2/(r+\beta)$, $\beta > 0$, for particular values of the cut-off parameter β. Each eigenfunction is a finite polynomial times an exponential and the eigenvalues are exactly those for the pure Coulomb problem (i.e. $\beta = 0$).

In a recent paper De Meyer and Vanden Berghe (1990) studied the Schrödinger equation with the potential $V(r) = -Ze^2/(r+\beta)$. They obtained accurate numerical results by means of an algorithm based on an iterative solution of the secular equation derived with a scaled basis set and the properties of the Lie algebra SO(2, 1). This method, which had been applied to other problems by Fernández *et al* (1985, 1986), appears to converge fast enough if the scaling parameter (or tilting transformation) is properly chosen. The results of De Meyer and Vanden Berghe (1990) are even more accurate than those obtained by Singh *et al* (1985) through numerical integration of an eigenvalue equation derived from the Schrödinger one by means of a nonlinear transformation of variables.

De Meyer and Vanden Berghe (1990) showed that one can obtain analytical solutions for the above-mentioned problem for particular values of the truncation parameter β. If n and l are respectively the principal and angular momentum quantum numbers those authors proved that the eigenvalues $E_{n,l}(\beta)$ obey $E_{l+1,l}(\beta = l+2) = E_{l+2,l+1}(\beta = 0) = -Z/[2(l+2)^2]$, the latter being the well known eigenvalues of the hydrogen atom in atomic units. In addition to this, De Meyer and Vanden Berghe (1990) showed that exact s-state solutions can be systematically generated for certain values of the parameter β obtained from the roots of finite polynomials.

Because the truncated Coulomb potential has several physical applications (Singh *et al* 1985, De Meyer and Vanden Berghe 1990 and references therein) exact closed-form solutions may be of great value even though they are only available for particular values of β. Such exact results may serve, for instance, as benchmark values for approximate methods.

The purpose of this comment is to generalize the results of De Meyer and Vanden Berghe (1990) and derive exact analytical results for other states. We do this by straightforward application of a systematic procedure based on the well known power series method which is customarily used to obtain the eigenstates and eigenvalues of most solvable quantum mechanical models.

0305-4470/91/061351+03$03.50

The starting point is the radial part of the time-independent Schrödinger equation which in atomic units reads

$$y''(r)+[2E+2/(r+\beta)-l(l+1)/r^2]y(r) \tag{1}$$

in which E is the energy and $y(0)=0$. Without loss of generality we choose $Z=1$ because $E(Z)=Z^2E(Z=1)$ and $\beta(Z)=\beta(Z=1)/Z$.

If the solution $y(r)$ is written

$$y(r)=r^{l+1}\,\mathrm{e}^{-\alpha r}\sum_{j=0}^{\infty}u_j r^j \qquad \alpha^2=-2E \tag{2}$$

then the coefficients u_j have to obey the following three-term recurrence relation:

$$a_j u_{j+1}+b_j u_j+c_j u_{j-1}=0 \tag{3a}$$

where

$$\begin{aligned} &a_j=\beta(j+1)(j+2l+2) \qquad b_j=j(j+2l-2\alpha\beta+1)-2(l+1)\alpha\beta \\ &c_j=2[1-\alpha(l+j)]. \end{aligned} \tag{3b}$$

One obtains exact analytical solutions when the sum in (2) reduces to a finite polynomial. It follows from the equations above that if $c_{\nu+1}=0$ and $u_{\nu+1}=0$ then $u_j=0$ for all $j>\nu$. These two equations completely determine values of E and β that lead to exact solutions. From the former one obtains

$$\alpha=1/(\nu+l+1) \qquad E_{n,l}=-1/[2(\nu+l+1)^2] \qquad n=\nu+l \tag{4}$$

which are energies of the pure Coulomb problem. The corresponding physical β values are obtained from the positive roots of $u_{\nu+1}=0$. The case $\nu=0$ leads to $\alpha=0$ and $E=0$ which is only possible in the limit $l\to\infty$. For this reason the lowest energy value for each value of l corresponds to $\nu=1$ for which one obtains the above-mentioned relation between the eigenvalues of this model and those of the hydrogen atom derived by De Meyer and Vanden Berghe (1990). For other states (4) gives us a more general expression which can be expressed in compact form as $E_{l+\nu,l}(\beta=\beta_{\nu l})=E_{l+\nu+1,l+1}(\beta=0)$, where $\nu=1,2,\ldots$, and $\beta_{\nu l}$ is a positive root of $u_{\nu+1}=0$. When $\nu=1$ we obtain the results of De Meyer and Vanden Berghe (1990) for the nodeless states:

$$\begin{aligned} &E_{l+2,l}=-1/[2(l+2)^2] \qquad y_{n,l}(r)=r^{l+1}[1+r/(l+2)]\,\mathrm{e}^{-r/(l+2)} \\ &\beta=l+2. \end{aligned} \tag{5}$$

One can obtain as many solutions as desired from the roots of the equations mentioned above. For instance, the next case, $\nu=2$, leads to

$$\begin{aligned} &E_{l+3,l}=-1/[2(l+3)^2] \qquad \beta=(l+3)\{3(l+2)-[(l+2)(l+6)]^{1/2}\}/[2(l+2)] \\ &u_0=1 \qquad u_1=1/(l+3) \\ &u_2=-(l+2)\{[(l+2)(l+6)]^{1/2}-l\}/\{(2l+3)(l+3)^2[3(l+2)-[(l+2)(l+6)]^{1/2}\}. \end{aligned} \tag{6}$$

As u_0, $u_1>0$ and $u_2<0$ the wavefunction has one node in $(0,\infty)$. It is worth mentioning that when $l=0$ the equations developed here lead to the equations for the s states obtained by De Meyer and Vanden Berghe (1990) by the transformation of the truncated Coulomb potential into a pure Coulomb problem with Dirichlet boundary conditions $y(\beta)=y(\infty)=0$.

As one proceeds further the expressions for E, β and the coefficients u_j become more and more involved. The manipulation of the three-term recurrence relation is greatly facilitated by the use of computer algebra but the analytical computation of the roots of $u_{\nu+1}=0$ becomes the bottleneck of the calculation and as a consequence results for large values of ν are more easily obtained numerically. However, the method proposed here is useful to investigate the analytical properties of the solutions. For instance, the numerator of $u_{\nu+1}$ is a polynomial function of β of degree ν. For the case $\nu=2$ discussed above only one of the two roots is positive. On the other hand, when $\nu=3$ the three roots of $u_4=0$ are positive and the results are threefold degenerate in the sense that three values of β are consistent with one value of the energy. We do not show such expressions here because they are rather long and involved and do not add much to the present discussion.

In this comment we have developed a systematic method for obtaining exact closed-form eigenvalues and eigenfunctions for the truncated Coulomb potential for particular values of the truncation parameter. The present treatment of the problem generalizes that of De Meyer and Vanden Berghe (1990) who only obtained exact results for the s states and nodeless states with arbitrary l values. As illustrative examples we have explicitly derived two infinite sets of solutions corresponding to the nodeless eigenfunctions and to those with just one node.

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