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1990 J. Phys. A: Math. Gen. 23 1323

(http://iopscience.iop.org/0305-4470/23/7/034)

J. Phys. A: Math. Gen. **23** (1990) 1323–1328. Printed in the UK

COMMENT

Exact bound-state solutions of the potential $V(r) = -Ze^2/(r+\beta)$

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Received 23 October 1989

Abstract. High-accuracy approximations of the bound-state energies of the potential $V(r) = -Ze^2/(r+\beta)$ are obtained by means of the dynamical group method. Certain bound-state solutions of the Schrödinger problem are constructed in analytic closed form.

1. Introduction

In a recent paper [1] attention has been drawn to the problem of determining the energy eigenvalues of the cut-off Coulomb potential

$$V(r) = -\frac{Ze^2}{r+\beta} \qquad (\beta > 0) \tag{1}$$

which serves as a model of the potential due to a smeared charge. Within the framework of the shifted $1/N$ expansion method an approximation formula for an estimate of energy eigenvalues for any angular momentum state has been established in [1]. In particular, the s-wave bound states are compared with the results of Mehta and Patil [2] which have been obtained from a dispersion theoretical study.

Before discussing exact analytic eigenstates of the potential (1) we shall establish high-accuracy approximations of the bound-state eigenvalues by means of the dynamical group approach. This technique has been successfully applied in the past to a variety of perturbed Coulomb potentials, e.g. a class of screened Coulomb potentials [3], the exponential cosine screened Coulomb potential [4], the Hulthén potential [5], etc. Without going into the details of the technique which can be found in [3–5] let us mention that first an energy functional $\Omega(E)$ is constructed out of the stationary Schrödinger equation which is multiplied on the left by $r(r+\beta)$ and in which rp^2 and r are replaced by the SO(2, 1) Lie algebra operators $K_1 + K_3$ and $K_1 - K_3$ respectively. Furthermore, this energy functional is tilted into a parameter-dependent functional

$$\Omega(E) \longrightarrow \tilde{\Omega}(E,\theta) = \mathrm{e}^{-\mathrm{i}\theta K_2}\,\Omega(E)\,\mathrm{e}^{\mathrm{i}\theta K_2} \tag{2}$$

where K_2 is the operator which together with K_1 and K_3 closes into the non-compact Lie algebra SO(2, 1), θ being the tilting angle. Introducing the orthonormal group state

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0305-4470/90/071323+06$03.50

basis $|nl\rangle$ in which the compact generator K_3 is diagonal

$$\begin{aligned} K_3 \,|nl\rangle &= n \,|nl\rangle \\ (K_1 \pm \mathrm{i}K_2) \,|nl\rangle &= [(l+1\pm n)(\pm n - l)]^{1/2} \,|n \pm 1 l\rangle \\ (K_3^2 - K_1^2 - K_2^2) \,|nl\rangle &= l(l+1) \,|nl\rangle \end{aligned} \tag{3}$$

the non-zero matrix elements of $\bar{\Omega}(E,\theta)$ associated with the potential (1) with $Ze^2 = 1$ are given by:

$$\begin{aligned} \langle nl \mid \bar{\Omega}(E,\theta) \mid nl\rangle &= (\tfrac{1}{4} - \tfrac{3}{2}E\omega^2)n^2 + (\beta/2\omega - \omega - E\beta\omega)n + \tfrac{1}{2}l(l+1)(\tfrac{1}{2} + E\omega^2) \\ \langle n \pm 1 l \mid \bar{\Omega}(E,\theta) \mid nl\rangle &= \tfrac{1}{2}(\beta/2\omega + \omega + E\beta\omega \pm \tfrac{1}{2} + (2n \pm 1)E\omega^2)[(n \mp l)(n \pm l \pm 1)]^{1/2} \\ \langle n \pm 2l \mid \bar{\Omega}(E,\theta) \mid nl\rangle &= \tfrac{1}{4}(-\tfrac{1}{2} - E\omega^2)[(n \mp l)(n \mp l \pm 1)(n \pm l \pm 1)(n \pm l \pm 2)]^{1/2} \end{aligned} \tag{4}$$

with

$$\omega = \mathrm{e}^{-\theta}. \tag{5}$$

Notice that for any fixed value of l the matrix $\langle n'l \mid \bar{\Omega}(E,\theta) \mid nl\rangle$ is a five-band matrix and that its elements are linear in E, i.e.

$$\langle n'l \mid \bar{\Omega}(E,\theta) \mid nl\rangle = a_{n'n} + Eb_{n'n}. \tag{6}$$

Since $\bar{\Omega}(E,\theta)$ leaves the l value unchanged its nth eigenstate associated with a particular l value can be expanded in the orthonormal SO(2, 1) group states as follows:

$$|\bar{\psi}_{nl}\rangle = \sum_{i=l+1}^{\infty} c_i \,|il\rangle \tag{7}$$

and the condition that $\bar{\Omega}(E_{nl},\theta) \mid \bar{\psi}_{nl}\rangle = 0$ yields [5]:

$$\begin{aligned} E_{nl} &= -\frac{\sum_i a_{ni}c_i}{\sum_i b_{ni}c_i} \\ c_j &= -\frac{\sum_{i,j(i\neq j)} a_{ji}c_i + \sum_{i,j(i\neq j)} b_{ji}c_iE_{nl}}{a_{jj} + b_{jj}E_{nl}} \qquad (j \neq n). \end{aligned} \tag{8}$$

The set of equations (8) have the appropriate form to establish a Gauss–Seidel iteration scheme [4, 5] for the approximation of the eigenvalue E_{nl}. If the scheme is convergent the consecutive approximations will tend to a limit which is the exact eigenvalue E_{nl}. In practice, it is found that the rate of convergence strongly depends upon the choice of the tilting parameter ω. In tables 1 and 2 we list for the $n = 1, 2, 3, 4$ states and for a range of β values, the approximate values of E_{nl} as they were obtained after an indicated number of iterations. The value of ω used is also indicated. It should be remarked that the rate of convergence is strongly ω dependent for the smaller β values. In fact, there is numerical evidence that the series of approximating values is an asymptotically convergent series and therefore in the domain of $\beta \ll 1$ an accuracy of only six decimal digits can be attained after 400 iterations. These results are shown in table 1. In contrast, for values of $\beta \geq 1$ the rate of convergence is generally so

Table 1. Energy eigenvalues ($-E_{nl}$) of the potential (1) with $Ze^2 = 1$ as a function of β ($\beta < 1$) for different excited states in atomic units. In square brackets are indicated the value of ω and the number of iterations.

β	1s	2s	2p	3s	3p
0.0001	0.499 820 [0.21, 450]	0.124 977 [1.20, 450]	0.124 992 [1.000 05, 200]	0.055 5490 [3.0001, 200]	0.055 5531 [2.03, 350]
0.001	0.498 044 [0.21, 450]	0.124 759 [1.20, 450]	0.124 917 [1.005, 200]	0.055 4884 [3.055, 300]	0.055 5309 [2.04, 350]
0.01	0.482 107 [0.23, 400]	0.122 742 [1.24, 450]	0.124 177 [1.05, 200]	0.054 8935 [2.15, 400]	0.055 3112 [2.05, 350]
0.1	0.387 544 [0.25, 300]	0.109 508 [1.37, 450]	0.117 535 [1.2, 200]	0.050 8100 [2.30, 400]	0.053 3093 [2.12, 350]
β	3d	4s	4p	4d	4f
0.0001	0.055 5541 [1.8, 350]	0.031 2472 [4.0005, 300]	0.031 2489 [3.0005, 400]	0.031 2494 [2.9, 300]	0.031 2496 [2.4, 250]
0.001	0.055 5408 [1.8, 350]	0.031 2229 [4.005, 300]	0.031 2396 [3.005, 400]	0.031 2438 [2.9, 250]	0.031 2455 [2.4, 250]
0.01	0.055 4081 [1.85, 350]	0.030 9787 [3.1, 350]	0.031 1468 [3.05, 400]	0.031 1877 [2.9, 250]	0.031 2055 [2.4, 250]
0.1	0.054 1366 [1.90, 350]	0.029 2169 [3.3, 350]	0.030 2949 [3.11, 400]	0.030 6484 [3.0, 250]	0.030 8136 [2.4, 250]

high that the accuracy of the approximations is completely determined by the accuracy of machine floating-point arithmetics. In table 2 bound-state energy values are listed with a precision of 12 decimal digits; these can serve as benchmark values for other approximation techniques. Finally, it should be indicated that, although the number of iterations mentioned in the tables seems rather high, the calculation efforts are nevertheless extremely low.

Close inspection of table 2 shows that the eigenvalues corresponding to the states $|n = l+1, l\rangle$ with $\beta = l+2$ seem to be rigorously given by the formula:

$$E_{l+1,l}(\beta = l+2) = -\frac{1}{2(l+2)^2} \qquad (l \geq 0) \tag{9}$$

which coincides with the formula for the eigenvalues $E_{l+2,l+1}(\beta = 0)$ of the pure Coulomb potential. Since it can hardly be believed that this is merely a coincidence we shall prove (9) by constructing in closed form the corresponding eigenstates. We make a distinction between the cases $l = 0$ and $l \geq 1$.

2. Exact s-wave bound states

The radial Schrödinger equation for the potential (1) with $Ze^2 = 1$ is given by

$$\frac{d^2y}{dr^2} + \left(2E + \frac{2}{r+\beta} - \frac{l(l+1)}{r^2}\right) y(r) = 0 \tag{10}$$

Table 2. Energy eigenvalues ($-E_{ni}$) as a function of β ($\beta \geq 1$). Conventions and notation are the same as in table 1.

β	1s	2s	2p	
1.0	0.180 367 050 302 [1.1, 200]	0.0695 806 627 209 [2.14, 350]	0.082 862 420 4409 [1.7, 200]	
2.0	0.125 000 000 000 [1.2, 200]	0.0544 740 424 109 [2.8, 200]	0.065 732 007 1888 [2.6, 200]	
3.0	0.098 215 640 0099 [2.0, 200]	0.045 979 036 3680 [3.2, 200]	0.055 555 555 5556 [2.8, 100]	
4.0	0.081 868 074 5499 [2.2, 200]	0.040 287 379 2663 [3.6, 200]	0.048 598 494 1002 [3.0, 100]	
5.0	0.070 670 280 2201 [2.3, 100]	0.036 119 245 5637 [4.0, 200]	0.043 458 403 5678 [3.2, 100]	
10.0	0.043 438 719 2643 [4.0, 100]	0.024 810 356 9956 [6.0, 100]	0.029 446 515 7059 [4.0, 100]	
15.0	0.032 071 427 3534 [4.5, 100]	0.019 439 283 7178 [7.0, 100]	0.022 825 578 4915 [5.0, 100]	
β	3s	3p	3d	
1.0	0.036 814 197 6453 [3.184, 350]	0.041 787 661 9249 [2.7, 350]	0.045 010 006 4657 [2.0, 150]	
2.0	0.030 640 352 5593 [3.824, 300]	0.035 263 924 1315 [3.16, 250]	0.038 787 135 7145 [2.5, 150]	
3.0	0.026 884 267 6256 [4.31, 250]	0.031 054 596 7323 [3.7, 150]	0.034 479 644 4021 [3.0, 100]	
4.0	0.024 232 233 4305 [4.8, 200]	0.028 008 531 6175 [3.9, 100]	0.031 250 000 0000 [3.2, 100]	
5.0	0.022 212 315 7296 [5.2, 200]	0.025 658 945 5530 [4.3, 100]	0.028 705 688 9891 [3.5, 100]	
10.0	0.016 341 468 8665 [6.7, 150]	0.018 748 153 0514 [5.6, 100]	0.021 024 301 6457 [4.0, 100]	
15.0	0.013 311 370 1906 [8.0, 150]	0.015 168 945 9759 [6.5, 100]	0.016 971 771 0564 [5.0, 100]	
β	4s	4p	4d	4f
1.0	0.022 756 978 1 [4.22, 350]	0.025 134 401 7727 [3.74, 350]	0.026 625 059 9928 [3.37, 300]	0.027 588 159 8846 [2.6, 200]
2.0	0.019 651 191 5589 [5.0, 300]	0.021 986 758 6724 [4.27, 300]	0.023 706 656 0757 [3.83, 200]	0.024 972 051 5698 [3.3, 150]
3.0	0.017 668 201 1559 [5.5, 300]	0.019 854 092 6772 [4.73, 200]	0.021 590 815 5272 [4.25, 150]	0.022 960 237 9736 [3.8, 100]
4.0	0.016 220 234 7926 [6.0, 250]	0.018 255 292 1756 [5.01, 200]	0.019 947 639 9842 [4.6, 150]	0.021 342 109 5966 [4.2, 100]
5.0	0.015 088 441 0635 [6.25, 200]	0.016 987 444 5484 [5.4, 150]	0.018 616 105 5722 [4.9, 100]	0.020 000 000 0000 [4.7, 100]
10.0	0.011 638 307 1155 [7.9, 200]	0.013 060 936 8874 [7.0, 100]	0.014 373 461 1533 [6.2, 100]	0.015 576 600 0898 [5.8, 100]
15.0	0.009 749 622 28609 [9.5, 200]	0.010 893 305 6586 [8.0, 100]	0.011 979 730 0989 [7.0, 100]	0.013 007 413 6328 [6.5, 100]

with boundary conditions

$$y(0) = y(\infty) = 0. \tag{11}$$

Putting $l = 0$ in (10) and performing the change of variables $\rho = r + \beta$ we obtain the differential equation of the pure Coulomb problem

$$\frac{d^2y}{d\rho^2} + \left(2E + \frac{2}{\rho}\right) y(\rho) = 0 \tag{12}$$

but with the modified boundary conditions:

$$y(\beta) = y(+\infty) = 0. \tag{13}$$

The pure Coulomb eigenstates which solve (12) and satisfy the conditions $y_c(0) = y_c(+\infty) = 0$ are known to be given by [6]:

$$y_c(\rho) = (2\alpha\rho)\, e^{-\alpha\rho} \sum_{p=0}^{n_c'} \frac{(-1)^p}{(n_c' - p)!\,(p+1)!\,p!} (2\alpha\rho)^p \qquad (n_c' = 0, 1, 2, \ldots) \tag{14}$$

where

$$\alpha = \frac{1}{(n_c' + 1)} \tag{15}$$

and

$$E = -\frac{1}{2(n_c' + 1)^2}. \tag{16}$$

Also n_c' counts the number of zeros of the solution $y_c(\rho)$ in $]0, +\infty[$. Next we investigate whether any of the Coulomb states (14) can obey the boundary conditions (13). If $n_c' = 0$ this can only happen for $\beta = 0$ which leads to a triviality. But, with $n_c' = 1$, it turns out that

$$y_c(\beta) = 0 \Leftrightarrow \beta = 2 \tag{17}$$

showing that

$$y(r) = (r+2)e^{-(r+2)/2}[1 - (r+2)/2] \sim r(1 + r/2)\, e^{-r/2} \tag{18}$$

is a solution of (10) (with $l = 0$) satisfying (11). Since this solution clearly has no zeros in $]0, +\infty[$ it must be identified with a 1s state and on account of (16) our formula (9) is already valid for $l = 0$.

This approach allows us to derive also exact energy values for certain irrational β values. For example, with $n_c' = 2$ the condition $y_c(\beta) = 0$ gives rise to a quadratic equation in β with roots $3(3 \pm \sqrt{3})/2$. The largest root $\beta = 7.098\ 076\ 21\ldots$ yields a solution $y(r)$ which has no zeros in $]0, +\infty[$ and thus corresponds to a 1s state, whereas the lowest root $\beta = 1.901\ 923\ 79\ldots$ yields a solution which has one zero in $]0, +\infty[$ and thus corresponds to a 2s state. Hence, according to (16)

$$E_{1,0}(\beta = 3(3 + \sqrt{3})/2) = E_{2,0}(\beta = 3(3 - \sqrt{3})/2) = -\tfrac{1}{18}. \tag{19}$$

Clearly, this way of constructing exact s-wave bound states can be continued with higher values of n_c'.

3. Exact bound-state solutions for $l \neq 0$

It is clear that when $l \neq 0$ the differential equation (10) can no longer be transformed into the Coulomb equation by a change of variables. Instead we look in analogy with (18) for solutions of (10) of the form

$$y(r) = r^{\mu} e^{\nu r}(1 + \lambda r) \qquad \lambda \neq 0 \tag{20}$$

satisfying (11). Direct substitution of (20) into (10) gives rise to a system of five nonlinear equations in the five parameters μ, ν, λ, E and β. On condition that $\beta \neq 0$ and $\lambda \neq 0$ this system has the unique solution:

$$\begin{aligned} &\mu = l + 1 \qquad \nu = -\frac{1}{l+2} \qquad \lambda = \frac{1}{l+2} \\ &E = -\frac{1}{2(l+2)^2} \qquad \beta = l + 2 \end{aligned} \tag{21}$$

and since $\lambda > 0$ the proposed eigenstate (20) has no zeros on $]0, +\infty[$ and must be associated with the quantum number $n = l + 1$. This finishes the proof of (9) for all $l \geq 1$. Moreover, it provides an alternative proof of (9) for the case $l = 0$ whereby one can verify that the solution (20) reduces to the form (18).

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