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On the Spectrum of the Screened Coulomb Potential $V(r) = -r^{-1}e^{-C/r}$

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Abstract: We analyse recent contradictory results and conclusions about the spectrum of the screened Coulomb potential $V(r) = -r^{-1}e^{-C/r}$. The well known Hellmann-Feynman theorem shows that all the bound states of the Coulomb potential ($C = 0$) remain bounded as C increases. We derive a simple approximate analytical expression for the eigenvalues for sufficiently small values of the screening parameter C and an approximate asymptotic expression for the asymptotic behaviour of the s-state eigenvalues when $C \to \infty$. Present results are expected to resolve the discrepancy about the spectrum of the quantum-mechanical model just mentioned.

Keywords: screened Coulomb potential; radial Schrödinger equation; Hellmann-Feynman theorem; critical values

1. Introduction

There has recently been some interest in the screened Coulomb potential $V(r) = -r^{-1}e^{-C/r}$, $C > 0$. Stachura and Hancock[1] applied some approximate methods to the radial Schrödinger equation and conjectured that there are critical values C_n of the screening parameter C so that bound states disappear into the continuum when $C > C_n$. Later Xu et al[2] carried out accurate calculations by means of the powerful generalized pseudospectral method and argued that there may not be such critical values of the screening parameter. More precisely, the results of Xu et al strongly suggest that all the bound states of the Coulomb potential ($C = 0$) remain bounded for all values of $C > 0$.

The purpose of this letter is the analysis of those contradictory results and conclusions. In Section 2 we show that the well known Hellmann-Feynman theorem (HFT)[3,4] provides useful information about the spectrum of the model just mentioned. We also propose a simple approximate analytical expression for the eigenvalues of the Schrödinger equation for small values of C and an asymptotic expression for large values of this screening parameter. Finally, in Section 3 we summarize our main results and draw conclusions.

2. Theoretical analysis of the eigenvalue equation

In what follows, we focus on the radial part of the Schrödinger equation

$$-\frac{1}{2}\frac{d^2}{dr^2}\psi(r) + U(r)\psi(r) = E\psi(r),$$
$$U(r) = \frac{l(l+1)}{2r^2} + V(r),\ V(r) = -\frac{e^{-C/r}}{r}, \tag{1}$$

where $l = 0, 1, \ldots$ is the angular momentum quantum number and $C > 0$. The boundary conditions are

$$\lim_{r\to 0}\psi(r) = 0,\ \lim_{r\to\infty}\psi(r) = 0. \tag{2}$$

Stachura and Hancock[1] stated that $U(r)$ becomes repulsive for a sufficiently large value of l and illustrated this fact for $C = 0.1$ and $l = 7$ in their figure 8. However, they did not appear to realize that

$$\lim_{r\to\infty} rU(r) = -1. \tag{3}$$

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Their figure does not reveal this fact because the scale is rather too coarse. Since $U(r)$ does not become repulsive for any value of l and C we cannot state that there are critical values of C. On the other hand, the numerical results of Xu et al[2] suggest that all the bound states of the Coulomb problem remain bounded for all values of C.

The HFT[3,4] states that all the eigenvalues increase with C

$$\frac{dE}{dC} = \left\langle \frac{e^{-C/r}}{r^2} \right\rangle > 0, \tag{4}$$

but it does not mean that some some of them may become positive by increasing the value of C.

By means of the change of variables $\rho = r/C$ the eigenvalue equation can be rewritten as

$$-\frac{1}{2}\frac{d^2}{d\rho^2}\varphi(\rho) + \left[\frac{l(l+1)}{2\rho^2} - C\frac{e^{-1/\rho}}{\rho}\right]\varphi(\rho) = C^2 E\varphi(\rho). \tag{5}$$

The HFT

$$\frac{dC^2E}{dC} = -\left\langle \frac{e^{-1/\rho}}{\rho} \right\rangle < 0, \tag{6}$$

clearly shows that C^2E decreases with C. If we take into account that

$$\lim_{C\to 0} C^2 E = 0, \tag{7}$$

then we can safely conclude that all the bound states of the Coulomb potential remain bounded as C increases.

Both Stachura and Hancock[1] and Xu et al[2] resorted to approximations to $V(r)$ of the form

$$V^{[K]}(r) = -\frac{1}{r}\sum_{j=0}^{K}\frac{1}{j!}\left(-\frac{C}{r}\right)^j. \tag{8}$$

The case $K = 1$ is of particular interest because the resulting eigenvalue equation

$$-\frac{1}{2}\frac{d^2}{dr^2}\psi(r) + \left[\frac{l(l+1)+2C}{2r^2} - \frac{1}{r}\right]\psi(r) = E\psi(r), \tag{9}$$

can be solved exactly. Its eigenvalues are given by

$$E_{nl} = -\frac{1}{2(n+L-l)^2},\ L = -\frac{1}{2} + \sqrt{\left(l+\frac{1}{2}\right)^2 + 2C}, \tag{10}$$

where $n = 1, 2, \ldots$ is the principal quantum number. This expression yields satisfactory results for sufficiently small values of C. In fact, the approximate eigenvalues shown in Table 1 for $C = 0.1$ agree reasonably well with the accurate ones obtained by Xu et al[2]. This simple approximation suggests that there are bound states for all values of l when C is sufficiently small (in particular, we may point out the case $l = 7$, $C = 0.1$ discussed by Stachura and Hancock[1] in their figure 8).

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Table 1. Approximate eigenvalues E_{nl} for $C = 0.1$ obtained from equation (10) ($\nu = n - l - 1$)

ν	$l = 0$	$l = 1$	$l = 2$	$l = 3$
0	-0.365	-0.117	-0.0541	-0.0308
1	-0.106	-0.0532	-0.0306	-0.0198
2	-0.0497	-0.0303	-0.0197	-0.0138
3	-0.0287	-0.0195	-0.0137	-0.0101
4	-0.0187	-0.0136	-0.0101	-0.00776
5	-0.0131	-0.0100	-0.00774	-0.00613
6	-0.00972	-0.00769	-0.00612	-0.00497
7	-0.00749	-0.00608	-0.00496	-0.00411
8	-0.00595	-0.00493	-0.00410	-0.00346
9	-0.00483	-0.00408	-0.00345	-0.00295

In order to obtain an approximate asymptotic expression for the eigenvalues for large values of C we expand $V(r)$ about its minimum at $r = C$

$$V(r) \approx -\frac{1}{eC} + \frac{1}{2eC^3}(r - C)^2. \tag{11}$$

The radial Schrödinger equation with this approximate potential is exactly solvable for $l = 0$. Consequently, the eigenvalues E_{n0} behave approximately as

$$E_\nu \approx -\frac{1}{eC} + \sqrt{\frac{1}{eC^3}}\left(\nu + \frac{1}{2}\right),\ \nu = n - 1 = 0, 1, \ldots, \tag{12}$$

for sufficiently large values of C. It is clear that

$$\lim_{C\to\infty} CE_\nu = -\frac{1}{e}, \tag{13}$$

in agreement with the result conjectured by Xu et al[2] from their accurate numerical eigenvalues. The accuracy of the eigenvalues E_{n0} under the harmonic approximation (12) increases with C and decreases with $n = \nu + 1$.

The eigenvalues given by the asymptotic harmonic approximation (12) shown in Table 2 agree quite well with the accurate results of Xu et al[2]. As stated above, the accuracy of E_ν increases with C and decreases with ν.

Table 2. Eigenvalues E_ν obtained from the harmonic approximation (12)

C	$\nu = 0$	$\nu = 1$	$\nu = 2$
10^2	-3.38(-3)	-2.8(-3)	-2.2(-3)
10^3	-3.583(-4)	-3.39(-4)	-3.20(-4)
10^4	-3.6485(-5)	-3.588(-5)	-3.527(-5)
10^5	-3.6692(-6)	-3.650(-6)	-3.631(-6)

3. Conclusions

We have shown that the arguments put forward by Stachura and Hancok[1] about the existence of critical values of the screening parameter C are not correct. The HFT (6) and equation (7) clearly show that the bound states of the Coulomb problem remain bounded as C increases. Present approximate analytical expression (10) confirms this fact for small values of C. Besides, our approximate eigenvalues agree with the accurate ones obtained by Xu et al[2]. The latter results already follow the HFT (6). In

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addition to what has just been said, we have put forward a simple proof for the asymptotic behaviour of the eigenvalues at large values of C conjectured by Xu et al from their numerical results.

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