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Letters to the Editor

BOUND *s*-STATE OF AN ELECTRON IN THE SCREENED COULOMB FIELD

СВЯЗАНИЕ *s*-СОСТОЯНИЯ ЭЛЕКТРОНА В ЭКРАНИРОВАННОМ КУЛОНОВСКОМ ПОЛЕ

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There are many papers devoted to the approximative and/or numerical solutions of the Schrödinger equation for an electron with the screened Coulomb potential energy

$$V(r) = -\frac{e^2}{4\pi\varepsilon_0 r}\exp(-\varkappa r)\,, \tag{1}$$

as can be seen from references in recently published papers [1, 2] dealing with this problem. In this short note we should like to draw attention to the fact that the potential energy (1) can be, for $\varkappa r < 1$, well approximated by the function

$$U(r) = -\frac{e^2\varkappa}{4\pi\varepsilon_0}\,\frac{1+\exp(-2\varkappa r)}{\mathrm{sh}\,(2\varkappa r)}\,,$$

for which the *s*-state Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}r^2\frac{\mathrm{d}R(r)}{\mathrm{d}r} + [U(r)-E]\,R(r) = 0 \tag{3}$$

can be solved analytically [3].

The energy eigenvalues of the equation (3) can be, according to [3], written in the form

$$E_n^0/E_1^H = n^{-2}(1-\varkappa a_1 n^2)^2\,, \tag{4}$$

where E_1^H is the energy of the hydrogen ground state, a_1 is the Bohr radius, and $n = 1, 2, \ldots \leqq (\varkappa a_1)^{-1/2}$. The corresponding wave functions can be found in [3]. Here, we present only the normalized wave function corresponding to the ground state energy E_1^0:

$$\Psi_{100}(r, \vartheta, \varphi) = \left[\frac{1}{\pi a_1^3}(1-\varkappa^2 a_1^2)\right]^{1/2}\exp\left(-\frac{r}{a_1}\right)\frac{\mathrm{sh}\,(\varkappa r)}{\varkappa r}\,. \tag{5}$$

When the difference

$$V(r) - U(r) = -\frac{e^2\varkappa}{4\pi\varepsilon_0}\,\frac{\exp(-\varkappa r)}{\mathrm{sh}\,(\varkappa r)}\left[\frac{\mathrm{sh}\,(\varkappa r)}{\varkappa r} - 1\right]$$

is approximated as

$$U'(r) = -\frac{e^2\varkappa}{4\pi\varepsilon_0}\,\frac{\exp(-\varkappa r)}{\mathrm{sh}\,(\varkappa r)}\,\frac{(\varkappa r)^2}{6} \tag{6}$$

and $U'(r)$ is considered to be the perturbation to the potential energy $U(r)$, then by the use of the function (5) we obtain for the correction ΔE_1 to the ground state energy of an electron with potential energy (1) the following result:

$$\frac{\Delta E_1}{E_1^H} = \frac{1}{6}\varkappa a_1(1-\varkappa^2 a_1^2)\left(1-\frac{1}{(1+\varkappa a_1)^3}\right). \tag{7}$$

In Table 1, our computed values of the energy $E_1 = E_1^0 + \Delta E_1$ are compared with numerical solutions of the Schrödinger equation with the potential energy (1) as given by Rogers et al. [4]. As can be seen, a very good agreement is achieved for $\varkappa a_1 \leqq 0.5$.

Table 1

$\frac{1}{\varkappa a_1}$	E_1^0/E_1^H (4)	$\Delta E_1/E_1^H$ (7)	$(E_1^0-\Delta E_1)/E_1^H$	E_1/E_1^H [4]
100	0.98010	0.00005	0.98015	0.9801
50	0.9604	0.0002	0.9606	0.9606
20	0.9025	0.0011	0.9036	0.9036
10	0.8100	0.0041	0.8141	0.8141
7	0.7347	0.0077	0.7424	0.7424
5	0.6400	0.0135	0.6535	0.6535
4	0.5625	0.0191	0.5816	0.5818
3	0.4444	0.0285	0.4729	0.4737
2	0.2500	0.0440	0.2940	0.2962

The potential energy (2) can be rewritten in the form

$$U(r) = -\frac{e^2\varkappa}{4\pi\varepsilon_0}\,\frac{\exp(-\varkappa r)}{\mathrm{sh}\,(\varkappa r)}\,. \tag{8}$$

In papers [1] and [5] the Hulthén potential

$$U_H(r) = -\frac{e^2\varkappa}{4\pi\varepsilon_0}\,\frac{\exp(-\varkappa r)}{1-\exp(-\varkappa r)}\,, \tag{9}$$

which can be written as

$$U_H(r) = -\frac{e^2\varkappa}{4\pi\varepsilon_0}\,\frac{\exp(-\varkappa r/2)}{2\mathrm{sh}\,(\varkappa r/2)}\,,$$

was used as a basis for the perturbation calculation. However, the potential energy (2) represents a better approximation to the potential energy (1) in the range $\varkappa r < 1$, since

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$$V(r)/U(r) = \mathrm{sh}\,(\varkappa r)/\varkappa r = 1 + (\varkappa r)^2/6 + \dots,$$

while

$$V(r)/U_H(r) = 1 - \exp(-\varkappa r)/\varkappa r = 1 - \varkappa r/2 + \dots .$$

This is the reason why the very good agreement in our first-order perturbation calculations of the ground state energy with $\varkappa a_1 \leqq 0.5$ was obtained.

Finally, we notice that for $(\varkappa a_1)^3/2 \ll 1$ one can write

$$E_1^0 + \Delta E_1/E_1^H \doteq (1 - \varkappa a_1)(1 - \varkappa a_1 + (\varkappa a_1)^2/2)\,. \tag{10}$$

In a semiclassical treatment [6] we have derived the formula

$$E_1/E_1^H = (1 - \varkappa a_1)\exp(-\varkappa a_1)\,. \tag{11}$$

Here, neglecting the third and higher powers of $\varkappa a_1$ in the power series of the exponencial function, the relation (10) is obtained again.

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