VIRTUAL LEVELS FOR A SCREENED COULOMB POTENTIAL

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The question of the appearance of virtual levels in a screened Coulomb potential is considered. We calculate the value of d_c—the critical Debye radius at which the last bound state of the hydrogenlike atom in a screened Coulomb potential vanishes.

DEBYE screening causes the level system of a hydrogenlike atom situated inside a metal for example, to differ noticeably from the levels of the isolated atom. It is obvious that when the Debye radius is sufficiently small there are no bound states at all. It is therefore of interest to consider the values of d at which states with E = 0 (virtual levels) can appear in the screened Coulomb potential

$$V(r) = -\frac{e^2}{r} e^{-r/d} \tag{1}$$

In the spherically symmetrical case the Schrodinger equation $\hat{H}\psi = E\psi = 0$ is reduced by means of the substitution $\psi = u/r$ to the form

$$u''(x) = -\alpha \frac{e^{-x}}{x} u(x), \tag{2}$$

where $x = r/d$ and $\alpha = 2d/a$ ($a = \hbar^2/me^2$ is the Bohr radius). It is necessary to determine for what values of α Eq. (2) has a solution satisfying the boundary conditions

$$u(0) = 0, \quad u(\infty) = \text{const} = 1. \tag{3}$$

If we seek the solution in the form of a series in α:

$$u(x) = 1 + \sum_{n=1}^{\infty} (-\alpha)^n u_n(x), \tag{4}$$

then we can easily obtain for $u_n(x)$ the formula

$$u_n(x) = \underbrace{\int_1^\infty \ldots \int_1^\infty}_{n} \frac{dt_1\, dt_2 \ldots dt_n}{t_1^2 (t_1^2 + t_2^2) \ldots (t_1^2 + t_2^2 + \ldots + t_n^2)} \times e^{-x(t_1 + t_2 + \ldots + t_n)}, \tag{5}$$

which obviously satisfies condition (3) when $x = \infty$. Condition (3) will be satisfied if α is the root of the equation

$$1 + \sum_{n=1}^{\infty} (-\alpha)^n a_n = 0, \tag{6}$$

whose coefficients, in accordance with (5), are determined by the integrals

$$a_n = u_n(0) = \int_1^\infty \frac{dt_1}{t_1^2} \int_{1+t_1}^\infty \frac{dt_2}{t_2^2} \ldots \int_{1+t_{n-1}}^\infty \frac{dt_n}{t_n^2} \tag{7}$$

and cannot be obtained exactly for arbitrary n. However, in view of the inequality

$$1/(n!)^2 \leqslant a_n \leqslant 1/n!$$

the series (6) converges rapidly and to determine at least the first root it is possible to use the first few terms.

From (7) we get

$$a_1 = 1, \quad a_2 = 1 - \ln 2 = 0.307,$$
$$a_3 = 1 + \ln 2 - {}^3/_2 \ln 3 = 0.0452.$$

Four more coefficients, a_4, a_5, a_6, and a_7, reduce to single integrals. By numerical integration we have calculated

$$a_4 = 0.0039, \quad a_5 = 0.0002.$$

Then, by solving (6), we can find $\alpha_1 = 1.68$. Thus, there are no bound states if

$$d < d_c = {}^1/_2 \alpha_1 a = 0.84a. \tag{8}$$

For an approximate determination of the next roots, we use the WKB method. It is useful to note beforehand that an equation similar to (2), namely

$$v'' = -\alpha e^{-x} v, \quad v(x) = J_0(2\sqrt{\alpha} e^{-x/2}) \tag{9}$$

admits of an exact solution in the form of a Bessel function. In this case

$$\alpha_n = {}^1/_4 \varkappa_n^2 \cong {}^1/_4 \pi^2 (n - {}^1/_4)^2 \quad \text{for } n \gg 1, \tag{10}$$

where κ_n are the roots of the equation $J_0(\kappa_n) = 0$. We obtain similarly for (2) when $\alpha \gg 1$

$$u(x) \cong \cos\left(\sqrt{\alpha} \int_x^\infty \frac{dx}{\sqrt{x}} e^{-x/2} - \frac{\pi}{4}\right), \tag{11}$$

and then we get for the roots of (6) the relation

$$\sqrt{\alpha} \int_0^\infty \frac{dx}{\sqrt{x}} e^{-x/2} = \pi\left(n - \frac{1}{4}\right) \tag{12}$$

whence

$$\alpha_n \cong {}^1/_2\pi(n - {}^1/_4)^2 \qquad \text{for } n \gg 1. \tag{13}$$

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