ELECTRONIC LEVELS OF ATOMS OF SUPER-HEAVY ELEMENTS

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On the basis of the Dirac equation, the behavior of electronic ns-levels in the field of a nucleus of finite size with $Z > 137$ is investigated in the neighborhood of $\epsilon \sim -m$ and $\epsilon \sim +m$. The critical values $Z = Z_{cr}$ are found, the existence of quasilevels for $\epsilon \sim -m$ and $Z > Z_{cr}$ is shown and an interpretation of them is given.

1. The question of the properties of electronic levels of super-heavy nuclei has taken on renewed interest recently in connection with the obtaining of new transuranic elements. In order to estimate the position of electronic ns levels, we shall for simplicity choose the potential of a nucleus with charge Ze in the form $V = -\alpha Z/r$ for $r > r_0$ and $V = -\alpha Z/r_0$ for $r < r_0$, where r_0 is the nuclear radius. From the conditions for matching the solutions of the Dirac equation at $r = r_0$, we then find, for $Z > 137$ and $mr_0 \ll 1$ (m is the electron mass), the following equation for determining the level energy ϵ:

$$\varphi_0 + \varphi_\varepsilon = -n\pi, \qquad (1)$$

where on the left the part depending on ϵ is equal to

$$\varphi_\varepsilon = \arg\Gamma\left(ig - \frac{\gamma\varepsilon}{\lambda}\right) + g\ln\frac{\lambda}{m} + \tan^{-1}\frac{g}{(1+\gamma/W)},$$

and

$$\varphi_0 = g\ln 2mr_0 - \arg\Gamma(1+2ig) - \tan^{-1}\frac{g}{\gamma}\tan\gamma.$$

Here

$$\gamma = \alpha Z,\quad g = \sqrt{\gamma^2 - 1},\quad \lambda = \sqrt{m^2 - \varepsilon^2},\quad W = (m+\varepsilon)/\lambda.$$

Equation (1) coincides with the corresponding equation of the paper by Pomeranchuk and Smorodinskiĭ[1] if the following correction is made in the latter: $\xi(\gamma) = \gamma\cot\gamma - 1$ should be replaced by $(1 - \gamma\cot\gamma)^{-1}$. For $\epsilon = -m$ and $n = 1$, we find from (1) the equation for the determination of Z_{cr}:

$$g\ln 2mr_0\gamma = \arg\Gamma(1+2ig) + \tan^{-1}\frac{g}{\gamma}\tan\gamma - n\pi. \qquad (2)$$

Z_{cr} has a weak dependence on r_0 and is equal to 178 for $r_0 = 12 \times 10^{-13}$ cm and 172 for $r_0 = 8 \times 10^{-13}$ cm (instead of the values 200 and 175 of reference 1). For nuclei on the β-stability curve[2] extrapolated to the region of super-heavy nuclei and for $r_0 = 1.2 \times 10^{-13} A^{1/3}$ cm, we find $Z_{cr} = 174$.

2. We now consider the character of the discrete levels near the limit of the continuous spectrum: $\epsilon = m$ ($Z > 137$). Noting that for $\epsilon \to +m$, $\lambda \to 0$, and using the asymptotic formula for $\arg\Gamma(ig - \gamma\epsilon/\lambda)$ for $\gamma\epsilon/\lambda \to \infty$, we find from (1)

$$\tan^{-1}\frac{\tanh\pi g}{\tan\pi N} = -\pi n + \psi_0 - g\ln 2mr_0,$$

$$\varepsilon = m/\sqrt{1+\gamma^2/N^2},$$

$$\psi_0 = \arg\Gamma(1+2ig) + \tan^{-1}\frac{g}{\gamma}\tan\gamma - g\ln\gamma - \tan^{-1}g, \qquad (3)$$

where $N = \gamma\epsilon/\lambda$ has the significance of an "effective" principal quantum number. Furthermore, we find from (3),

$$N = n + \frac{1}{\pi}\tan^{-1}\frac{\tanh\pi g}{\tan(\psi_0 - g\ln 2mr_0)}, \qquad (4)$$

whereas for a pure Coulomb field for $Z < 137$ we have $N = n + \sqrt{1-\gamma^2}$.[3] As r_0 is decreased the levels are pushed downward. From (3) it follows that the rate at which the levels with principal quantum number N are pushed is characterized by the derivative

$$dN/dr_0 = g(\tan^2\pi g\cos^2\pi N + \sin^2\pi N)/r_0\pi\tanh\pi g,$$

which is a minimum for $N = n$ [so that $(\pi r_0/g) \times dN/dr_0 = \tanh\pi g$], i.e. when the spectrum of the cut-off Coulomb field in the region $\epsilon \sim m$ and $Z > 137$ coincides with the spectrum of the Coulomb field for $Z = 137$. dN/dr_0 is a maximum for $N = n + 1/2$ [then $(\pi r_0/g)\, dN/dr_0 = (\tanh\pi g)^{-1}$], i.e. when the spectrum differs most from the spectrum of the pure Coulomb field for $Z = 137$. This effect is especially important for Z only slightly exceeding 137.

3. Let us now illustrate on the example of a potential well of radius r_0 the appearance of quasi-levels in the region $\epsilon < -m$ after the pushing of the lowest discrete level to $-m$. For $U = U_{cr} + \Delta$

(U is the well depth, U_{cr} corresponds to Z_{cr}, $\Delta > 0$ and small), the lowest discrete level disappears. Matching the external (e) and internal (i) solutions of the Dirac equation[3] for $\epsilon = -m - w$ ($w > 0$ and small):

$$G_i = \sin kr, \quad G_e = A \sin(pr + \alpha),$$

$$F_i = \frac{p}{U}\left(\cos kr - \frac{\sin kr}{kr}\right),$$

$$F_e = -\frac{Ap}{w}\left(\cos(pr + \alpha) - \frac{\sin(pr + \alpha)}{pr}\right),$$

$$k = \sqrt{(\varepsilon + U)^2 - m^2}, \quad p = \sqrt{\varepsilon^2 - m^2},$$

we get

$$\cot\beta = (1/pr_0)(1 - \pi w/U\delta), \quad \beta = \alpha + pr_0,$$

$$\delta = (r_0^2/\pi)(U_{cr} - m)(\Delta - w).$$

In this case $G_e \ll F_e$ so that G_e and G_i can be disregarded in what follows. The ratio of the amplitude F_e to F_i, which is equal to $2mU_{cr}\delta/\pi p \sin\beta$, is anomalously small for $\beta \sim \pi/2$, i.e. for

$$w = \Delta(mr_0^2U_{cr} + \pi^2)/(mr_0^2U_{cr} + 2\pi^2). \quad (5)$$

This indicates the possible existence in this energy region of a quasistationary state — a quasilevel.

In fact, solving the Dirac equation with the condition of outgoing waves at infinity $\sim e^{ipr}/r$ and $\epsilon = -m - w - i\Gamma$, we find formula (5) for w, and a level width

$$\Gamma = w^{3/2}(\sqrt{2m}\pi^2r_0^2)/(2\pi^2 + mr_0^2U_{cr}). \quad (6)$$

One can give an interpretation of the behavior of the electron-positron system starting from the second-quantized Hamiltonian of the system. For $U < U_{cr}$ the state Φ^0, in which the lower continuum is filled, is finite and neutral, just as for $U = 0$.

The state Φ', in which the lowest discrete level ϵ, (with degeneracy η_1) is also filled, has a charge $-\eta_1 e$ and is finite in the neighborhood of $U = U_{cr}$, since for $U = U_{cr}$ the gap separating Φ' from the continuous spectrum of states with the same charge is finite (this gap is $\epsilon_2 - \epsilon_1$ where ϵ_2 is the next level after ϵ_1). But then for $U > U_{cr}$ all the neutral states are infinite, since they are obtained from Φ' by the application of η_1 annihilation operators corresponding to the lower continuum. Since as shown above there are quasilevels in the lower continuum, this corresponds to a quasi-stationary state Φ^{*0} which decays with emission of η_1 positrons with a lifetime $1/2\Gamma$.

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[2] N. N. Kolesnikov, JETP 30, 889 (1956), Soviet Phys. JETP 3, 844 (1957).

[3] A. I. Akhiezer and V. B. Berestetskiĭ, Квантовая электродинамика (Quantum Electrodynamics), Fizmatgiz, (1959).

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