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Interior Electron Shells in Superheavy Nuclei*

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The interior electron shells for superheavy nuclei ($90 \leqq Z \leqq 250$) have been investigated. Their binding energies are tabulated together with the vacuum polarization corrections for the various levels.

Introduction

It is known that Sommerfeld's finestructure formula does not hold for Z-values larger than 137, but that it is possible to go beyond this value if one changes the singularity of the Coulomb potential by the more realistic assumption of an extended nucleus[1-4]. Up to now this has been done for a potential constant inside the nucleus corresponding to a conducting sphere rather than for a homogeneous charged sphere.

For the electronic structure of superheavy nuclei it is important to clarify qualitatively and quantitatively the level structure of the K- and L-electrons for high Z elements. Therefore, in Section I, the electron energies and wave functions for a schematic square well potential are studied. In this case it is particularly simple to investigate the behavior of the electron wave functions in the limit $E \to -m$, e.g. when the bound electron levels drop into the positron continuum. In Section II we study the more realistic case where the Coulomb potential is that of a homogeneously charged sphere with radius $R = 1.2 \cdot A^{1/3}$ fm. All eigenstates of the first three radial quantum numbers $n = 1, 2, 3$ are calculated. The vacuum polarization corrections are also included.

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I. The Square-Well Potential

It is possible to give explicitly analytic solutions of the Dirac equation for a square well potential. This is particularly useful in order to investigate the qualitative behavior of the electron wave functions in the limit $E \to -m$, e.g. the case where the bound electron orbits drop into the "positron sea".

For a spherical symmetric square-well potential

$$V(r)=\begin{cases} -V_0 & \text{for } r \leqq R_0 \\ 0 & \text{for } r > R_0 \end{cases} \tag{1}$$

the Dirac equation has the form*

$$\begin{aligned} u' - \frac{\kappa}{r} u &= (m-E+V(r))\, w \\ w' + \frac{\kappa}{r} w &= (m+E-V(r))\, u, \end{aligned} \tag{2}$$

where $u(r)$, $w(r)$ are the radial wave functions of the upper and the lower 2-spinor which form the 4-spinor, respectively.

The only solutions of s-levels ($\kappa = -1$) inside the well, which can be normalized, are

$$\left.\begin{aligned} u_1 &= c_1 \left(\frac{\sin x}{x} - \cos x\right) \\ w_1 &= c_1\, S \sin x \end{aligned}\right\} \quad \text{for} \quad r \leqq R_0 \tag{3}$$

with

$$S = \sqrt{\frac{E+V_0+m}{E+V_0-m}}\ \operatorname{sign} \kappa$$

$$x = r\, k_1, \qquad k_1 = \sqrt{(E+V_0)^2 - m^2}.$$

Similarly we find that

$$\begin{aligned} u_2 &= -c_2 \sqrt{\frac{m-E}{m+E}} \left(1 + \frac{1}{k_2 r}\right) e^{-k_2 r}, \\ w_2 &= c_2\, e^{-k_2 r}, \end{aligned} \tag{4}$$

$$k_2 = \sqrt{m^2 - E^2} \tag{5}$$

are the only s-wave functions in the region outside the well which drop down sufficiently fast at infinity. The energy is determined by fitting the

* We choose units with $\hbar = c = 1$.