LAMB SHIFT AND ENERGY LEVEL OF A TIGHTLY BOUND ELECTRON

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The K-absorption edge in mercury has been calculated to within terms of order α^2mc^2 (where $\alpha^2mc^2 = 2$ ry), with the object of verifying the presence of the Lamb shift, which is of order αmc^2. Here, we consider $Z\alpha$ to be of the order of unity, since Z is large.

Earlier rough calculations[1] to within order αmc^2 of all effects other than the Lamb shift gave a value of 6129 ry for the K-absorption edge and left an apparent discrepancy of only several Rydbergs with experiment to be accounted for by the Lamb shift. However, the experimental values were incorrectly quoted in this article, and the actual discrepancy was ~ 20 ry.

To improve on the calculation of effects of order mc^2 and αmc^2 other than the Lamb shift, a relativistic self-consistent-field calculation with exchange (Hartree-Fock calculation) was carried out by one of us (D.F.M.). Just as in the nonrelativistic case,[2] the energy of the electron system can be expressed in terms of one-electron radial integrals; complete expressions have been given by Swirles[3] and Grant.[4] To within order αmc^2, the K-absorption edge is given by $\epsilon_{1s} + \delta\epsilon_{1s}$, where ϵ_{1s} is the eigenvalue of the $1s$ state, and $\delta\epsilon_{1s}$ is the shift arising from the magnetic interaction between the K electrons. The eigenvalue was found to be 6152 ry, and $\delta\epsilon_{1s}$, -15 ry, giving a net value of 6137 ry. This is in good agreement with similar calculations by Cohen,[5] who obtains 6138 ry.

Inclusion of the Lamb shift completes the effects of order αmc^2. This calculation was carried out[6] without employing an expansion in $Z\alpha$, giving a result of -38 ry when combined with that of the vacuum polarization.[7] The resulting theoretical value of 6099 ry is to be compared with the experimental value[8] of 6107.7 ± 0.6 ry for the K-absorption edge, showing that inclusion of the Lamb shift markedly improves the agreement.

Corrections of order α^2mc^2 are contributed by the rearrangement energy and by the finite size of the nucleus. The former was evaluated by repeating the relativistic self-consistent-field calculations for the ionized atom, $Hg^+(1s)^{-1}$, giving a result of 4 ry.

The correction from the finite size of the nucleus was calculated using[9]

$$G_0^2\delta y\,|_{R_1} - G_0^2\delta y\,|_{R_2} = \int_{R_1}^{R_2} \left\{ \frac{G_0^2}{G^2}(G^2+F^2)(\delta E - \delta V) + G_0^2(E+m-V)(\delta y)^2 \right\} dr, \quad (1)$$

where F, G, and F_0, G_0 are the perturbed and unperturbed Dirac radial functions, multiplied by r, respectively, $y = F/G$, $y_0 = F_0/G_0$, and $\delta y = y - y_0$. Here, R_1 was chosen to be a radius just outside the nuclear radius, and R_2 to be an appreciable fraction of the radius of the K shell. The δy was calculated by numerical integration of the differential equation from which Eq. (1) was obtained. The correction to the energy level from a nucleus with shape represented by an inverted Fermi distribution[10] was -3.9 ry, effectively cancelling the rearrangement energy.

We believe that the discrepancy of ~ 8 ry comes mainly from the inadequacy of the self-consistent-field method in describing correlation in angle of the two K electrons, which tend to stay apart because of their mutual repulsion.

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