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Relativistic Effect on the L_3-Shell Binding-Energy Increase in Ion-Atom Collisions

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The binding-energy increase of the L_3-shell electrons with different magnetic quantum numbers during ion-atom collisions is estimated relativistically. The calculations have been made for a straight-line trajectory by the use of relativistic screened hydrogenic wave functions. The obtained results indicate that at small impact parameters the electronic relativistic effect considerably enhances the binding-energy increase.

KEY WORDS: Binding-Energy Increase/ Magnetic-Qunatum Number Dependence/ Relativistic Effect/

I. INTRODUCTION

In recent years the alignment of inner-shell electrons in ion-atom collisions has received considerable attention. Experimentally the process can be observed as angular distribution of the collisionally induced X-rays or Auger electrons. Many experimental studies on the alignment in L_3-shell ionization by charged-particle impact have been reported.[1] The experimental results for the anisotropy $\mathscr{A}_0$ as a function of the projectile energy are in good agreement with the theoretical predictions. However, for low-energy projectiles the experimental data scatter with each other and there is discrepancy between theoretical values based on different assumptions.

The anisotropy parameter for L_3-shell ionization is defined as[2]

$$\mathscr{A}_0 = \frac{\sigma(3/2) - \sigma(1/2)}{\sigma(3/2) + \sigma(1/2)}, \qquad (1)$$

where $\sigma(m)$ is the ionization cross section for L_3-shell electron with the magnetic quantum number m. The L_3-shell ionization cross section has been usually calculated in the plane-wave Born approximation (PWBA)[3] or the semiclassical approximation (SCA).[4]

It is well known that in the L-shell ionization process for low-energy projectiles three effects become important: the electronic relativistic effect of the target electron, the Coulomb deflection of the projectile by the target atom, and the increased binding energy of the target electron due to presence of the projectile. The Coulomb-deflection effect for different m states has been estimated by Pálinkás *et al.*[5] and by Jitschin *et al.*[6] The relativistic SCA calculations for $\sigma(m)$ have been performed with hyperbolic trajectories by Rösel *et al.*[7]

On the other hand, following the method of Brandt and Lapicki,[8] Sarkadi[9] has

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derived the nonrelativistic expressions for m-dependent binding-energy increase as a function of impact parameter. However, considering the fact that most experiments for alignment in L-shell ionization by heavy charged-particle impact have been made for heavy elements and we are interested in low-energy projectiles, it is interesting to calculate the m-dependent L_3-shell binding-energy shift relativistically.

In the present work, the L_3-shell binding-energy increase during ion-atom collisions has been estimated for $|m|=1/2$ and $|m|=3/2$ states by the use of relativistic hydrogenic (Dirac) wave functions. The calculations are based on the method of Brandt and Lapicki[8] and made in the manner similar to the relativistic calculations for the m-averaged binding-energy increase.[10]

II. BINDING-ENERGY INCREASE

According to the first-order perturbation theory, the change in the binding energy of the target electron during ion-atom collisions can be expressed as[10]

$$\Delta E=\int\phi^*(\boldsymbol{r})\frac{\alpha Z_1}{|\boldsymbol{R}-\boldsymbol{r}|}\phi(\boldsymbol{r})\,d\boldsymbol{r}, \tag{2}$$

where $\phi(\boldsymbol{r})$ is the unperturbed wave function for the L_3-shell electron, Z_1 is the atomic number of the projectile, $\boldsymbol{R}$ and $\boldsymbol{r}$ are the coordinates of the projectile and the electron, respectively. The relativistic units ($\hbar=m=c=1$) are used.

The relativistic hydrogenic wave function for L_3-shell electron with magnetic quantum number m is given by[11]

$$\phi^m_{L3}=\begin{pmatrix} g(r) & \chi^m_{-2}(\hat{\boldsymbol{r}}) \\ if(r) & \chi^m_2(\hat{\boldsymbol{r}}) \end{pmatrix}, \tag{3}$$

where $\chi^m_\kappa(\hat{\boldsymbol{r}})$ is the spin-angular momentum wave function and $\hat{\boldsymbol{r}}$ is a unit vector of the direction $\boldsymbol{r}$. The large and small parts of radial wave function are written by

$$g(r)=N(1+W)^{1/2}\exp(-\lambda r), \tag{4a}$$

$$f(r)=-N(1-W)^{1/2}\exp(-\lambda r), \tag{4b}$$

where $N=[\zeta^{2\gamma+1}/2\Gamma(2\gamma+1)]^{1/2}$, $\zeta=\alpha Z_{2L}$, $\gamma=(4-\zeta^2)^{1/2}$, $W=\{(1+\gamma)/2\}^{1/2}$, α is the fine structure constant, $Z_{2L}=Z_2-4.15$ is the effective nuclear charge seen by the L_3-shell electron, and Z_2 is the atomic number of the target.

Substituting Eq. (3) into Eq. (2) and using the multipole expansion of $1/|\boldsymbol{R}-\boldsymbol{r}|$, we obtain the m-dependnet L_3-shell binding-energy shift:

$$\Delta E^m=\alpha Z_1[I_0-(-1)^{|m|+1/2}\frac{1}{5}I_2], \tag{4}$$

where

$$I_0=\frac{1}{R}\int_0^R Q(r)\,r^2dr+\int_R^\infty Q(r)\,rdr, \tag{5a}$$

$$I_2=\frac{1}{r^3}\int_0^R Q(R)\,r^4dr+R^2\int_R^\infty Q(r)\frac{dr}{r}, \tag{5b}$$

with $Q(r)=g^2(r)+f^2(r)$ and $R=|\boldsymbol{R}|$.

Following the method of Brandt and Lapicki,[8] we use the semiclassical approximation and describe the projectile by a straight-line trajectory with an impact parameter b. Then the dominant contribution of I_0 and I_2 as a function of R comes from the value at the point of the closest approach and we can assume that R can be set to be equal to b. Under this approximation the scaled binding-energy shifts in units of Rydberg are written as a function of impact parameter by

$$\frac{\Delta E^{\pm 1/2}}{Z_1 Z_{2L}}=\frac{2}{\Gamma(2\gamma+1)}\frac{1}{y}\Big\{\gamma(2\gamma+1,\ y)+\frac{1}{5y^2}\gamma(2\gamma+3,\ y)+y\Gamma(2\gamma,\ y)+\frac{y^3}{5}\Gamma(2\gamma-2,\ y)\Big\}, \tag{6}$$

$$\frac{\Delta E^{\pm 3/2}}{Z_1 Z_{2L}}=\frac{2}{\Gamma(2\gamma+1)}\frac{1}{y}\Big\{\gamma(2\gamma+1,\ y)-\frac{1}{5y^2}\gamma(2\gamma+3,\ y)+y\Gamma(2\gamma,\ y)-\frac{y^3}{5}\Gamma(2\gamma-2,\ y)\Big\}. \tag{7}$$

with $y=\zeta b$.

Here $\Gamma(x)$ is the gamma function, and $\gamma(a,\ x)$ and $\Gamma(a,\ x)$ are the incomplete gamma functions defined as follows:

$$\gamma(a,\ x)=\int_0^x \exp(-t)\,t^{a-1}\,dt,$$

and

$$\Gamma(a,\ x)=\int_x^\infty \exp(-t)\,t^{a-1}\,dt.$$

In the zero impact-parameter limit Eqs. (6) and (7) approach to the same value:

$$\frac{\Delta E^{\pm m}}{Z_1 Z_{2L}}=\frac{1}{\gamma}. \tag{8}$$

On the other hand, in the limit of $\gamma=2$ Eqs. (5) and (6) reduce to the nonrelativistic expressions obtained by Sarkadi:[9]

$$\frac{\Delta E^{\pm 1/2}}{Z_1 Z_{2L}}=\frac{2}{y}\Big\{1+\frac{6}{y^2}-e^{-y}\Big(\frac{6}{y^2}+\frac{6}{y}+4+\frac{7}{4}y+\frac{y^2}{2}+\frac{y^3}{12}\Big)\Big\}, \tag{9}$$

$$\frac{\Delta E^{\pm 3/2}}{Z_1 Z_{2L}}=\frac{2}{y}\Big\{1-\frac{6}{y^2}+e^{-y}\Big(\frac{6}{y^2}+\frac{6}{y}+2+\frac{y}{4}\Big)\Big\}. \tag{10}$$

III. RESULTS AND DISCUSSION

The relativistic calculations of increase in the binding energy of L_3-shell electron with $|m|=1/2$ and $3/2$ have been performed for Ag, Au, Pb, and U. The results are shown in Figs. 1-4 as a function of impact parameter and compared with the nonrelativistic values. The scaled binding-energy increase is given in units of Rydberg and the impact parameter is expressed in $a_{2L}=a_0/Z_{2L}$, where a_0 is the first Bohr radius. The nonrelativistic value of $\Delta E_L/Z_1Z_{2L}$ has a universal property for Z_2 while the relativistic value depends on Z_2.

It can be seen from Fig. 1 that in the case of Ag ($Z_2=47$) the relativistic effect is not so important, but there is considerable difference between the values of $|m|=1/2$ and 3/2. The scaled binding-energy increase for $|m|=1/2$, which is equal to that for $|m|=3/2$ at $b=0$, increases with increasing b and then decreases. There is a peak around at $b=2a_{2L}$. On the other hand, the binding-energy increase for $|m|=3/2$ is a monotone decreasing function of b. Therefore, in the region $b>0$ the binding-energy shift for $|m|=1/2$ is always larger than that for $|m|=3/2$.

For larger Z_2 values, the relativistic effect becomes important. This can be seen in Figs 2-4 for Z_2 values between 79 and 92. The general behaviour of the relativistic curves with $|m|=1/2$ and 3/2 is the same as that for Ag, but the relativistic effect enhances the binding-energy increase. The difference between the relativistic and nonrelativistic values is largest at $b=0$ and becomes gradually smaller with increasing b. In the case of high b values the relativistic energy shift tends to approach to the nonrelativistic one. The peak position for $|m|=1/2$ in the relativistic case is almost same as that in the nonrelativistic case.

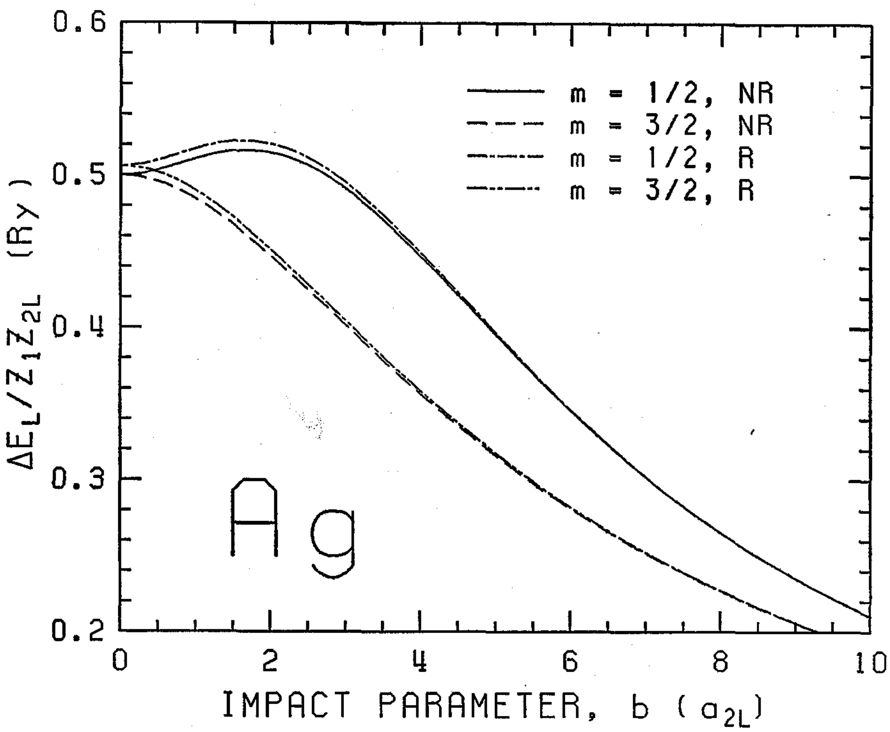

Fig. 1. The increase in scaled binding energy of L_3-shell electron, $\Delta E^m/Z_1Z_{2L}$, as a function of impact parameter b for silver. The solid line represents the nonrelativistic result for $|m|=1/2$ and the dashed curve for $|m|=3/2$, while the dash-dotted line corresponds to the relativistic result for $|m|=1/2$ and the dash-double-dotted curve for $|m|=3/2$.

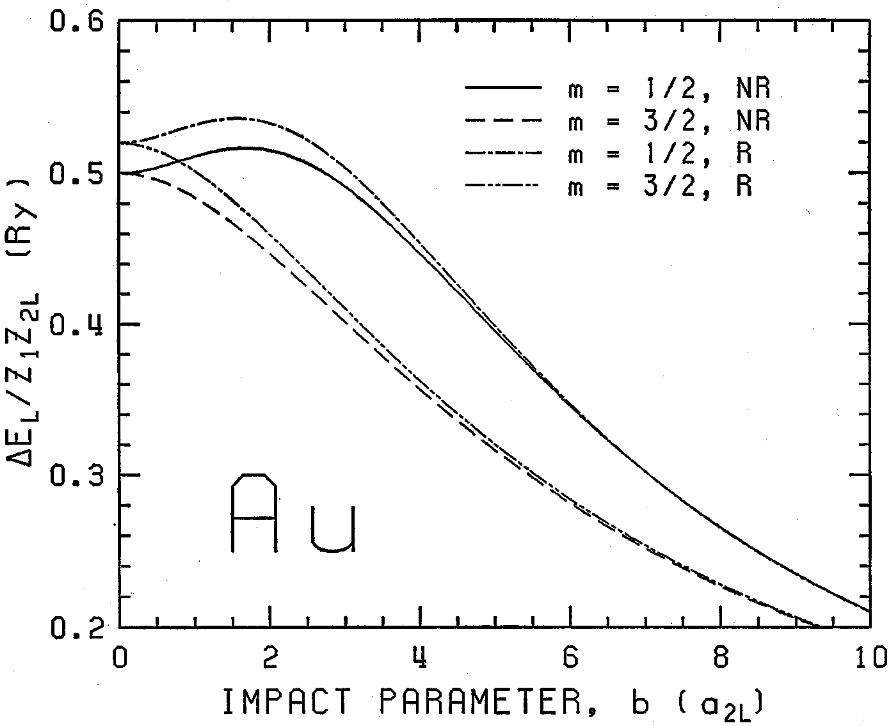

Fig. 2. The same as Fig. 1, but for gold.

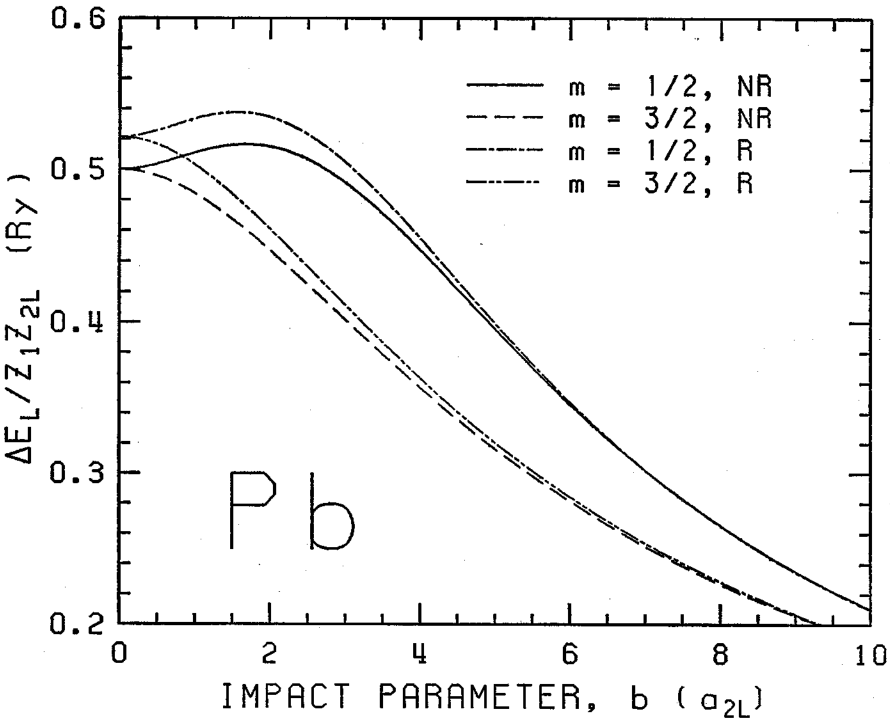

Fig. 3. The same as Fig. 1, but for lead.

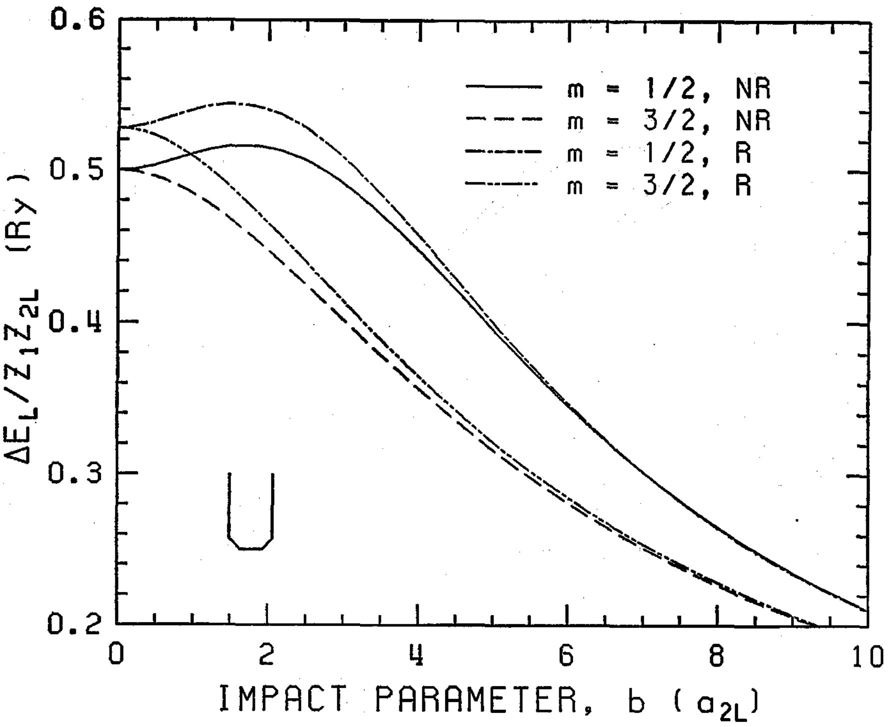

Fig. 4. The same as Fig. 1, but for uranium.

It should be noted that the behaviour of the m-dependent L_3-shell binding-energy increase is different from the m-averaged one. The latter is a slowly decreasing function of b.[10] On the other hand, as can be seen from Figs. 1-4, the energy shift for $|m|=3/2$ is more rapidly decreasing with b and that for $|m|=1/2$ has a peak around at $b=2a_{2L}$.

IV. CONCLUSION

The relativistic calculations of m-dependent L_3-shell binding-energy increase have been made for a straight-line trajectory by the use of screened hydrogenic wave functions. The obtained results indicate that the general behaviour of the scaled binding-energy shift as a function of impact parameter does not change from the nonrelativistic one, but the relativistic effect considerably enhances the binding-energy increase at small impact parameters for high Z_2 elements.

Most experimental studies have been made with high-Z_2 targets and impact-parameter-dependent L_3-shell ionization cross sections are large for small impact parameters. Considering these facts, the anisotropy parameter in Eq. (1) may change when the present results are incorporated into the m-dependent L_3-shell ionization cross sections. It is hoped to perform relativistic calculations of m-dependent L_3-shell ionization cross sections for heavy elements by the use of the present results.

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