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Relativistic Calculations of the 1s-2s Excitation Cross Sections of Hydrogen-Like Ions by Heavy-Charged Particle Impact

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The cross sections for the $1s$–$2s$ excitation of hydrogen-like ions by heavy-charged particle impact have been calculated using the relativistic wave functions for the target electron in the Born and distortion approximations. The obtained results are compared with the nonrelativistic values. It is found that the electronic relativistic effect in the $1s$–$2s$ excitation is less important than in the K-shell ionization. The effect of increased binding energy due to presence of the projectile is discussed by comparing the cross scetions in the Born approximation with those in the distortion approximation.

KEY WORDS: $1s$–$2s$ Esxcitation/ Electronic Relativistic Effect/ Distortion Approximation/

I. INTRODUCTION

The $1s$–$2s$ excitation of hydrogen atom or hydrogenic ions have been an interesting problem in atomic physics. Many theoretical calculations have been reported using various models. It is well known that for low-energy projectiles the simple Born approximation becomes unreliable and the perturbation of the eigenstates of the target atom due to presence of the projectile should be considered. In order to take into account this effect, Bates[1] introduced the distortion approximation in the impact-parameter approach and calculated the excitation cross sections of hydrogen atoms by protons and α particles. He showed that the inclusion of the distortion greatly reduces the cross sections obtained in the first Born approximation in low-energy region. Detailed calculations on hydrogen and helium atoms have further confirmed his results.[2]

Up to the present, the distortion approximation has been applied only for the case of hydrogen and helium atoms by proton and α-particle impact. Accordingly all the calculations reported are nonrelativistic ones. In the present work, the relativistic calculations of the $1s$-$2s$ excitation cross section of hydrogenic ions by charged-particle impact have been made and the electronic relativistic effect on the excitation cross section has been investigated. The relativistic hydrogenic (Dirac) wave functions are used for target electron, while the projectile is treated nonrelativistically because of low velocity. The effect of increased binding energy of the target electron due to presence of the projectile has been studied by comparing the cross sections in the first Born approximation with those in the distortion approximation.

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II. THEORY

A general formalism of the distortion approximation has been given by Bates[3] and McDowell and Coleman.[4] Here we follow their approach.

Consider the system that the target atom is at rest at the origin of the coordinate and the incident ion moves along a straight line with constant velocity v. The Z axis is chosen in the direction of the projectile and the impact parameter, the distance of the projectile from the Z axis, is taken to be ρ.

The collision is described by the time-dependent Schrödinger equation

$$\mathrm{i}\frac{\partial}{\partial t}\Psi(r, t) = H\Psi(r, t)\,, \tag{1}$$

where r is the position vector of the target electron. The Hamiltonian for the motion of electron is the sum of that for the target ion and the time-dependent perturbation:

$$H = H_0 + V(r, R)\,,$$
$$H_0 = -\frac{1}{2}\nabla^2 - \frac{Z_2}{r}\,,$$
$$V(r, R) = \frac{Z_1 Z_2}{R} - \frac{Z_1}{|R-r|}\,,$$

where R is the position vector of the projectile and Z_1 and Z_2 are the nuclear charge of the projectile and target ion, respectively. Throughout the present work, atomic units are used.

We expand the electronic wave function in terms of hydrogenic wave functions of the target atom:

$$\Psi(r, t) = \sum_n a_n(t)\varphi_n(r)\exp(-\mathrm{i}\varepsilon_n t)\,. \tag{2}$$

Here $\varphi_n(r)$ is the hydrogenic wave function for the state n and ε_n is the energy eigenvalue of this state, *i.e.*

$$H_0\varphi_n(r) = \varepsilon_n\varphi_n(r)\,. \tag{3}$$

The summation in Eq. (2) means a sum over discrete states and an integration over the continuum.

Susbstituting Eq. (2) into Eq. (1), we obtain

$$\mathrm{i}\frac{\partial}{\partial z}a_n(z) = \frac{1}{v}\sum_s a_s(z)V_{ns}\exp(-\mathrm{i}\alpha_{ns}z)\,, \tag{4}$$

where

$$z = vt\,,$$
$$V_{ns} = \int\varphi_n^*(r)V(r, R)\varphi_s(r)\,\mathrm{d}\boldsymbol{r}\,, \tag{5}$$

and

$$\alpha_{sn} = (\varepsilon_s - \varepsilon_n)/v\,.$$

When the initial state is the ground state of the target atom and denoted as 0, the initial condition of Eq. (4) is given by

$$a_s(-\infty) = \delta_{s0}\,. \tag{6}$$

The cross section describing excitation from the ground state to the state n can be expressed as

$$Q_n = 2\pi\int_0^\infty |a_n(+\infty)|^2 \rho\, d\rho\,. \tag{7}$$

In the impact-parameter description of the first Born approximation, $a_0(z)=1$ and all other states except for $s=n$ are set euqal to 0, *i.e.* $a_s(z)=0$ for $s\neq n$. Then Eq. (4) can be written by[5]

$$a_n(\infty) = -\frac{\mathrm{i}}{v}\int_{-\infty}^{\infty} V_{n0} \exp(-\mathrm{i}\alpha_{0n} z)\, dz\,. \tag{8}$$

The equivalence of this expression to the first Born approximation in the quantum mechanical treatment[6] has been verified by Arthurs.[7]

If we consider only the term with $s=0$, Eq. (4) is solved as

$$a_0(z) = \exp\left[-\frac{\mathrm{i}}{v}\int_{-\infty}^{z} V_{00}\, dz'\right]. \tag{9}$$

Using Eq. (9) and keeping the terms with $s=0$ and $s=n$, Eq. (4) can be written by

$$\mathrm{i}\frac{\partial}{\partial z} a_n(z) = \frac{1}{v}\{V_{nn} a_n(z) + V_{n0} \exp[-\mathrm{i}\alpha_{0n} z - \int_0^z V_{00}\, dz']\}\,. \tag{10}$$

From Eq. (10), the transition amplitude is obtained as

$$a_n(\infty) = -\frac{\mathrm{i}}{v}\int_{-\infty}^{\infty} V_{n0} \exp[-\mathrm{i}\alpha_{0n} z - \mathrm{i}\beta_{0n}]\, dz\,, \tag{11}$$

where

$$\beta_{0n} = \frac{1}{v}\int_0^z (V_{00} - V_{nn})\, dz'\,. \tag{12}$$

Comparing Eqs. (8) and (11), it can be seen that the distortion approximation is a higher approximation than the first Born approximation and takes into account the perturbation of the binding energy of the target electron during ion-atom collision.

The relativistic hydrogenic wave functions are given by[8]

$$\Psi(r) = \begin{pmatrix} g_\kappa(r)\ \chi_\kappa^\mu(\hat{r}) \\ \mathrm{i}f_\kappa(r)\ \chi_{-\kappa}^{\mu}(\hat{r}) \end{pmatrix}, \tag{13}$$

where κ is the relativistic quantum number, μ is the magnetic quantum number,

$\chi_\kappa^\mu(\hat{r})$ is the spin-angular function, and $\hat{r}$ is the unit vector of the direction of r. The large and small components of the radial wave function are

$$g_\kappa(r) = N(1+W)^{1/2}(c_0+c_1)\, r^{\gamma-1}\mathrm{e}^{-\lambda-1}\,, \tag{14a}$$

and

$$f_\kappa(r) = -N(1-W)^{1/2}(a_0+a_1 r)\, r^{\gamma-1}\mathrm{e}^{-\lambda-1}\,, \tag{14b}$$

where the parameters, N, W, a_0, a_1, c_0, c_1, γ, and λ for 1s and 2s states are given in Ref. 8.

Using the wave functions in Eq. (13), the relativistic matrix elements for the 1s–2s excitation are obtained as

$$V_{00} = -Z_1 N_1^2 \left[\frac{1}{R}\frac{\gamma(2\gamma+1,\, 2\lambda_1 R)}{(2\lambda_1)^{2\gamma+1}} + \frac{\Gamma(2\gamma,\, 2\lambda_1 R)}{(2\lambda_1)^{2\gamma}}\right], \tag{15}$$

$$\begin{aligned} V_{nn} = -Z_1 N_2^2\, [&\{(1+W_2)c_0^2+(1-W_2)a_0^2\}\, J_0 \\ &+2\{(1+W_2)c_0c_1+(1-W_2)a_0a_1\}\, J_1 \\ &+\{(1+W_2)c_1^2+(1-W_2)a_1^2\}\, J_2]\,, \end{aligned} \tag{16}$$

$$\begin{aligned} V_{n0} = -Z_1 N_1 N_2 [&\{(1+W_1)^{1/2}1+W_2)^{1/2}c_0 \\ &+(1-W_1)^{1/2}(1-W_2)^{1/2}a_0\}\, L_0 \\ &+\{(1+W_1)^{1/2}(1+W_2)^{1/2}c_1 \\ &+(1-W_1)^{1/2}(1-W_2)^{1/2}a_1\}\, L_1]\,, \end{aligned} \tag{17}$$

where N_n, λ_n, and W_n correspond to the parameters for the ns electron, a_0, a_1, c_0, and c_1 are the parameters for the 2s state, and

$$\begin{aligned} J_k = \frac{1}{R(2\lambda_2)^{2\gamma+k+1}}\{&\gamma(2\gamma+k+1,\, 2\lambda_2 R) \\ &+2\lambda_2 R\Gamma(2\gamma+k,\, 2\lambda_2 R)\}\,, \end{aligned} \tag{18}$$

$$\begin{aligned} L_k = \frac{1}{R(\lambda_1+\lambda_2)^{2\gamma+k+1}}\{&\gamma[2\gamma+k+1,\, (\lambda_1+\lambda_2)R] \\ &+(\lambda_1+\lambda_2)R\Gamma[2\gamma+k,\, (\lambda_1+\lambda_2)R]\}\,. \end{aligned} \tag{19}$$

The functions $\gamma(a, x)$ and $\Gamma(a, x)$ are the first and second incomplete Gamma functions.[9]

Letting $\gamma = W_1 = W_2 = 1$ in Eqs. (17), (18), and (19), we can obtain the non-relativistic expressions:[1]

$$V_{00} = -\frac{Z_1}{R}[1-\mathrm{e}^{-2Z_2R}(Z_2R+1)]\,, \tag{20}$$

$$V_{nn} = -\frac{Z_1}{R}[1-\frac{\mathrm{e}^{-Z_2R}}{8}(8+6Z_2R+2Z_2^2R^2+Z_2^3R^3)]\,, \tag{21}$$

$$V_{0n} = -\frac{4\sqrt{2}}{27}Z_1Z_2(1+\frac{3}{2}Z_2R)\,\mathrm{e}^{-3Z_2R/2}\,. \tag{22}$$

III. RESULTS AND DISCUSSION

We have performed the relativistic and nonrelativistic calculations for the $1s$–$2s$ excitation cross sections in the first Born approximation and in the distortion approximation. All the numerical calculations in the present work have been made with the FACOM M–382 computer in the Data Processing Center of Kyoto University.

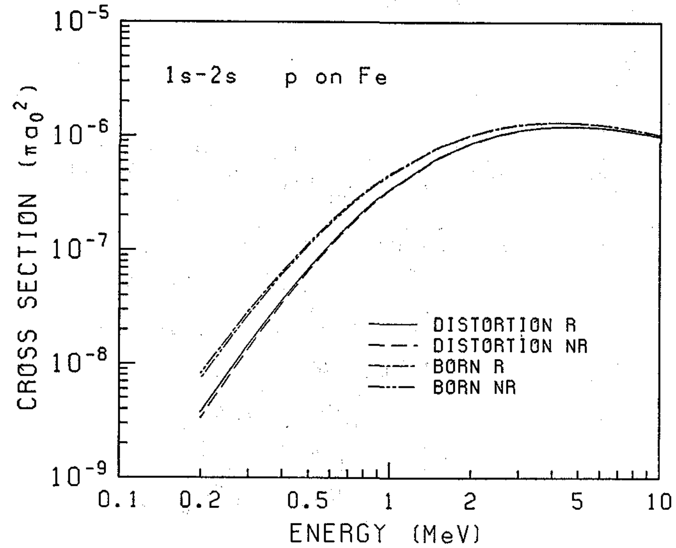

Fig. 1. Cross section for $1s$–$2s$ excitation of Fe^{25+} ion by proton impact. ——— Relativistic distortion approximation; — — - nonrelativistic distortion approximation; — - — - relativistic first Born approximation; — - - - — nonrelativisitic first Born approximation.

In Fig. 1, the $1s$–$2s$ excitation corss sections for protons on Fe^{25+} ion are plotted as a function of proton energy. In the low-energy region, the electronic relativistic effect increases the excitation cross section, while the distortion effect in the target state reduces it. However, it can be seen from the figure that the relativistic effect is much smaller than the distortion effect. The perturbation of the binding energy of the target ion plays a dominant role in the $1s$–$2s$ excitation process. For high-energy projectiles, all the curves become almost equal with each other, and both relativistic and distortion effects are negligibly small. Furthermore, the nonrelativistic and relativistic values in the first Born approximation are in good agreement with with the wave-mechanical cross sections in the nonrelativistic[6] and relativistic[10] plane-wave Born approximation.

Figure 2 shows the $1s$–$2s$ excitation cross sections of Sn^{49+} ion by proton impact. In this case, the electronic relativistic effect is more important than in the case of Fe^{25+}, but still small. The $1s$–$2s$ cross sections for U^{91+} by proton bombardment are shown in Fig. 3. Even for high-Z_2 ions such as U^{91+}, the electronic relativistic effect is not so large, and the distortion of the target electron plays more important role in the excitation cross section.

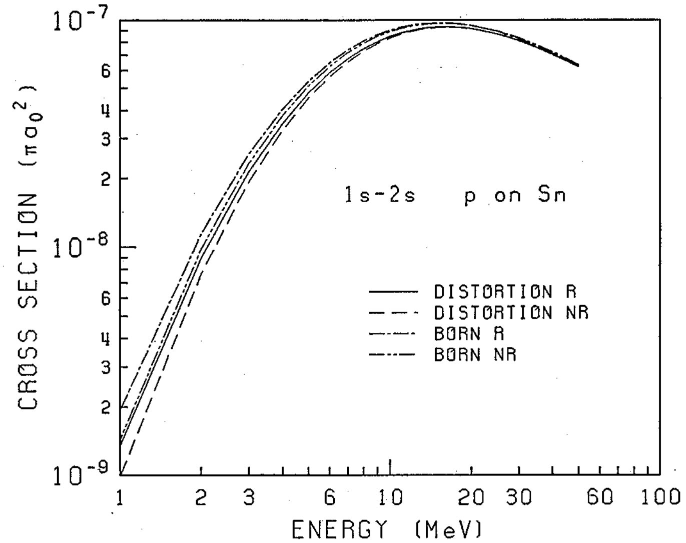

Fig. 2. Cross section for 1s–2s excitation of Sn^{49+} ion by proton impact. See caption of Fig. 1.

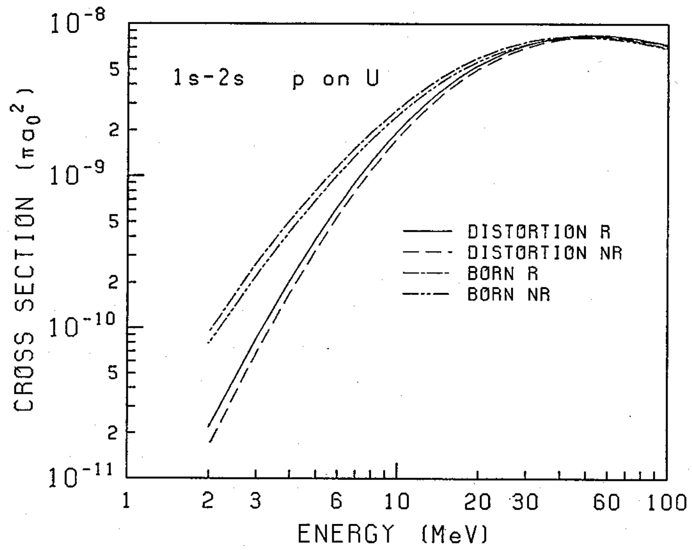

Fig. 3. Cross section for 1s–2s excitation of U^{91+} ion by proton impact. See caption of Fig. 1.

In Fig. 4, the reduced cross sections of Fe^{25+} ion by $^{16}O^{8+}$-ion impact are plotted as a function of the projectile energy divided by its mass. The reduced cross section is defined as the ratio to the square of the projectile charge, Z_2^2. When the reduced cross section is plotted against the reduced projectile energy, the curve for the non-relativistic first Born approximation coincides with that in Fig. 1. Comparing Figs. 1 and 4, it is seen that reduction of the cross section in the distortion approximation becomes pronounced for the highly-charged particle.

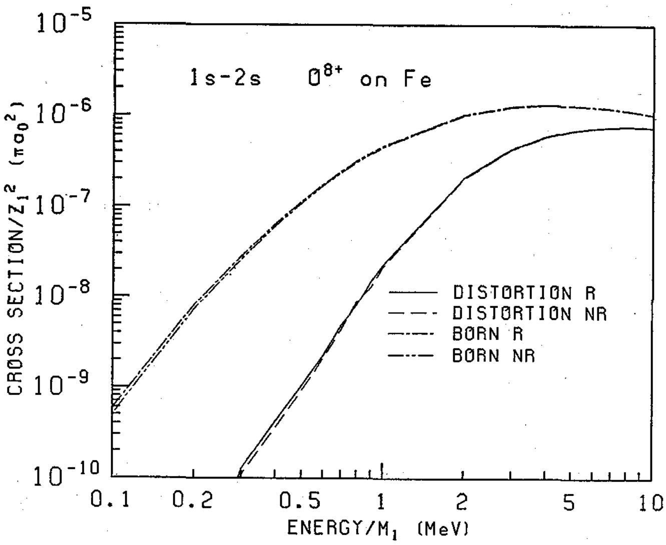

Fig. 4. Reduced cross section for $1s$–$2s$ excitation of Fe^{25+} ion by $^{16}O^{8+}$-ion impact. See caption of Fig. 1.

In the case of K-shell ionization cross section, it is well known that the electronic relativistic effect for low-energy projectiles is large even for medium-Z_2 targets, such as copper ($Z_2=29$).[11] This is explained by the fact that the ionization cross section is approximately proportional to the square of the momentum wave function of the initial bound electron at the minimum momentum transfer during ionization, and the relativistic wave function in the momentum space has larger high-momentum component than the nonrelativistic one.[12]

On the other hand, the $1s$–$2s$ excitation cross section depends not only on the initial-state, but also for the final-state wave function. The effect of relativity acts on both states and the ratio of the relativistic to nonrelativistic cross sections is a weak function of the momentum transfer. The relativistic effect changes with the target atomic number, but its dependence on the projectile energy is not so large.

In conclusion, we have calculated the $1s$–$2s$ excitation corss sections of hydrogenic ions by charged-particle impact in the distortion approximation, using relativistic wave functions for the target electron. It is found that the electronic relativistic effect is small and not so important in comparison with the distortion effect of the target state. In the present work, we assume the projectile can be represented by a straight-line trajectory. However, in the low-energy region where the relativistic effect and distortion effect are important, the Coulomb deflection of the projectile path would be appreciable. It is hoped to perform similar calculations with Rutherford trajectory.

The projectile is considered as a bare ion. In this case, charge transfer from the target ion to the projectile is important. Furthermore, Kingston *et al.*[12] showed that the $2p$ states strongly affect the $1s$–$2s$ excitation cross section of hydrogen atom by proton impact, because the matrix elemnet for $1s$–$2p_0$–$2s$ sequence is large. It is interesting to calculate the relativistic $1s$–$2s$ cross sections by the use of coupledchannel equations involving $1s$, $2s$, and $2p$ states.

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