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Relativistic Coulomb Continuum Wave Function at Zero Kinetic Energy in Ion-Atom Collisions

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A relativistic continuum wave function in the Coulomb field at zero kinetic energy limit is expressed in terms of Bessel function. The result is compared with the exact Coulomb continuum wave functions at low energies and the possibility for application of the present result as an approximate wave function in the final state for inner-shell ionization in ion-atom collisions is discussed.

KEY WORDS: Coulomb continuum state/ Relativistic wave function/ Ion-atom collision/

I. INTRODUCTION

In recent years, extensive experimental data on inner-shell ionization cross sections in ion-atom collisions have been accumulated and a careful comparison between these data and various theoretical models becomes possible. The plane-wave Born approximation (PWBA)[1] and the semiclassical approximation (SCA)[2] are most frequently used to interpretate the experimental results.

In order to describe the final electron state, it is usual to use the continuum wave function in the nuclear Coulomb field. This continuum wave function is given in terms of the confluent hypergeometric function and it is not so convenient to evaluate the transition matrix elements even in the case of the simple PWBA or SCA theory based on the first-order Born approximation.

For L-subshell ionization by heavy-ion impact, we have shown that the measured ionization cross sections deviate from the predictions of the first-order theories and the higher-order process plays an important role.[3] In our paper, we used the continuum Coulomb wave function at the threshold energy (zero kinetic energy) for the final state and calculated the L-subshell ionization cross sections in the second-order SCA model. In this way, we could avoid tedious numerical integrations involving the hypergeometric functions, because the final-state wave function is expressed in the form of the Bessel function. This simplification can be justified from the fact that most electrons ejected in ion-atom collisions are concentrated in the energy region near to the threshold.

In the previous work,[4] we calculated the Coulomb continuum wave functions

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with zero kinetic energy and compared them with those in low-energy region. We found that for small radial distances the zero-energy wave functions can well reproduce the behavior of the continuum wave function with low kinetic energies for various angular momenta.

However, all the calculations have been done using the nonrelativistic hydrogenic wave functions. On the other hand, most experimental studies on L-subshell ionization have been performed for medium or heavy target elements where the electronic relativistic effects are known to be important.[5] It is useful to perform the higher-order calculations for L-shell ionization cross sections in ion-atom collisions by the use of relativistic wave functions, in the manner similar to the nonrelativistic case.[3]

In the present work, we derive the relativistic continuum wave functions at zero kinetic energy and compare them with the wave functions with various kinetic energies and orbital angular momenta. The validity of application of the present results to the calculations of inner-shell ionization cross sections in ion-atom collisions is discussed.

II. RELATIVISTIC WAVE FUNCTION AT ZERO KINETIC ENERGY

The solution of the Dirac equation for the free electron in the Coulomb field is given by[6]

$$\psi=\begin{pmatrix} G(r) & \chi_{\kappa}^{\mu}(\hat{r}) \\ \mathrm{i}F(r) & \chi_{-\kappa}^{\mu}(\hat{r}) \end{pmatrix}, \tag{1}$$

where χ_{κ}^{μ} is the spin-angular function, r is the radial distance, $\hat{r}$ is the unit vector of the direction $\mathbf{r}$, $\kappa=\mp(j+1/2)$ for $j=l\pm 1/2$, l is the orbital angular momentum, j is the total angular momentum, μ is its projection, and $G(r)$ and $F(r)$ are large and small components of the radial wave functions, respectively.

The radial wave function is

$$rF=\frac{\mathrm{i}(W-1)^{1/2}(2pr)^{\gamma}\mathrm{e}^{\pi y/2}|\Gamma(\gamma+\mathrm{i}y)|}{2(\pi p)^{1/2}\Gamma(2\gamma+1)}J_{-}, \tag{2}$$

$$rG=\frac{(W+1)^{1/2}(2pr)^{\gamma}\mathrm{e}^{\pi y/2}|\Gamma(\gamma+\mathrm{i}y)|}{2(\pi p)^{1/2}\Gamma(2\gamma+1)}J_{+}, \tag{3}$$

where W is the total energy in units of the electron rest mass, p is the momentum, $\gamma^2=\kappa^2-(\alpha Z)^2$, Z is the atomic number, α is the fine structure constant, $y=ZW/p$, $\Gamma(x)$ is the gamma function,

$$J_{\pm}=\mathrm{e}^{\mathrm{i}pr+\mathrm{i}\eta}(\gamma+\mathrm{i}y)F(\gamma+1+\mathrm{i}y,\ 2\gamma+1;\ 2\mathrm{i}pr)\pm\mathrm{C.C.}, \tag{4}$$

$F(\alpha,\beta;x)$ is the confluent hypergeometric function, and c.c. denotes complex conjugate. The factor η is given by

$$\mathrm{e}^{2\mathrm{i}\eta}=-(\kappa-\mathrm{i}y/W)/(\gamma+\mathrm{i}y). \tag{5}$$

The solutions are normalized in the energy scale and when ψ_W and ψ_{W} are solutions corresponding to energies W and W',

$$\int \psi_W \psi_{W'} \mathrm{d}\mathbf{r} = \delta(W - W'), \tag{6}$$

where $\delta(x)$ is the Dirac delta function.

Throughout the present work, we use the atomic units, i.e. $\hbar = e = m_e = 1$, where e is the charge and m_e is the rest mass of the electron.

At the zero kinetic energy limit, $W \to 1$, i.e. $p \to 0$, Eqs. (2) and (3) approach to

$$rF = -Z^{1/2} \alpha J_{2\gamma}[(8Zr)^{1/2}], \tag{7}$$

and

$$rG = (2r)^{1/2} \left\{ J_{2\gamma-1}[(8Zr)^{1/2}] - \frac{\gamma + \kappa}{(2Zr)^{1/2}} J_{2\gamma}[(8Zr)^{1/2}] \right\}, \tag{8}$$

where $J_z(x)$ is the Bessel function.

These results coincide with the expressions given by Trautmann *et al.*[7] except for the normalization constant.

In the case of the nonrelativistic limit, $\gamma \to |\kappa|$, the large component, Eq. (8), reduces to

$$rG \sim (2r)^{1/2} J_{2l+1}[(8Zr)^{1/2}], \tag{9}$$

which is equivalent to the expression used in the previous work[4], except for normalization.

III. RESULTS AND DISCUSSION

In the nonrelativistic case,[4] the electron wave function can be written in a universal form for the atomic number Z, when the radial distance r is replaced by r/Z and the kinetic energy E by Z^2E. On the other hand, the relativistic wave function has no such universal property because γ depends on Z.

In the manner similar to the nonrelativistic case, the comparison between the continuum wave function with zero kinetic energy and that with small kinetic energies is made graphically. Figure 1 shows the results for hydrogen atom with $\kappa = -1$. The left side indicates the large component and the right side represents the small component. The symbols, a, b, c, and d correspond to the kinetic energy with $E =$ 0.01, 0.02, 0.05, and 0.10 hartree, respectively. The exact continuum wave function at the given energy is shown by the solid curve, while the zero-energy wave function is plotted by the dashed curve. Similar results for $\kappa = 1$ and -2 are shown in Figs. 2 and 3.

It can be seen from the figures that for low energies and at small radial distances the zero-energy wave function is in good agreement with the continuum wave functions with low energies both for large and small components. The discrepancy between two wave functions becomes larger for larger radial distance and for higher kinetic energy.

In Fig. 4, a similar comparison for $\kappa = 1$ and for uranium ($Z = 92$) is shown. In this case, the symbols a, b, c, and d correspond to the kinetic energy of 100, 200, 300, and 1000 hartree, respectively. It is clear that the almost same trend as for hydrogen

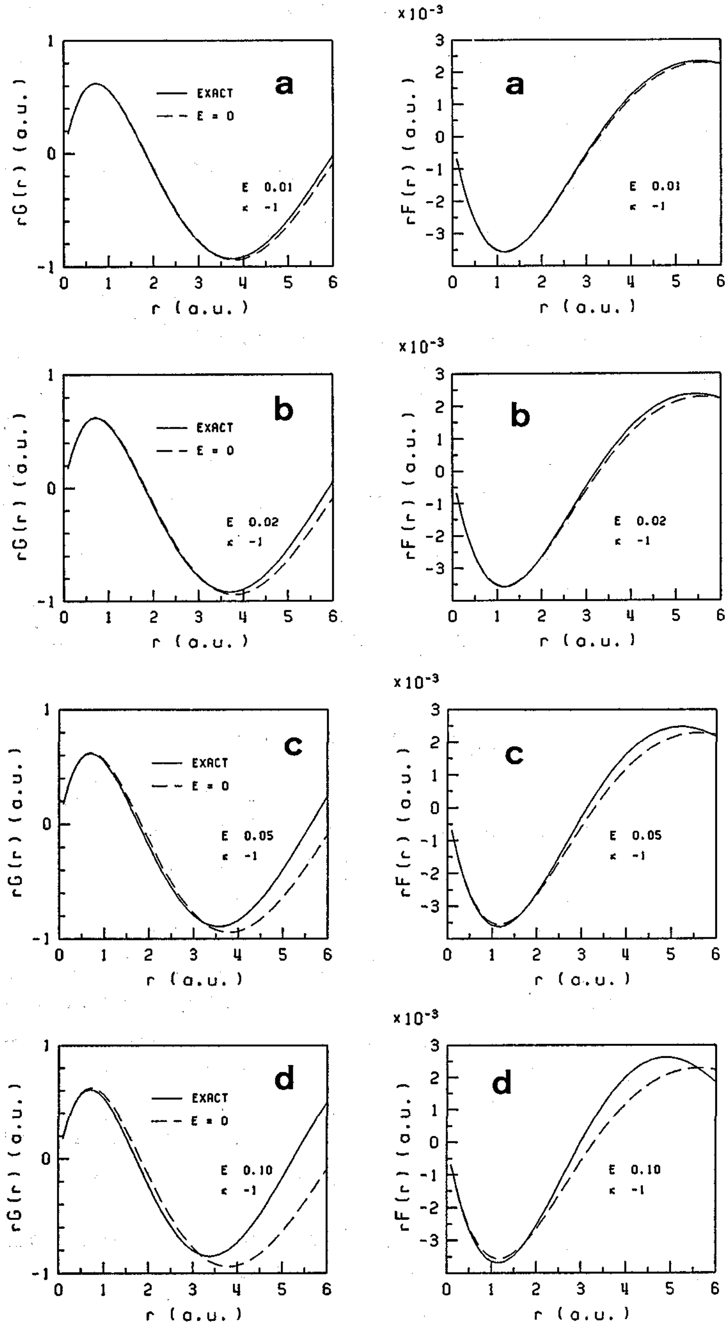

Fig. 1. Comparison of large and small components of zero-energy wave function with those of exact continuum wave functions for $\kappa=-1$ and for hydrogen. The solid lines correspond to the relativistic continuum wave functions with a) $E=0.01$, b) $E=0.02$, c) $E=0.05$, and d) $E=0.10$ hartree, while the dashed lines indicate those with $E=0$.

is observed also in the case of uranium. For $\kappa=1$ and -2, similar results can be obtained.

As has been described above, there is no scaling property in the relativistic wave

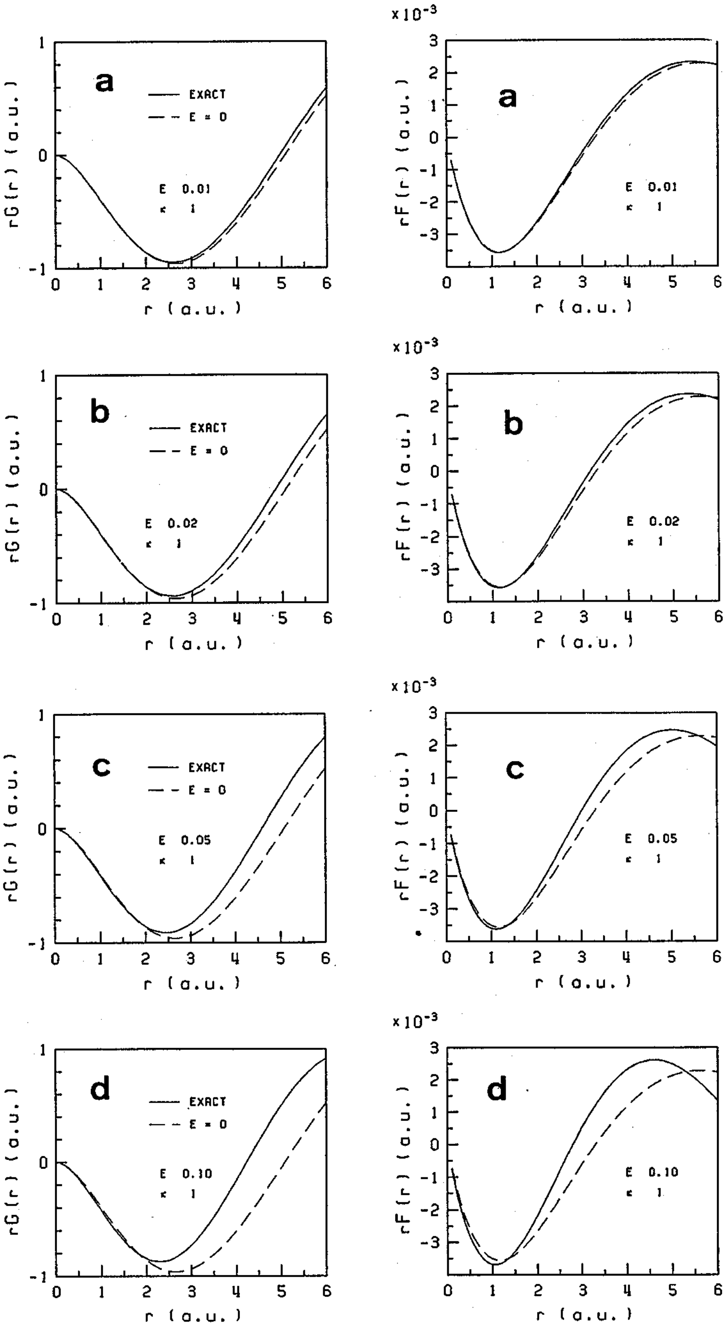

Fig. 2. Same as Fig. 1, but for $\kappa=1$.

function. However, if we plot the wave functions as a function of r/Z, instead of r, we can obtain an approximate universal behavior of the continuum wave functions between hydrogen and uranium.

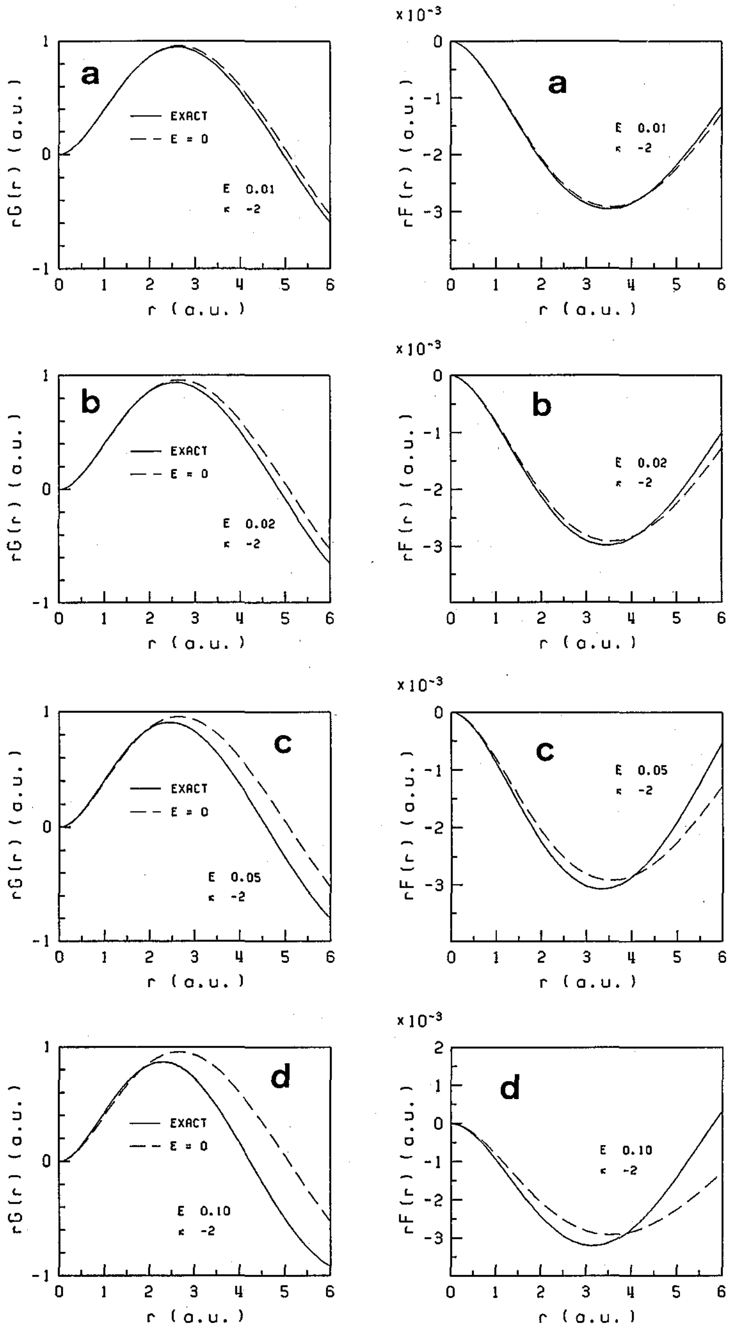

Fig. 3. Same as Fig. 1, but for $\kappa=-2$.

From these results, we can say that at small radial distance, $r/Z \leq 4.0$ a.u., and for low energies, $E \leq 0.02\ Z^2$ hartree, the wave function at zero kinetic energy limit can well reproduce the behavior of both large and small components of the relativistic

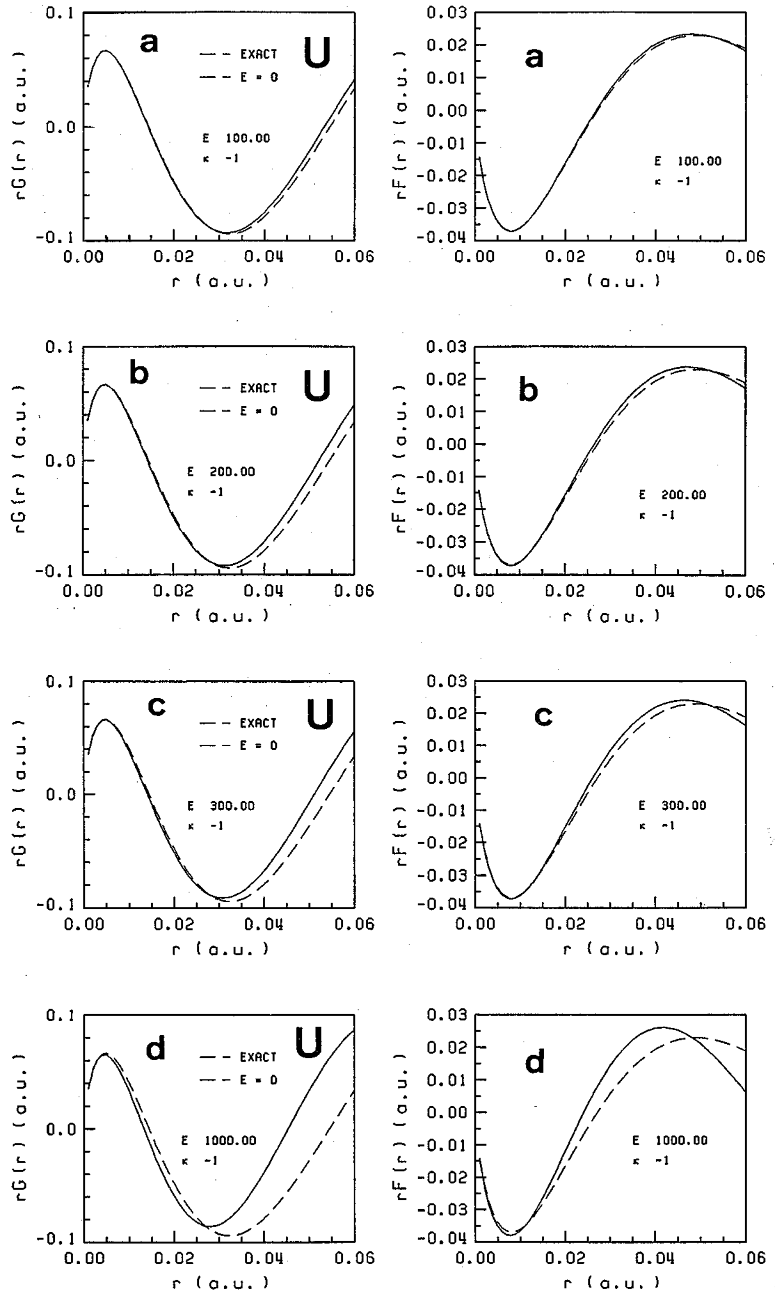

Fig. 4. Same as Fig. 1, but for $\kappa = -1$ and for uranium ($Z = 92$). The symbols correspond to a) $E = 100$, b) 200, c) 300, and d) 1000 hartree, respectively.

Coulomb continuum wave function with the finite kinetic energy. This conclusion is same as that obtained in the nonrelativistic case.[4]

Since the dominant contributions of the transition matrix element for inner-shell ionization process in ion-atom collisions comes from the region near to the mean radial distance of the inner-shell electrons to be ejected and most electrons ejected have small kinetic energies, the use of the zero-energy wave function for the relativistic calculations of inner-shell ionization cross sections by heavy-ion impact is quite adequate.

As in the nonrelativistic case, the discrepancy between the zero-energy wave function and the exact one at the given kinetic energy becomes larger for larger κ values. However, for low-energy projectiles, where the electronic relativistic effects and the higher-order process are important, the contributions from high partial waves are generally negligible. This fact indicates that the present zero-energy wave function is useful to perform higher-order calculations of inner-shell ionization cross section by low-energy heavy ions relativistically. The calculations for L-subshell ionization cross sections by heavy-ion impact by the use of the present wave functions are in progress.

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