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Approximate Continuum Wave Function for Inner-Shell Ionization in Ion-Atom Collisions

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An approximate electronic wave function for final state in inner-shell ionization during ion-atom collisions has been tested. The continuum wave function with zero kinetic energy is expressed in terms of the Bessel function and compared with the exact continuum wave functions with various kinetic energies and orbital angular momenta. The applications of this wave function to the calculations of inner-shell ionization cross sections are discussed.

KEY WORDS: Ion-atom collision/ Inner-shell ionization/ Continuum wave function/

I. INTRODUCTION

The inner-shell ionization is one of the most interesting processes in ion-atom collisions. Various theoretical models have been developed to calculate the inner-shell ionization cross sections by heavy charged-particle impact. It is well known that the plane-wave Born approximation (PWBA)[1] and the semiclassical approximmation (SCA)[2] give the theoretical cross sections in good agreement with the experimental values. In most theories, the hydrogenic wave functions have been employed.

However, owing to the final continuum state, the calculation of ionization cross sections is in general more tedious and time-consuming than that of excitation cross sections. The electronic wave function for the continuum state in the nuclear Coulomb field is usually expressed in terms of the confluent hypergeometric function, which is not so convenient to evaluate the transition matrix element.

We have introduced the approximate continuum wave function in our previous work for the second-order SCA calculations of L-shell ionization cross sections by heavy-ion bombardments.[3] This wave function corresponds to the continuum Coulomb wave function with zero kinetic energy and is expressed in terms of the Bessel function.

It is the purpose of the present paper to test the validity of application of this approximate wave function to the calculation of inner-shell ionization cross sections. For this purpose, the approximate wave function is compared with the exact Coulomb continuum wave functions with various kinetic energy and orbital angular momenta.

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II. CONTINUUM COULOMB WAVE FUNCTION

The continuum wave function with momentum k in the Coulomb field of the nucleus with nuclear charge Z is given by[4]

$$\psi_l(r) = \frac{N_{kl}}{kr} F_l(-Z/k, kr) , \tag{1}$$

where N_{kl} is the normalization constant, r is the radial distance of the electron from the nucleus, l is the orbital angular momentum, and $F_l(\eta, \rho)$ is the Coulomb wave function.[5] Atomic units ($m=\hbar=e=1$) are used. The Coulomb wave function can be written in terms of the confluent hypergeometirc function and computed by means of a series-exapnsion method.[5]

On the other hand, the continuum wave function with zero kinetic energy in the Coluomb field is expressed by[3,6]

$$\psi_l(r) = Z^{3/2} \ (2/\rho)^{1/2} \ J_{2l+1}[(8\rho)^{1/2}] , \tag{2}$$

where $\rho=Zr$ and $J_l(x)$ is the Bessel function of order l.

III. RESULTS AND DISCUSSION

The comparison of the approximation wave functions with the exact ones is

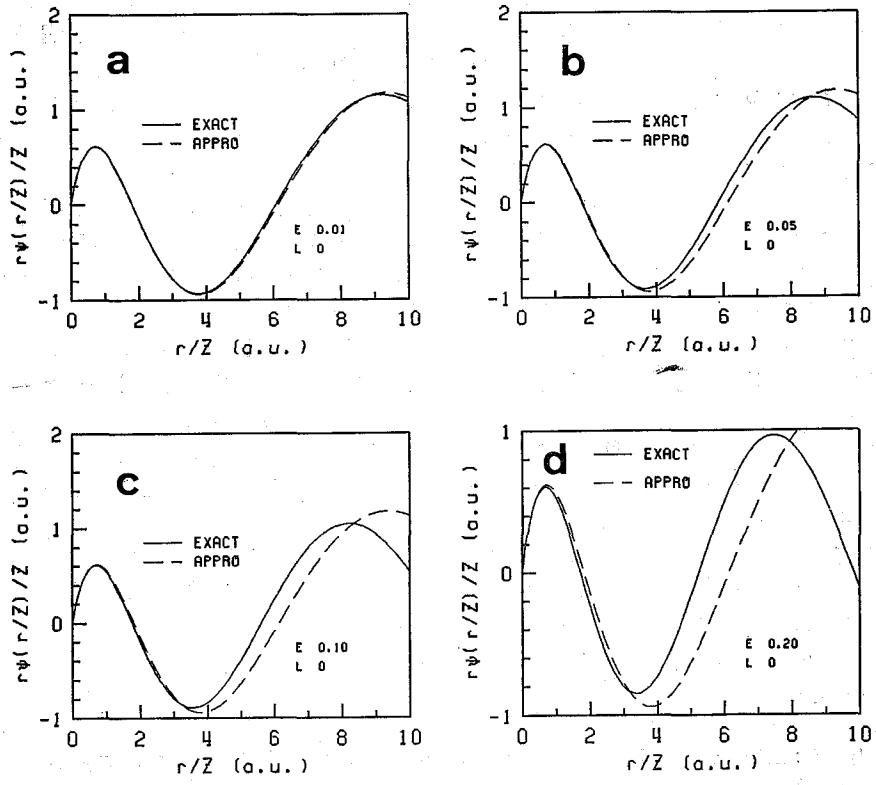

Fig. 1. Comparison of approximate continuum wave function with exact wave functions for $l=0$. The solid line represents the exact wave function and the dashed line indicates the approximate one. a) $E=0.01$ Ry, b) $E=0.05$, c) $E=0.1$, and d) $E=0.5$.

made graphically for $l=0$, 1, and 2. The exact wave functions with kinetic energies $E=0.01$, 0.05, 0.1, and 0.2 Ry are considered, because in the inner-shell ionization the ejected electrons with small kinetic energies are important. As can be seen from Eq. (2), the approximate wave function, as a function of r, depends on Z and l.

It is well known that the first-order PWBA cross section and the SCA cross section with straight-line trajectory show a universal behavior according to Z. Considering this fact, the wave functions are calculated as a function of r/Z, instead of r.

The calculated results of $r\psi_l(r/Z)/Z$ for $l=0$, 1, and 2 as a function of r/Z are shown in Figs. 1, 2, and 3, respectively. As expected from the assumption for the approximate wave function, it can be seen that for low enregies, $E \leqq 0.05$ Ry, the approximate wave function is in good agreement with the exact wave functions. When the energy becomes higher, the exact wave function oscillates more quickly than the approximate one.

It is also clear from the figures that at small radial distances, $r/Z \leqq 4.0$, a.u., the approximate wave function reproduces well the behavior of the exact wave function. If the dominant part of the transition matrix element for the ionization process comes from this region, the use of the present approximate wave function for the calculation of ionization cross sections is quite adeaquate. This corresponds to the case of

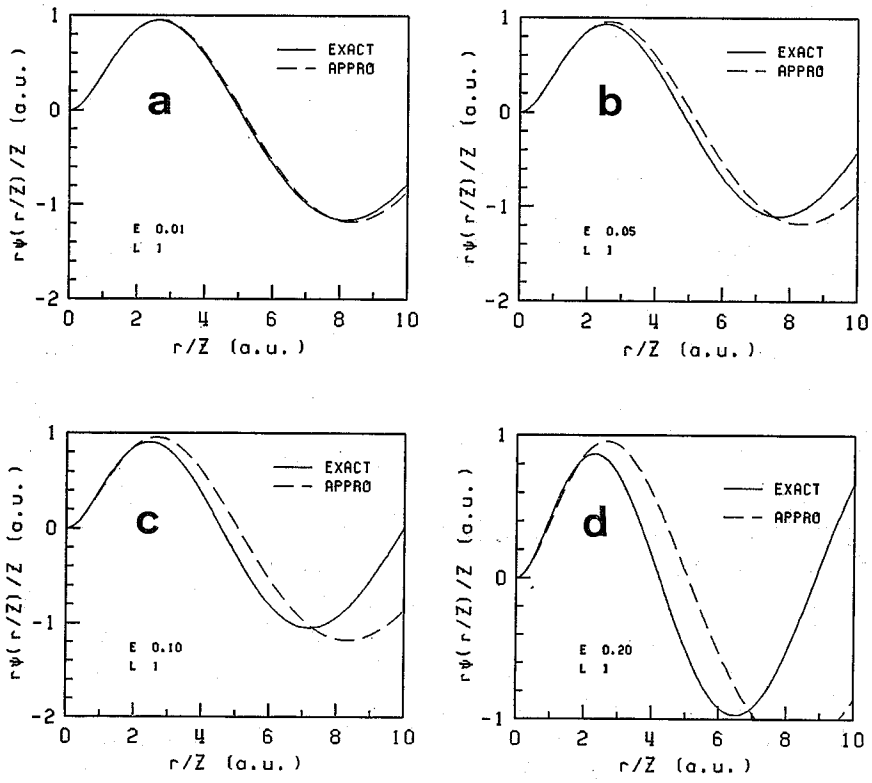

Fig. 2. Same as Fig. 1, but for $l=1$.

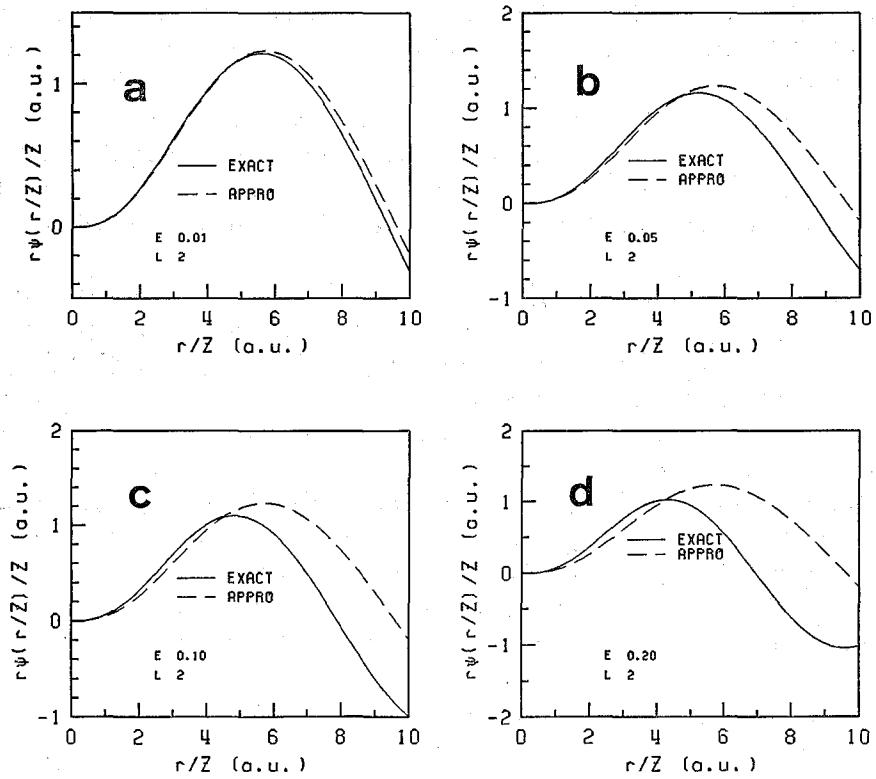

Fig. 3. Same as Fig. 1, but for $l=2$.

ionization by low-energy projectiles.

For larger l values, the discrepancy between the approximate and exact wave functions arises at smaller r. For fixed values of r, the discrepancy is larger for larger l than for small l. Since high partial waves are important when the projectile energy is high, their contributions to the inner-shell ionization cross sections for low-energy projectiles are usually small. This fact also indicates the validity of the present approximate wave function to the inner-shell ionization process by low-energy projectiles.

In conclusion, we have compared the approximate Coulomb wave function with zero kientic energy with the exact Coulomb continuum wave functions in the low-energy region. At low energies, $E \leqq 0.05$, the present wave function is a good approximation to the exact continuum wave function. It is found also that the approximate wave function can reproduce well the behavior of the exact one for small radial distances, $r/Z \leqq 4.0$. The agreement is better for smaller l values. These results indicate that the present approximation is useful to calculate inner-shell ionization cross sections by low-energy projectiles.

The advantage of the present approximate wave function consists in the fact that the matrix element for the ionization process can be calculated analytically in the form of simple algebric functions, as has been shown in our previous work.[3] It

is hoped that more PWBA and SCA calculations are made with the present approximate wave function for the final state.

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