Excitation of positive ions by heavy particles

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The Coulomb-Born approximation has been used to study the excitation of positive ions by heavy-particle impact. Slater-type wave functions are used for the ionic target states. This choice enables us to calculate the excitation rate coefficients between arbitrary initial and final states. We calculate the differential and total cross sections and alignment parameters for excitation of He^+ ions from the ground state to the $2p$ state by proton impact. The alignment parameters for the projectile velocity range considered here are found to be positive in contrast to negative values of the corresponding parameters for electron-impact excitation of the same target states.

INTRODUCTION

Excitation is one of the important processes among ion-atom or ion-ion inelastic collisions. Other inelastic processes like capture or ionization can be mediated through excitation. For example, if heavy particles like protons or α particles can first excite an atomic or ionic electron to its higher excited states then the excited electron can be captured or ionized rather easily, instead of direct capture or ionization. This may be one of the reasons we can talk about simultaneous excitation and capture or ionization. Moreover, excitation of ions by heavy ionic projectiles is different from excitation of ions by electron impact. Because of the fact that electrons are indistinguishable, exchange of electrons can take place for electron-impact excitation, which is not possible for the excitation by heavy particles. Furthermore, the Coulomb force between the incident electron and the electron associated with the target nucleus is repulsive in nature, whereas for protons or α particles as the projectile the analogous Coulomb force is attractive. It would be worthwhile to see how this attractive force influences the cross sections.

By virtue of the strongly dominant Coulomb force, the Coulomb-Born (CB) approximation for scattering of positive ions is more accurate than the Born approximation for scattering of neutral atoms, since the perturbation series is expected to converge more rapidly. In the initial applications[1,2] of the CB approximation and its variants for electronic impact, use of partial-wave analysis was made. But partial-wave analysis has some limitations. First, it is not suitable at high energies, as one then requires the inclusion of a large number of partial waves. Secondly, in the case of impact by heavy particles, it is a formidable task to deal with the partial-wave analysis. To free the method of calculation from the above limitations the necessity of a straightforward evaluation of the scattering amplitude without resorting to partial-wave analysis is apparent.

During the last decade much attention has been drawn to the excitation of positive ions by electron impact. References to important works in this line can be found in the review by Henry.[3] In contrast, very little effort has been made for excitation of positive ions by heavy-particle impact. Simony *et al.*[4] presented a method for calculating excitation cross sections by the impact of charged particles of arbitrary nuclear charge. In their formulation they included Coulomb distortion effects both in initial and final states within the framework of the Coulomb-projected-Born approximation. But in their actual calculation they neglected Coulomb distortion effects from the initial state and computed cross sections for $1s$-$2s$ excitation of hydrogenlike ions by electron impact. Potter and Macek[5] calculated cross sections for $1s$-$2s$ excitation of the He^+ ion by proton impact. They used the closed-form expression of Oh *et al.*[6] for the $1s$-$2s$ amplitude with minor changes for proton impact. Winter *et al.*[7] calculated charge-transfer and excitation cross sections for the $H^+ + He^+$ system using the coupled-molecular-state approach with and without plane-wave translational factors. They however, presented cross sections for center-of-mass energies up to 14 keV. Recently Scheibner *et al.*[8] investigated the role of plasma screening in fine-structure excitation of $n=2$ states of hydrogenic ions in collision with protons. They obtained substantial reduction of unscreened cross-section values[9] due to plasma screening.

To our knowledge there is no calculation for $1s$-$2p$ excitation of He^+ ion by proton impact in the Coulomb-Born approximation. But there are many such calculations for the $e^- + He^+$ system. From those calculations it is our understanding that very near to the threshold energy, the plane-wave Born (PB) approximation results for the $1s$-$2p$ transition are an order of magnitude less than both the corresponding CB results and the experimental data (cf. Ref. 6). Up to a few times the threshold energy, the discrepancy is about 20%. Beyond this energy range total cross sections and alignment parameters may be, to order m/M, identical in the CB and PB approximations where m and M are electron and proton masses, respectively. This near-threshold energy range corresponds to a projectile velocity v less than 5 a.u. When we talk about heavy-particle collisions, we consider higher or lower projectile energy depending on how large the projectile velocity is. In these cases, $v \leq 5$ a.u. corresponds to the energy region where the PB approximation may not give good results. So it is necessary to employ a better approximation like the CB approximation, which is definitely more complex than the PB approximation. Moreover, Oh, Macek, and Kelsey[6] argue that PB results lose information regarding anisotropy for all energies. The alignment parameters we report in this paper are concerned with this anisotropy; we believe that the CB approximation will provide better results than the PB approximation.

In the present theoretical investigation we employ the CB approximation to study the excitation of positive ions by heavy-particle impact. In the next section we present an approximate form of the CB amplitude for the system

$$A^+ + B^+(n,l,m) \rightarrow A^+ + B^+(n',l',m') ,$$

where A^+ is a bare ion like a proton or α particle and B^+ is a one-electron ion like He^+. We then choose initial and final target ionic states as a combination of Slater-type orbitals of various angular momenta, which allow us to evaluate the amplitude as well as to select the arbitrary initial and final target states. The Coulomb distortion effect has been included in both initial and final channels. Atomic units are used throughout the calculation.

1s-2p AMPLITUDE

The CB amplitude for the excitation of an initial state ϕ_m of a He^+ ion into a final state ϕ_n by proton impact can be obtained[10,11] as

$$f = -\frac{\mu A_Z}{2\pi} \int \int \chi(-i\alpha_n, -\mathbf{K}_n, \rho)\phi_n^*(\mathbf{r}) \times \left[\frac{1}{\rho} - \frac{1}{r'}\right]\phi_m(\mathbf{r}) \times \chi(-i\alpha_i, \mathbf{K}_i, \rho) d\mathbf{r}\, d\rho , \quad (1)$$

where the Coulomb wave functions χ are defined as

$$\chi(-i\alpha_n, \mathbf{K}_n, \rho) = e^{-\pi\alpha_n/2}\Gamma(1+i\alpha_n)e^{-i\mathbf{K}_n\cdot\rho} \times {}_1F_1[-i\alpha_n; 1; i(K_n\rho + \mathbf{K}_n\cdot\rho)] ,$$

$$\chi(-i\alpha_i, \mathbf{K}_i, \rho) = e^{-\pi\alpha_i/2}\Gamma(1+i\alpha_i)e^{-i\mathbf{K}_i\cdot\rho} \times {}_1F_1[-i\alpha_i; 1; i(K_i\rho - \mathbf{K}_i\cdot\rho)] ,$$

$$r' = m_1\mathbf{r} - \rho ,$$

$$m_1 = M_T/(M_T+1) ,$$

where $\alpha_n = \mu A_Z/K_n$, $\alpha_i = \mu A_Z/K_i$, $\mathbf{K}_i$ and $\mathbf{K}_n$ are initial and final momentum vectors, respectively, and M_T is the target mass. μ is the reduced mass and A_Z is the projectile charge. The first term in Eq. (1) corresponding to the interaction $1/\rho$ will not contribute to the matrix element due to the orthogonality of the initial- and final-state wave functions. To evaluate the second term we choose initial and final bound states as a combination of Slater-type orbitals of different angular momenta. The six-dimensional integral for the scattering amplitude is then reduced to a one-dimensional integral, following closely the method of Deb and Sil,[10] and this one-dimensional integral is then evaluated numerically by the Gaussian quadrature method.

RESULTS AND DISCUSSION

We apply this method to calculate cross sections for excitation of a He^+ ion from the ground state to the $2p$ state by proton impact. Since most of the contribution to the total cross sections comes from extremely forward angles we use the transformation

$$\cos\theta = 1 - \frac{1}{K_i^2}\left[\frac{1+Z}{1-Z}\right] ,$$

where Z represents Gaussian quadrature points and θ is the scattering angle. Unlike the case of electron-impact excitation of He^+ (cf. Ref. 10), the present calculation involves numerical cancellation among the terms of equal orders. To avoid this problem the computation has been done in double precision. Moreover, we employed the approximation $K_i - K_n \simeq 1 - \mu(\varepsilon_n - \varepsilon_i)/K_i$.

In Fig. 1 we plot the differential cross sections (in units of a_0^2) for proton impact excitation of He^+ ion from ground-state to $2p$ states. These cross sections fall very fast as θ increases. For example, as θ varies from 0.1 to 0.4 mrad differential cross sections fall off almost three orders of magnitude, whereas for electron-impact excitation these cross sections fall at a slower rate. The primary reason for that is the mass asymmetry between proton and electron. Since the proton is much heavier than

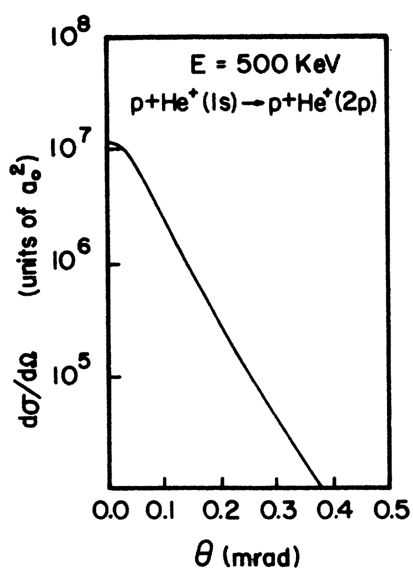

FIG. 1. Differential cross sections (in units of a_0^2) as a function of scattering angle in milliradians.

the electron, it does not get deflected as much as the electron (as projectile) does. Another, possibly less important, reason is the following. As one can notice from the theory the internuclear distance R has been approximated by ρ, the distance between the projectile and the center of mass of the target electron. But the matrix element consisting of the interaction $1/\rho$ does not contribute due to the orthogonality of the initial and final bound states. The only contributing term of the matrix element consists of the interaction between the proton and the target electron which is attractive in nature. This attractive Coulomb force may prevent the incident proton from being deflected much.

We also calculate total cross sections σ_0 and σ_1 for calculating Fano-Macek alignment parameters[6,12]

$$A_0^{\text{col}}=(\sigma_0-\sigma_1)/(\sigma_0+2\sigma_1) .$$

These parameters are required to determine the anisotropy of the source atom or molecule for collision in a gas. Light emitted in the subsequent decay manifests this anisotropy through its angular distribution and polarization. In Fig. 2 we plot these parameters as a function of energy. For energy greater than 100 keV the alignment parameters remain positive and tend to unity as the energy increases. This means that total cross sections for excitation of $2p_0$ are larger than the corresponding quantities for $2p_1$ states. Here we note that the alignment parameters for electron-impact excitation of He^+ at similar velocities are negative[6] In other words, proton-impact excitation is different from electron-impact excitation of ionic targets.

More refined methods such as the close coupling (CC) approximation may be used to yield more reliable results at low energies since only the first few partial waves are important. But at higher energies it is necessary to include quite a large number of partial waves, the evaluation of which becomes very difficult as well as too much time consuming. In such cases the present technique can provide an useful means for obtaining corrections for higher partial waves. For example, let us write

$$\sigma^{\text{CC}}=\sum_{l=0}^{N}\sigma_l^{\text{CC}} ,$$

where σ^{CC} is the total cross section in the CC approximation and σ_l^{CC} are contributions from the lth partial wave. Here N is a large integer for high energies. Calculating the contributions for the first few partial waves in the CC approximation one may correct for the contributions of higher partial waves by adding the full CB contributions (in the present method) and then subtracting the contributions of the same number of partial waves in the CB approximation, namely,

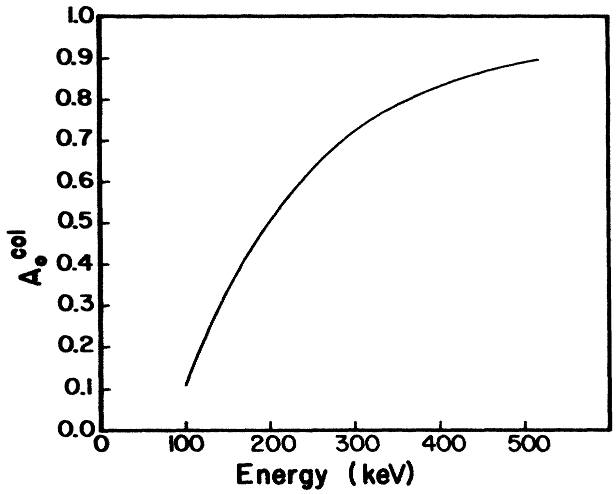

FIG. 2. Fano-Macek alignment parameters as a function of incident proton energy in keV.

$$\sigma^{\text{CC}}=\sum_{l=0}^{L}\sigma_l^{\text{CC}}+\sigma^{\text{CB}}-\sum_{l=0}^{L}\sigma_l^{\text{CB}} ,$$

where $\sigma^{\text{CB}},\sigma_l^{\text{CB}}$ are analogous to $\sigma^{\text{CC}},\sigma_l^{\text{CC}}$ and L is a suitable value of l up to which the CC calculation is possible without much difficulty.

SUMMARY

In the present investigation we have extended our earlier method[10] for the excitation of positive ions from an arbitrary initial state to an arbitrary final state by heavy-particle impact. This extension involves some changes and approximations to our earlier method. The calculation is done within the framework of the Coulomb-Born approximation, which is a better approximation for electron-ion or ion-ion collision than the Born approximation usually valid for neutral target atoms. Here we have calculated differential and total cross sections, and hence the Fano-Macek alignment parameters for $p^+ + He^+$ ion collision at several energies. We find that the alignment parameters are positive at projectile velocities where the corresponding parameters for electron-impact excitation are negative.

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