Sequential over-barrier ionization of multi-electron atoms in the tens-to-hundreds keV/u energy range*

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Our previous work on the classical over-barrier ionization model for helium double ionization is extended to the complex multi-electron system of Ne. The total and q-fold ionization cross sections are calculated at energies ranging from a few tens to several hundred keV/u. The calculation results are in good agreement with the experimental data, and the energy dependence of the cross sections suggests that the multi-ionization of a strong perturbated complex atom is probably the sequential over-barrier ionization process.

Keywords: multi-electron system, multi-ionization, over-barrier ionization

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1. Introduction

The multi-ionization (MI) of an atom impacted by a heavy ion is a fundamental process in atomic physics,[1] as well as plasma, fusion and atmospheric physics, and many other techniques. Because of its importance and broad range of applications, it is necessary to improve our understanding of this process.

As the simplest two-electron system, the ionization of helium atoms has been investigated widely in both theory and experiments.[2−10] Plane-wave Born approximation (PWBA),[11] continuum distorted-wave eikonal initial-state (CDW-EIS),[12] classical trajectory Monte Carlo (CTMC)[13] and multi-coupled channel (MCC)[14] methods have given good estimations of the single-ionization (SI) cross section.

Double-ionization (DI) has been interpreted well by using several models. For the extremely fast projectile, DI can be understood well by using McGuire's shake-off (SO) model,[15] in which the first electron is ionized through direct interaction, while the second is ejected through final-state rearrangement. For swift projectiles, two independent close binary encounters between the projectile and the two target electrons[15] are the main mechanism. For slow projectiles, the capture model[16] and its extensions[17] are valid. At low to intermediate energies (25–500 keV/u), our previous work on the classical over-barrier ionization (COBI) model[18−22] gives a good description of the DI of helium. In COBI, the DI mechanism in such an energy range is the over-barrier ionization process.

For more complex systems, such as neon, the current understanding of MI is not enough. In the framework of the independent-particle model (IPM), the relevant probabilities are constructed by the binomial distribution of single-electron probabilities. The statistical energy deposition models proposed by Russek and Thomas,[23] Cocke[24] and Muller *et al.*[25] have been used to successfully interpret the multi-ionization process for slow or fast collisions.

When the beam velocity is comparable to the orbital velocity of the target electron, the perturbation methods are invalid. The multi-electron and strong perturbation problems are two of the difficulties in describing MI. Recently, Kirchner *et al.*[26−28] proposed a complex quantum theory to calculate the total and q-fold cross sections of neon. The calculation results are in qualitative agreement with the experimental data.[29,30] Besides the first-principles theories, models that carry main physical ideas are also necessary to gain a better understanding of the underlying physics.

In this paper, we establish a multi-electron classical over-barrier ionization (ME-COBI) model to describe the MI of a multi-electron atom in the low-to-intermediate energy range. The aim of the present

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work is to obtain some useful information and examine whether the MI process of a strongly perturbated complex atom can be treated as a sequential over-barrier ionization process. The ME-COBI model is introduced briefly in Section 2, and in Section 3 the calculation results are compared with the available experimental data and the MI scenario is also discussed.

2. Model

The ME-COBI model is based on our previous work on COBI[18−22] and the OB models,[16] which give a good estimation of the ionization or the capture of helium. According to the capture model of OB,[16] an electron can be released from the target when the Coulomb potential barrier is lower than the electron binding energy. The release distance $R_{\rm r}$, below which the release becomes possible, is given as $R_{\rm r} = (Z + 2\sqrt{qZ})/I$, where Z and q are the charge of the projectile and the target core, respectively, and I is the electron binding energy of the target atom. On the other hand, capture takes place only if the release occurs within the capture distance $R_{\rm c}$, within which the electron potential energy in the ionic field of the projectile is larger than its kinetic energy in the projectile frame. We obtain the capture distance $R_{\rm c} = 2q/v^2$, with v being the velocity of the projectile.

The OB model[16] does not describe the electrons released outside the capture distance. Those electrons will not be ionized until they obtain enough kinetic energy to escape. When the projectile approaches distance $R_{\rm I}$, where the kinetic energy of the released electron converted from the Stark energy is larger than its binding energy, ionization takes place. Thus, ionization distance $R_{\rm I}$ satisfies the inequality $q/R_{\rm I} \geq I + q/R_{\rm r}$. So, in the COBI model, the electrons released outside the capture distance will not be ionized until the ion enters ionization distance $R_{\rm I}$.

For the release, the capture and ionization do not take place instantly, but gradually occur. The corresponding one-electron probabilities $P_{\rm r}$, $P_{\rm c}$ and $P_{\rm I}$ for release, capture and ionization need to be taken into account. The probabilities at any collision parameter are obtained as the ratios of the collision durations, in which the release, the capture and the ionization take place, to the orbital period of the target electron. As a result, the one-electron probabilities are

$$P_{\rm r} = \frac{2}{vT}\sqrt{R_{\rm r}^2 - b^2},$$

$$P_{\rm c} = \frac{2}{vT}\sqrt{R_{\rm c}^2 - b^2},$$

$$P_{\rm I} = P_{\rm r} - P_{\rm c} = \frac{2}{vT}\left(\sqrt{R_{\rm r}^2 - b^2} - \sqrt{R_{\rm c}^2 - b^2}\right),$$

where b is the collision parameter, v is the collision velocity and T is the orbital period of the target electron.

In the ME-COBI model, the one-electron ionization probability is used to construct the relevant multi-electron ionization probabilities within the framework of the IPM. The out-shell electron of neon is distinguished by subscripts n; $R_{{\rm r}n}$, $R_{{\rm c}n}$, and $R_{{\rm I}n}$ are the distances for the n-th released target electron. They satisfy the following equations:

$$R_{{\rm r}n} = \frac{Z_n + 2\sqrt{q_n Z_n}}{I_n},$$

$$\frac{q_n}{R_{{\rm c}n}} = \frac{1}{2}v^2,$$

$$\frac{q_n}{R_{{\rm I}n}} = I_n + \frac{q_n}{R_{{\rm r}n}},$$

where q_n and Z_n are the charge of the projectile and the target seen by the n-th target electron. The values of q_n and Z_n are determined by the method adopted by Niehaus in the MCOBM,[17] in which the released electrons stay in the quasi-molecular states surrounding the target and projectile core from outside and lose their abilities to screen both nucleuses.

The value of ionization probability $P_{{\rm I}n}$ for the n-th released electron can be calculated from $R_{{\rm I}n}$. By using the binomial distribution, the q-fold ionization cross section (σ_{q+}) of a neon atom can be calculated by integrating the above one-electron ionization probabilities for the out-shell (2p and 2s) electrons at all collision parameters. Then, the total ionization cross section ($\sigma_{\rm T}$) can be obtained as $\sigma_{\rm T} = \sum_q q \times \sigma_{q+}$.

3. Results and discussion

The total ionization cross section of the Ne impacted by the He^+ ion is calculated using the present model and plotted in Fig. 1. The experimental data[29,30] are also plotted in the same figure for comparison.

In Fig. 1, the results from the present model are in excellent agreement with the experimental data. The theory and the experiment both indicate that the total ionization cross section increases very rapidly at the energy of several tens of keV/u, reaches the maximum value at about 100 keV/u, and then drops off slowly for higher energies.

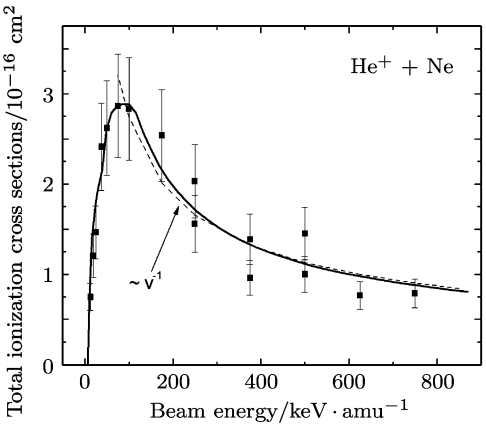


Fig. 1. Total ionization cross sections of Ne impacted by He^+, where the solid line represents the results from the present model, the dashed line denotes the results from the law of $\sim v^{-1}$, and the dots with error bars are the experimental data cited from Refs. [29] and [30].

To understand this, the ionization probability for the impact parameter $b = 0$ is discussed. The ionization cross section has an approximate expression of $\sigma_{\rm T} \approx \pi R_{\rm I}^2 P_{\rm I}(0)/2$,[20,22] where

$$P_{\rm I}(0) = \frac{2}{Tv}(R_{\rm r} - R_{\rm c}) = \left(\frac{2R_{\rm r}}{v}\frac{1}{T}\right)\left(\frac{R_{\rm r} - R_{\rm c}}{R_{\rm r}}\right).$$

Let

$$h = \frac{2R_{\rm r}}{v}\frac{1}{T}, \quad g = \frac{R_{\rm r} - R_{\rm c}}{R_{\rm r}}.$$

h is the ratio of collision duration $2R_{\rm r}/v$ to bound electron orbital period T. Obviously, this is the probability of the release process occurring within the collision duration, and decreases with the increasing v as $1/v$. g is the uncaptured fraction of the released electrons

$$g = 1 - \frac{2q}{R_{\rm r}}\frac{1}{v^2},$$

which increases very rapidly with the increasing v.

The uncaptured fraction g of the released electron increases as v^2, which is the main reason for the sharp increase in ionization cross section at low energies. The decrease in interaction time h causes the cross section to decrease as $1/v$ for higher energies. In the energy range from 50 to 200 keV/u, the uncaptured fraction g increases, while the interaction time h decreases; the competition between them leads to the appearance of the maximum at about 100 keV/u.

When the beam energy is larger than 100 keV/u, the results from the present model and the experiments show that the total ionization cross section drops off approximately as $1/v$. Such an energy dependence is quite different from the $1/v^2$ law,[31] which is valid for the fast ion–atom collision. For swift projectiles at MeV/u energy ranges, the perturbation is weak and the target electron is usually treated as a free one. The projectile kicks the electron away through the violent binary-encounter process, and such a forced impulse ionization determines that the cross section to the ionized target electron obeys the $1/v^2$ law.

At tens-to-hundreds of keV/u, the collision velocity is comparable to the orbital velocity of the target electron. The free electron and the forced impulse approximations break down, and the circulation period of electrons around the target core should be taken into account. The $1/v$ dependence of the total ionization cross section can be understood well by the picture of over-barrier ionization. For energies larger than 100 keV/u, the capture cross section drops off rapidly as about v^{-7}[16] and is much smaller than the ionization cross section. So, the present model gives the ionization probability as

$$P_{\rm I} = P_{\rm r} - P_{\rm c} \approx P_{\rm r} = \frac{2R_{\rm r}}{v}\frac{1}{T} \propto \frac{1}{v}$$

and the total ionization cross section as $\sigma_{\rm T} \propto P_{\rm I} \propto P_{\rm r} \propto 1/v$. This indicates that the energy dependence of the total ionization at an energy of several-hundred keV/u is mainly influenced by the total release probability $P_{\rm r}$.

The calculated q-fold MI cross sections of neon impacted by He^+ are compared with the experimental data in Fig. 2.

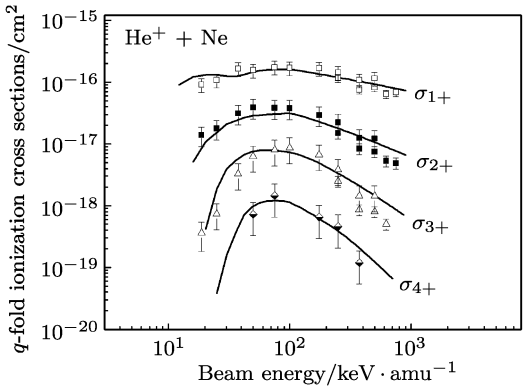


Fig. 2. The q-fold ($q = 1, 2, 3, 4$) MI cross sections of Ne impacted by He^+, where the solid lines represent the results obtained from the present model, and the dots with error bars are the experimental data cited from Refs. [29] and [30].

Figure 2 shows that the theoretical results are in very good agreement with the experimental data. The q-fold ionization cross sections have the same energy

dependences as the total cross section. They increase at an energy of several tens of keV/u, reach their maxima at about 100 keV/u, then drop off slowly. Such energy dependences also come from the competition between their total release probability h and uncapture fraction g.

The decreasing trend of the q-fold ionization cross section given by the present model is $\sigma_{q+} \propto v^{-q}$. If the MI mechanism of neon can be regarded as sequential over-barrier ionizations, then the experimental data should decrease with v with nearly the same trends as the predicted model. In Fig. 2, the experimental data of the q-fold ionization cross sections lie around the theoretical lines of $\sigma_{q+} \propto v^{-q}$, while they deviate from the binary-encounter law of $\sigma_{q+} \propto v^{-2q}$.

Within the framework of IPM, the energy dependence of $\sigma_{q+} \propto v^{-q}$ can also be understood well by using the picture of sequential over-barrier ionizations. With the projectile approach, the target electrons will be released one after the other to the side of the projectile. When they enter into their ionization distances, these electrons will be ionized one by one. The mechanisms of the sequential release and the over-barrier ionizations indicate that the energy dependence of the single-ionization cross section is determined by the first-electron release probability $P_{\rm r1}$. Thus, the q-fold cross sections are determined by the relevant q-fold release probabilities, and we have $\sigma_{q+} \propto \prod_{i=1}^{q} P_{{\rm r}i} \propto v^{-q}$.

4. Conclusion

In this work, a classical multi-electron over-barrier ionization model is presented to calculate the total and q-fold ionization cross sections of neon in the energy range from a few tens to several hundred keV/u. A good agreement between the calculation results and the experimental data suggests that the multi-ionization of strong perturbated complex atoms cannot be treated as violent binary encounters, but can be seen as originating from the sequential release processes occurring at larger distances.

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