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Plasma screening effects on resonant charge transfer in strongly coupled plasmas

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Abstract. – The resonant charge transfer process in collisions between positive ions has been investigated in strongly coupled plasmas. The ion-sphere model is applied to describe the interaction potential in strongly coupled plasmas. The electron transfer probability and the electron transfer cross-section are obtained as functions of the energies of the symmetric and antisymmetric states, ion-sphere radius, and collision energy. The results show that the plasma screening effects enhance the resonant electron transfer probability as well as the electron transfer cross-section in strongly coupled plasmas.

The charge transfer process in collisions between atoms and ions has received considerable attention, since this process is one of the most fundamental processes in many areas of physics such as astrophysics, atomic physics, chemical physics, and plasma physics [1–6]. Recently, the charge transfer process in plasmas has been of great interest since this process can be used for plasma diagnostics [6]. The charge transfer processes in collisions of positive ions in strongly coupled plasmas would be different from those of free ions due to the strong plasma screening effects by surrounding electrons. A most typical example of strongly coupled plasma may be seen in the system of ions inside a highly evolved star [7]. It is known that the Debye-Hückel potential describes the properties of low-density plasmas and corresponds to a pair correlation approximation. The plasma described by the Debye-Hückel model is known as the ideal plasma, since the average interaction energy between particles is smaller than the average kinetic energy of a particle [8, 9]. However, in strongly coupled plasmas, the potential energy would not be described by the ordinary Debye-Hückel model because of the strong collective effects of particle interactions. For a strongly coupled plasma, the ion-sphere model [10–13] is found to be more suitable than the cutoff model and has played an important part in elucidating the properties of the plasma. However, the charge transfer process in collisions between positive ions in strongly coupled plasmas has not been investigated as yet. It is known that the classical path approximation [1, 2, 6] is reliable for investigating the charge transfer process when the velocity of the projectile is small compared to the velocity ($v \approx 10^8$ cm/s) of the electron on its Bohr orbit. Thus, in this letter we investigate the plasma screening effects on the charge transfer process in collisions of positive ions in strongly coupled plasmas

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described by the ion-sphere model since the theoretical atomic spectroscopy is essential in the study of plasma parameters. The impact parameter analysis is applied to obtain the resonant charge transfer probability as a function of the impact parameter, energies of the symmetric and antisymmetric stationary states, ion-sphere radius, Debye length, and collision energy.

When the projectile velocity v is smaller than the velocity of the atomic electron in the target ion, the probability (P_{ct}) of the charge transfer process $X^{Z+} + X^{(Z-1)+} \rightarrow X^{(Z-1)+} + X^{Z+}$ in collision of an ion X^{Z+} with its parent ion $X^{(Z-1)+}$ along the collision orbit x with the impact parameter b can be obtained by the impact parameter analysis [6] in the following form:

$$P_{ct}(b,v) = \sin^2\left[\int_{-\infty}^{\infty} \mathrm{d}x \frac{\Delta E(x,b,v)}{2\hbar v}\right], \tag{1}$$

where $\Delta E(x,b,v) = E_A - E_S$, E_A and E_S are the energies of the antisymmetric and symmetric states of the molecular ion, respectively. Then, the charge transfer cross-section (σ_{ct}) is represented as

$$\sigma_{ct}(v) = 2\pi \int b\,\mathrm{d}b P_{ct}(b,v). \tag{2}$$

In strongly coupled plasmas, the concept of Debye screening as a cooperative phenomenon is no longer applicable, since the probability of finding other charged particles in a Debye sphere almost vanishes. Hence, the Debye-Hückel model is not reliable to describe the interaction potential in strongly coupled plasmas. To understand salient features of such a strongly coupled plasma, it is instructive to introduce the ion-sphere model [7, 10]. It is equivalent to the Wigner-Seitz sphere used in condensed-matter theory. The ion-sphere consists of a single ion and its surrounding negative-charge sphere. If the hydrogenic ion with nuclear charge Z is placed in a strongly coupled plasma, the interaction potential $V(\boldsymbol{r},\boldsymbol{r}')$ between the hydrogenic ion and the electron that can be obtained by the ion-sphere model becomes

$$V(\boldsymbol{r},\boldsymbol{r}') = \left(-\frac{Ze^2}{r} + \frac{e^2}{|\boldsymbol{r}-\boldsymbol{r}'|}\right)\left[1 - \frac{r}{2R_i}\left(3 - \frac{r^2}{R_i^2}\right)\right]\theta(R_i - r), \tag{3}$$

where $\boldsymbol{r}$ and $\boldsymbol{r}'$ are the positions of the bound electron and the projectile ion, respectively, $\theta(R_i - r)$ is the step function, the ion-sphere radius R_i $(= [3(Z-1)/4\pi n_e]^{1/3})$ is given by the plasma electron density n_e since the total charge within the ion-sphere is neutral. This ion-sphere potential (eq. (3)) is designed so that the potential and its first derivative vanish at the surface of the ion-sphere.

Recently, the eigenstates $R_{nl}(r)$ and energy eigenvalues E_{nl} of the radial Schrödinger equation for the hydrogenic ion with nuclear charge Z in nonideal plasmas have been obtained by using the Ritz variational method [11, 14] and the perturbation analysis with the ion-sphere model. For the ground state of the hydrogenic ion, the radial wave function is obtained by

$$R_{1s}(r) = 2\alpha_{1s}^{-3/2} e^{-r/\alpha_{1s}}, \tag{4}$$

where α_{1s} is the $1s$ variation parameter obtained by the minimization of the energy expectation value, *i.e.*, $\partial\langle E_{1s}(\alpha_{1s})\rangle/\partial\alpha_{1s} = 0$ [10]:

$$\alpha_{1s}(R_i) = \frac{a_Z}{1 - \delta_{1s}(R_i)/Z}, \tag{5}$$

where a_Z $(= \hbar^2/Zme^2)$ is the Bohr radius of the hydrogenic ion with nuclear charge Z and the effective screening correction $\delta_{1s}(R_i)$ is obtained by

$$\delta_{1s}(R_i) \cong \frac{(Z-1)(a_Z/R_i)^3}{1 - 3(1-1/Z)(a_Z/R_i)^3}. \tag{6}$$

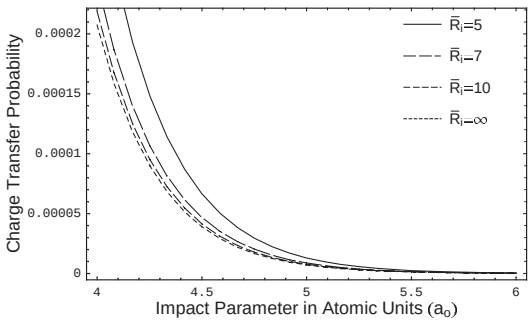

Fig. 1 – The charge transfer probability (P_{ct}) as a function of the impact parameter in atomic units (a_0) for the reaction $He^{2+} + He^{+} \to He^{+} + He^{2+}$ in strongly coupled plasmas for various values of the ion-sphere radius when $\bar{E}_c = 500$.

In order to specifically investigate the plasma screening effects on the charge transfer process in strongly coupled plasmas, we consider the charge transfer probability and cross-section for the reaction $He^{2+} + He^{+} \to He^{+} + He^{2+}$. When the internuclear separation R is greater than the Bohr radius a_0 ($= \hbar^2/me^2$), the energy difference ΔE ($= E_A - E_S$) between the antisymmetric and symmetric stationary states can be obtained by the energy expectation value $\langle E_{1s}\rangle$ and the screened variation parameter α_{1s} with the screening correction $\delta_{1s}(R_i)$ (eq. (6)):

$$\Delta E(R_i) = 4\bar{\alpha}_{1s}^{-2}(R_i)Ry(R/a_0)\exp\big[-2\bar{\alpha}_{1s}^{-1}(R_i)R/a_0\big], \tag{7}$$

where $\bar{\alpha}_{1s}$ ($\equiv 2\alpha_{1s}/a_0$) $= (1-\delta_{1s}/2)^{-1}$, Ry ($= me^4/2\hbar^2 \approx 13.6\,\mathrm{eV}$) is the Rydberg constant, and $R = (b^2 + x^2)^{1/2}$. Since the straight-line trajectory analysis is known to be reliable for large impact parameters [2], *i.e.*, $2\bar{\alpha}_{1s}^{-1}(R_i)b/a_0 > 1$, the charge transfer probability for $\bar{b} > 4$ is found to be

$$P_{ct}\big(\bar{b}, \bar{E}_c, \bar{\alpha}_{1s}\big) = \sin^2\left\{\left(\frac{\mu}{m}\right)^{1/2}\bar{\alpha}_{1s}^{-2}\bar{E}_c^{-1/2}\int_{-\infty}^{\infty}\mathrm{d}\bar{x}\big(\bar{b}^2+\bar{x}^2\big)^{1/2}\exp\left[-2\bar{\alpha}_{1s}^{-1}\big(\bar{b}^2+\bar{x}^2\big)^{1/2}\right]\right\}, \tag{8}$$

where μ is the reduced mass of the collision system, m is the electron rest mass, $\bar{E}_c$ ($= E_c/Ry = \mu v^2/2Ry$) is the scaled collision energy, $\bar{b}$ ($\equiv b/a_0$) is the scaled impact parameter, and $\bar{x} \equiv x/a_0$. Using the integral representation of the n-th order second-kind Bessel function K_n [15],

$$\int_1^{\infty}\mathrm{d}t e^{-\beta t}\big(t^2-1\big)^{n-1/2} = \frac{2^n\Gamma(n+1/2)}{\Gamma(1/2)}\frac{K_n(\beta)}{\beta^n}, \tag{9}$$

where Γ stands for the Gamma-function, the charge transfer probability for intermediate collision velocities in strongly coupled plasmas for the reaction $He^{2+} + He^{+} \to He^{+} + He^{2+}$ is found to be

$$P_{ct}\big(\bar{b}, \bar{E}_c, \bar{R}_i\big) = \sin^2\left\{2\left(\frac{\mu}{m}\right)^{1/2}\bar{\alpha}_{1s}^{-2}\big(\bar{R}_i\big)\bar{E}_c^{-1/2}\bar{b}^2\left[\frac{K_1(2\bar{\alpha}_{1s}^{-1}(\bar{R}_i)\bar{b})}{2\bar{\alpha}_{1s}^{-1}(\bar{R}_i)\bar{b}} + K_0\big(2\bar{\alpha}_{1s}^{-1}\big(\bar{R}_i\big)\bar{b}\big)\right]\right\}, \tag{10}$$

where $\bar{R}_i \equiv R/a_0$. The charge transfer cross-section in units of πa_0^2 is then obtained as

$$\begin{aligned}\sigma_{ct}\big(\bar{E}_c, \bar{R}_i\big)/\pi a_0^2 \;=\; 2\int_{\bar{b}_c}^{\infty}\bar{b}\,\mathrm{d}\bar{b}\sin^2\Bigg\{&2\left(\frac{\mu}{m}\right)^{1/2}\bar{\alpha}_{1s}^{-2}\big(\bar{R}_i\big)\bar{E}_c^{-1/2}\bar{b}^2\times\\ &\times\left[\frac{K_1(2\bar{\alpha}_{1s}^{-1}(\bar{R}_i)\bar{b})}{2\bar{\alpha}_{1s}^{-1}(\bar{R}_i)\bar{b}} + K_0\big(2\bar{\alpha}_{1s}^{-1}\big(\bar{R}_i\big)\bar{b}\big)\right]\Bigg\},\end{aligned} \tag{11}$$

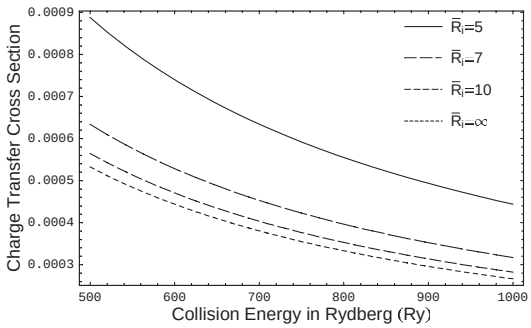

Fig. 2 – The charge transfer cross-section (σ_{ct}) in units of πa_0^2 as a function of the collision energy in Rydberg (Ry) for the reaction $He^{2+} + He^{+} \rightarrow He^{+} + He^{2+}$ in strongly coupled plasmas for various values of the ion-sphere radius.

where $\bar{b}_c$ ($= \max\{4\alpha_{1s}, 8/\bar{E}_c\}$) is the scaled cutoff impact parameter since the charge transfer probability is reliable for the domain $\bar{\alpha}_{1s}^{-1}\bar{b} \gg 1$ since the charge transfer probability is oscillating for small impact parameters.

Figure 1 represents the charge transfer probability as a function of the scaled impact parameter for the reaction $He^{2+} + He^{+} \rightarrow He^{+} + He^{2+}$ in strongly coupled plasmas for different values of the ion-sphere radius. As we see in fig. 1, the plasma screening effects significantly enhance the transfer probability. Figure 2 shows the charge transfer cross-section as a function of the scaled collision energy. In addition, the three-dimensional plot of the charge transfer cross-section is illustrated in fig. 3 as a function of the scaled collision energy and the ion-sphere radius. Thus, it is found that the charge transfer cross-section increases with decreasing the ion-sphere radius, *i.e.*, with increasing the plasma density, and decreases

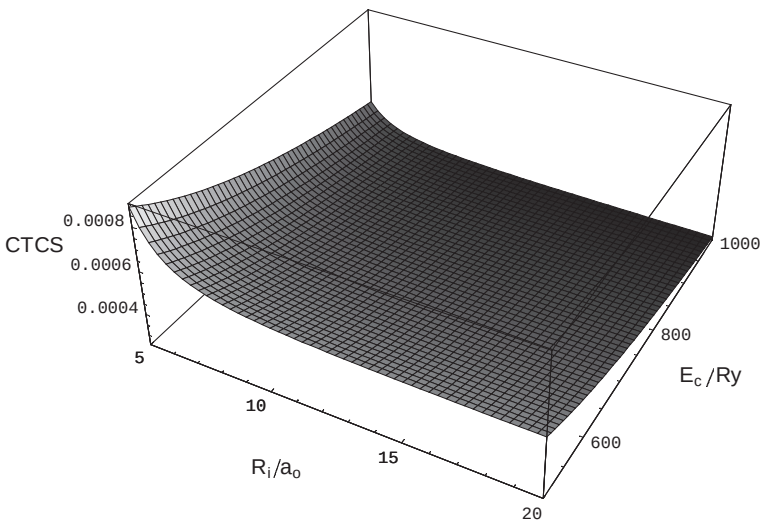

Fig. 3 – The three-dimensional plot of the charge transfer cross-section (CTCS) in units of πa_0^2 as a function of the collision energy in Rydberg (E_c/Ry) and the the ion-sphere radius in atomic units (R_i/a_0).

with the collision energy. Hence, it is important to note that the plasma screening effect increases the resonant charge transfer probability and cross-section in collisions of positive ions in strongly coupled plasmas since the screened variation parameter $\bar{\alpha}_{1s}^{-1}(R_i)$ decreases with increasing the ion-sphere radius. These results provide useful information on the charge transfer process in classical nonideal plasmas.

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