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Charge Transfer Cross Sections at Low Energies and Transfer Ionization at High Energies

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Abstract: We report a theoretical study of state-selective differential single-electron capture cross sections between Na^+ and Rb(5s, 5p) atoms. The experimental data have been obtained with laser cooled target in a magnetic optical trap. We also report a theoretical study of transfer ionization of He by protons at high collision energies and analyze the transfer ionization cross section with respect to single electron capture cross section in terms of a shakeoff model.

Key words: charge transfer; differential cross section; transfer ionization; ion-atom collision
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Charge transfer reaction between singly charged ions and atoms have been studied extensively since the 1960's. These earlier studies focused on the total charge transfer cross sections. In the 1990's, Nils Anderson and coworkers have examined the differential cross sections for alkali atoms by protons and by other alkali ions. They also have studied laser-excited target atoms. In these experiments, the scattering angles of the projectiles are determined. Due to the small scattering angles, the determination of the differential cross sections was quite difficult. In recent experimental development, it was recognized that the projectile scattering angles can be determined if the recoil momentum of the target is measured. For a precise determination of the momentum of the recoil ions, the target should be cooled to reduce the thermal momentum distributions. In the last few years, supersonic cooled He targets have been used in many collision experiments. With the advent of laser cooling, it is possible to cool the alkali target atoms. Here we report the theoretical calculations on the experimental results obtained from Kansas State University for collisions with laser cooled Rb atoms [1].

In the second part of this report, we address the transfer ionization (TI) of He at high collision velocities, in particular, the ratio of TI with respect to single electron capture cross section. This theoretical study is an attempt to understand the recent measurement of Schmidt et al [2] from Stockholm where this ratio has been related to the ratio of double to single photoionization cross sections at high photon energies. We will attempt to interpret both experimental results based on the shakeoff model.

1 Differential Charge-transfer Cross Sections at Low Energies

The theory for single electron charge transfer process is well established. Within the semiclassical impact parameter approximation, one obtains differential cross sections by first calculating scattering amplitudes as function of impact parameters and then performs eikonal approximation. The dif-

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ferential cross section is given by

$$\frac{d\sigma_{fi}}{d\theta} = 2\pi \sin\theta \mid A_{fi} \mid^2, \qquad (1)$$

where

$$A_{fi}(\theta) = \mu v \int_0^\infty b C_{fi}(b, \infty) e^{2(i/v) Z_T Z_P \ln b} \cdot J_m\left(2\mu v \sin\frac{\theta}{2}\right) db, \qquad (2)$$

here μ is the reduced mass, v is the relative velocity, and $m = |m_f - m_i|$, for the initial (m_i) and final (m_f) state magnetic quantum numbers, $Z_P(Z_T)$ is the projectile (target) charge, b is the impact parameter, and J is the Bessel function of the first kind. The charge transfer amplitude C_{fi} is calculated using the two-center atomic orbital close-coupling approximation where the time-dependent wavefunction is expanded in terms of atomic orbital at the two collision centers. In applying to $Na^+ +$ Rb collisions, we approximated it as a one-electron system where Na^+ and Rb^+ are treated as structureless cores and the active electron in such a core is approximated by a model potential, such that the first few bound states of Na and of Rb are well described.

In Fig. 1 we compare the measured and the calculated differential cross sections for (a) $Na^+ + Rb(5s) \rightarrow Na(3s) + Rb^+$ and (b) $Na^+ + Rb(5s) \rightarrow Na(3p) + Rb^+$ where the latter is the dominant channel for collisions at 7, 5 and 2 keV. The results for the dominant channel show good agreement but there are pronounced discrepancies for the weak channel at the low energy of 2 keV. We note that the theoretical results have been convoluted with an angular resolution of 73, 87 and 138 μrad for 7, 5 and 2 keV, respectively. In fact from the theoretical calculations the differential cross sections are found to oscillate rapidly with respect to the scattering angles, see Fig. 2. Due to the limitation of the angular resolution of the experiment, such oscillations are not seen clearly in the data.

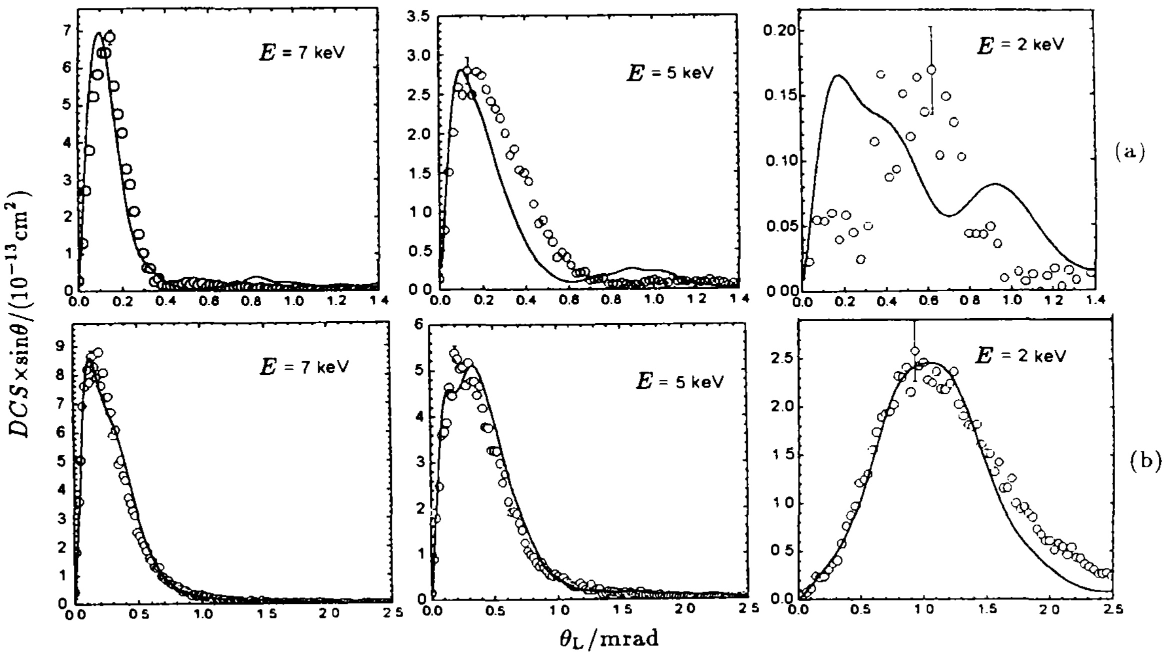

Fig. 1 Differential cross sections (DCS) for $Na^+ + Rb(5s) \rightarrow Na(3s) + Rb^+$ at 7, 5 and 2 keV impact energies. The theoretical results have been convoluted with the experimental angular resolutions.

We conclude that the current experiment, even with laser cooled target atoms, the limitation of the experimental resolution still prevents us from examining the oscillatory differential cross sections predicted by the theory.

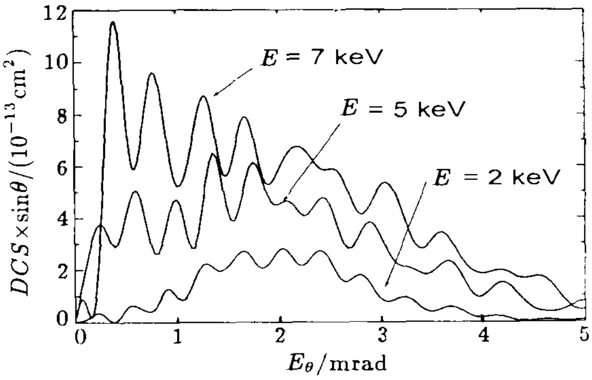

Fig. 2 Theoretical differential cross sections for $Na^+ + Rb(5s) \to Na(3s) + Rb^+$ at 7, 5 and 2 keV impact energies showing rapid oscillations not resolved in the experiments.

2 Transfer Ionization of He at High Energies

In a recent experiment, Schmidt et al measured the total cross sections for transfer ionization (TI) of He by protons in the 2.5—4.5 MeV energy region. Using the recoil ion momentum spectroscopy, they were able to differentiate the Thomas TI process from the kinematic TI (KTI) process. In the Thomas process, TI occurs first through a hard collision between the incident proton and an electron which is ejected at 45° with respect to the incident ion direction with velocity $\sqrt{2}v$. This electron subsequently collides with the second electron to ionize it and at the same time itself is captured by the proton. The target nucleus plays little role in the Thomas process and thus it is characterized by a small recoil momentum. For the KTI process, the first electron is captured at close impact, resulting at a large target recoil momentum while the second electron is ionized.

For fast collision, the capture of the first electron is a fast process and the resulting ionization may be approximated as a shakeoff process. This is analogous to double ionization at large photon energies where the ejection of a fast electron may result in the release of a shakeoff electron. Thus intuitively it is possible to consider KTI and double photoionization on an equal footing and compare the ratio of double photoionization to single photoionization (R_ν) with the ratio of TI to single electron capture cross sections (R_{TI}).

In Fig. 3 we show such ratios R_ν and R_{TI} vs the velocity of the first ejected electron. For R_ν, we calculate v by assuming that the first electron carries all the excessive photon energy. For R_{TI} we assume that the velocity of the first electron is the same as the velocity of the projectile. The dashed lines give the best known results for R_ν. For v below 8 arb. unit , the dashed lines are the experimental results. Above that, the dashed lines are from the theoretical estimate. There are three sets of R_{TI} shown in Fig. 3. The open squares and the solid circles are from measurements where different mechanisms of TI are not distinguished. These data are taken at lower energies too. For the data points from Schmidt et al, at v between 10 and 15, the open squares are from the total TI while the solid squares are only for KTI. It is clear that the R_{TI} for the KTI process only is reasonably close to R_ν. Thus there is an indication that the two processes may indeed be examined on the same ground within the shakeoff theory.

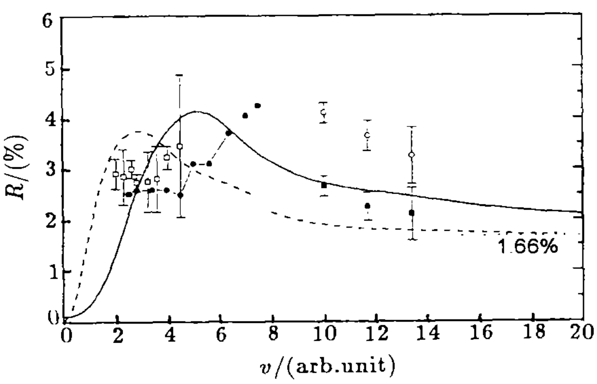

Fig. 3 Ratio of double to single photoionization of He (R_ν) and ratio of transfer ionization to single electron capture on He by proton impact (R_{TI}), as a function of the velocity of the fast ejected electron. Solid line: Shakeoff theory prediction. Experimental data, see text.

In the Shakeoff theory, the first electron in

He is ejected into the continuum with a momentum $\boldsymbol{k}$, or velocity $\boldsymbol{v}$. Let $\Psi(\boldsymbol{p}_1, \boldsymbol{r}_2)$ be the helium ground state wavefunction in the mixed coordinate and momentum space. If $\boldsymbol{p}_1 = \boldsymbol{v}$, then the spatial wavefunction of the second electron is described by

$$\Phi_v(\boldsymbol{r}_2) = \frac{\Psi(\boldsymbol{v}, \boldsymbol{r}_2)}{N_v}, \tag{3}$$

where $N_v^2 = \langle \Psi(\boldsymbol{v}, \boldsymbol{r}_2) | (\boldsymbol{v}, \boldsymbol{r}_2) \rangle$ is the normalization constant. In the Shakeoff model, one takes $\Phi_v(\boldsymbol{r}_2)$ to be the wavefunction of the remaining electron when the first electron is ejected at velocity $\boldsymbol{v}$, either by photoabsorption or by electron capture process. By projecting out all the bound states where the electrons ending up in the ground state or the excited states of He^+, the Shakeoff probability can then be calculated.

The Shakeoff probability has been calculated by Aberg in the limit that the first electron is ejected at an infinite velocity. Using accurate wavefunction of He by Kinoshita, the ratio was evaluated to be 1.66%. This is the Shakeoff limit often quoted in the literature. To compare with the experimental data shown in Fig. 3, it is essential that the shakeoff probability be evaluated at finite velocity. Using wavefunctions obtained from configuration interaction approach, we show the calculated shakeoff probabilities, in solid line in Fig. 3, over a broad range of velocity, and extending to the small-v limit. It is clear that the measured ratios of R_v and R_{KTI} are quite close to the predictions of the shakeoff model. This is an indication that the shakeoff picture is conceptually adequate in describing the transfer ionization process at high impact velocity, and in describing double photoionization at high photon energies.

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低能电荷转移截面和高能转移电离研究

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摘　要: 介绍了对于 Na^+ 离子和 Rb(5s, 5p)原子碰撞中态选择单电子俘获微分截面的理论计算，并与实验数据进行比较，实验结果是离子与在磁光学阱中用激光冷却的碱金属靶原子碰撞而测量到的；还对高能量质子引起的 He 原子的转移电离进行了理论研究，在 Shakeoff 模型的基础上，分析解释了转移电离截面与单电子俘获截面的比值，并与最新实验结果作了比较.

关键词: 电荷转移；微分截面；转移电离；离子-原子碰撞