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A Potential Parameter on the Stabilization Ratio of Double-electron Transfer in Slow Highly Charged Ions with Helium Collisions

DU Fan[1, 2], LU Rongchun[1], YU Deyang[1]

(*1. Institute of Modern Physics, Chinese Academy of Sciences, Lanzhou 730000, China;*
2. University of Chinese Academy of Sciences, Beijing 100049, China)

Abstract: We borrow the concept of virtual state to characterize the strong interacting feature of the two transferred electrons in slow highly charged ions with helium collisions. Consequently, a potential parameter ω is defined to distinguish the collision systems and to scale the double-electron transfer processes. The Q-value is taken into account according to the classical over-the-barrier model. Comparing with our previous experimental data, it is clearly shown that the true double capture or the autoionizing double capture dominates when $\omega \leqslant 1$ or $\omega \geqslant 2$, respectively. We clarify that the distinction of the collision systems is essentially the ratio between the average excitation energy and the average binding energy of the two transferred electrons at the scattered ion.

Key words: double-electron transfer; true double capture; autoionizing double capture; stabilization ratio

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1 Introduction

Double-electron transfer (DET) is one of the basic multi-electron processes in slow collisions of highly charged ions (HCIs) with helium atoms. In such a process, DET is usually divided into two subsequent stages: (i) the electron transfer and (ii) the subsequent stabilization. Both classical[1−3] and quantum[4−6] methods are developed to understand the first stage. These theories usually treat the projectile as a structureless charged point, which is reasonable for the electron transfer happening at large inter-nuclei distance of about 10 a.u., as well as the transferred electrons being populated in highly excited states. At the second stage, the doubly excited states stabilize via either photon emission which gives rise to true double capture (TDC), or Auger electron emission leading to autoionizing double capture (ADC). The stabilization of DET was experimentally investigated by both Auger spectrum[7−16] and optical spectrum[16−19], and it was found that ADC dominates if the two electrons are captured into same or similar n-shells and that TDC dominates when the two electrons are populated in asymmetrical configurations. It was also found that the impact velocity[18,20] and the projectile core properties[21] affect the stabilizing results. However, the initial population of the doubly excited recoiled ions is difficult to be calculated in very detail, and therefore the decay scheme is indistinct. We still lack a precise theory to describe the stabilization stage.

Sakaue *et al.*[22] measured the branching ratios of DET in I^{q+} (q = 10, 15, 20 and 25) with Ne, Ar,

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Biography: Du Fan(1986–), male, Huhhot, Inner Mongolia, China, Master student, working on the field of atomic and molecular physics

Corresponding author: YU Deyang, E-mail; d.yu@impcas.ac.cn.

Kr and Xe collisions at 1.5 q keV. They introduced the average principal quantum number $\langle n\rangle$ of the excited scattered ions and showed that Auger decay is dominant when $\langle n\rangle$ is sufficiently large. Recently, Lü *et al.*[23] investigated the relative ratio between TDC and ADC in slow A^{q+}-He (A=C, N, Ne, Ar, Kr, and $q = 4 \sim 7$) collisions. They defined a potential parameter $\Omega = I_{\max}/\left(I_1^{\mathrm{He}} + I_2^{\mathrm{He}}\right) - 1$ to distinguish the different collision systems, where $I_{\max}$ is the maximum bonding energy of the projectile vacancies, and I_1^{He} and I_2^{He} denote the first and second ionization energy of helium, respectively. They showed that TDC is the major channel when $\Omega < 1$ while ADC becomes dominant when $\Omega > 1$. They argued that the electrons are influenced by both the projectile ion and the recoiled He^{2+}, and the stabilization is determined by the competition of the Coulomb potential between the projectiles and the recoiled He^{2+}. However, to our best knowledge, the Auger electron spectra show that the emitted electron comes from the scattered ion rather than the quasi-molecular of the ion-helium system, which implies that during the stabilization the interaction between the electrons and the He^{2+} is negligible. In addition, Krok *et al.*[24] showed that the stabilization of excited ion does not depend on the target.

In this paper, we emphasize the strong interacting feature between the two transferred electrons, and present a practical approach to estimate the stabilization ratio $R_{\mathrm{TDC}} = \sigma_{\mathrm{TDC}}/\sigma_{\mathrm{DET}}$ (σ_{TDC} and σ_{DET} are the cross sections of TDC and DET, respectively). The Q-value is taken into account according to the classical over the barrier model. We show that the distinction of the collision systems is essentially the ratio between the average excitation energy and the average binding energy of the two transferred electrons at the doubly excited ion.

2 The model

Since the transferred electrons are always populated on excited states in HCI with helium collisions, the electron-nuclei interaction is greatly reduced. Due to the strong electron-electron correlation, the configuration mixing is large and the independent-particle model is no longer a good approximation[25−27]. Although the eigen energy of each electron is nonsense, the total energy is still a conserved quantity. Therefore, the two electrons in doubly excited states couple together and should be considered simultaneously, as if they are populated in a transient *virtual* state. According to energy conservation, the average binding energy of the virtual state is $\langle E_{\mathrm{b}}\rangle = (E_1 + E_2)/2$, while practically the electron binding energies E_1 and E_2 are calculated from any models about the electron transfer stage, e.g., the MCBM (Molecular Coulombic Barrier Model)[3].

According to this assumption, we propose a potential parameter ω to represent the ratio between the average excitation energy and the average binding energy:

$$\omega = \frac{I_{\max} - \langle E_{\mathrm{b}}\rangle}{\langle E_{\mathrm{b}}\rangle} = \frac{I_{\mathrm{MAX}}}{\langle E_{\mathrm{b}}\rangle} - 1 \ , \tag{1}$$

where $I_{\max}$ denotes the maximum bonding energy of the projectile vacancies. The average binding energy $\langle E_{\mathrm{b}}\rangle$ includes the contributions of the initial helium binding energies I_1^{He} and I_2^{He}, as well as the Q-value of the reaction

$$\langle E_{\mathrm{b}}\rangle = \frac{I_1^{\mathrm{He}} + I_2^{\mathrm{He}} + Q}{2} \ . \tag{2}$$

The Q-value can be deducted following the idea of the MCBM, which was expatiated by Niehaus[3]. Briefly, the superposed Coulomb potential has two troughs due to the projectile ion and the helium nuclei, and the charge transfer corresponds to a target electron to overcome the potential barrier. In atomic units, the potential at the inter-nuclei position is written as $V(r) = -q/(R-r) - t/r$, where q is the charge state of the ion, t represents the charge state of the target core, R is the distance between the two nuclei, and r represents the distance between the active electron and the target nuclei. The height of the barrier between the two nuclei is $V_{\max} = -\left(\sqrt{q} + \sqrt{t}\right)^2/R$ when $r = -R\sqrt{t}/\left(\sqrt{q} - \sqrt{t}\right)$. During approaching ("way in") the height of the barrier decreases and the electrons successively overcome the barrier and move around both nuclei. Taking into the Stark energy, the energy of the t-th electron in the superposed potential is $E_t = -I_t - q/R$,

where I_t is the ionization energy. The condition to overcome the barrier is $E_t \geqslant V_{\max}$, so the distance of overcoming the barrier is $R_t^{\text{in}} = (t+2\sqrt{qt})/I_t$. MCBM supposes that the energy of the electron keeps constant after it overcomes the barrier, because it moves around both nuclei and the Stark effect does not work anymore. Then its over-the-barrier energy is $E_t = -\left[1+1/\left(t/q+2\sqrt{t/q}\right)\right] I_t$. While separating ("way out"), the electrons are successively isolated by the raising barrier, and both captured by the ion in DET. Taking into account the Stark energy of the recoiled target again, the Q-value of the electrons can be deduced. The Q-values of the first and the second electrons are

$$Q_1 = -\frac{I_1}{2\sqrt{q}+1}\left[q-\frac{2\left(\sqrt{q}+1\right)^2}{\left(\sqrt{q-1}+\sqrt{2}\right)^2}\right], \quad (3)$$

$$Q_2 = -\frac{q-2}{2\left(\sqrt{2q}+1\right)} I_2 , \quad (4)$$

where $I_1 = 0.9$ a.u. and $I_2 = 2.0$ a.u., respectively. $Q = Q_1 + Q_2$ depends on the charge state q of the projectile ion, and contributes a notable part to the average binding energy.

If the average excitation energy $I_{\max} - \langle E_{\text{b}} \rangle$ is smaller than the average binding energy $\langle E_{\text{b}} \rangle$, the ADC channel closes. Even though the electron-electron interaction still works and may lead to the auto-transfer to Rydberg state[28−30], as shown in Fig. 1(a). Due to the weak electron-nuclei interaction, the electromagnetic transition is also reduced. Therefore, when $I_{\max} - \langle E_{\text{b}} \rangle$ is larger than $\langle E_{\text{b}} \rangle$, we further assume that, if only the ADC is possible in energy, it will dominates over TDC, as illustrated in Fig. 1(b).

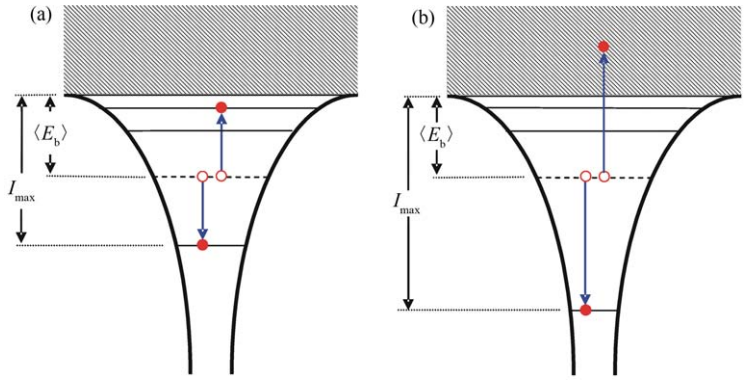

Fig. 1 (color online) Stabilization of double-electron transfer in slow HCI-He collisions. Due to the strong electron-electron correlation the eigen energy of each transferred electron is nonsense, but the total energy is still a conserved quantity. Accordingly, the two electrons are assumed populating in a *virtual* state with average binding energy of $\langle E_{\text{b}} \rangle$.
(a) If the average excitation energy $I_{\max} - \langle E_{\text{b}} \rangle$ is less than the average binding energy $\langle E_{\text{b}} \rangle$, ADC channel closes therefore TDC dominates. (b) Otherwise, due to the weak electron-nuclei interaction and strong electron-electron interaction, ADC channel dominates.

3 Result and discussion

The stabilization ratios R_{TDC} (as well as the autoionizing ratio $R_{\text{ADC}} = 1 - R_{\text{TDC}}$) in collisions of A^{q+} (A=C, N, O, F, Ne, S, Si, Ar, Ca and Kr, $q = 4 \sim 9$, 11, 16) with helium which is taken from our previous work[21,31] are illustrated as two functions of the potential parameter ω in Fig. 2. It clearly shows that TDC or ADC dominates when $\omega \leqslant 1$ or $\omega \geqslant 2$, repectively. In the region of $1 < \omega < 2$, the R_{TDC} decreases dramatically from about 90% to about 10%. According to this definition, the potential parameter ω distinguishes the collision system and can be employed as a scale to evaluate the stabilization stage.

We note that in very high charge states region (i.e., $\omega \gg 1$), the ADC channel dominates but the stabilization ratio R_{TDC} increases slowly with the parameter ω increases. The reason is that the radiative decay rate scales as q^4 while the autoioniza-

tion rate is independent of q[32]. This is consistent with the results of Cederquist *et al.*[33], who measured cross sections for TDC and ADC in slow collisions of Xe^{q+} with helium in the charge state regime $15 \leqslant q \leqslant 42$. The minor fluctuation of the stabilization ratio was studied by Krok *et al.*[24], who pointed out that $R_{\rm TDC}$ reaches a local maximum when the number of electrons and vacancies in the outer subshells is almost same. It also should be noted that the shell effect on the stabilization following multi-electron transfer (MET) was observed in slow Ar^{q+}-Ar collisions[34], where the branching ratios of MET vary dramatically with the inner shell open or close. However, although the K-shell of F^{7+} and $Ne^{7+,8+}$ is closed, the ADC dominates due to its vacancies is deep enough to open the ADC channel. The potential parameter is a more critical criterion than the shell effect[34].

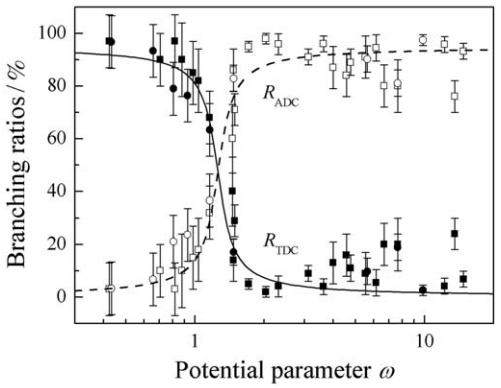

Fig. 2　The stabilization ratio $R_{\rm TDC}$ and the autoionizing ratio $R_{\rm ADC}=1-R_{\rm TDC}$ as functions of the potential parameter ω in slow ions with helium collisions. The slow ions we have considered, include C^{4+}, N^{4+}, O^{4+}, Ne^{4+}, C^{5+}, N^{5+}, O^{5+}, Ne^{5+}, C^{6+}, N^{6+}, O^{6+}, F^{6+}, Ne^{6+}, Ar^{6+}, Ca^{6+}, O^{7+}, F^{7+}, Ne^{7+}, S^{7+}, Ar^{7+}, Ca^{7+}, F^{8+}, Ne^{8+}, Ar^{8+}, Ca^{8+}, F^{9+}, Ne^{9+}, Si^{9+}, S^{9+}, Ar^{9+}, Ca^{9+} Si^{11+}, Ar^{11+} and Ca^{11+}.
The solid and open symbols represent $R_{\rm TDC}$ and $R_{\rm ADC}$, respectively. The data are taken from our previous work, Yu *et al.* [21] (■ and □) and Cao *et al.*[31] (● and ○). The solid and dashed lines are employed to guide the eye.

4 Conclusion

A potential parameter ω is defined to scale the DET process in HCI-He collisions, and in which the Q-value of the collision is taken into account. It is shown that TDC or ADC dominate when $\omega \leqslant 1$ or $\omega \geqslant 2$, respectively. In the region of $1 < \omega < 2$, the TDC channel decreases rapidly, and correspondingly the ADC channel increases. We introduce the transient *virtual* state hypothesis, and point out that the distinction of the collision systems is essentially the ratio between the average excitation energy and the average binding energy of the two transferred electrons at the scattered ion. The result agrees systematically with our previous experimental data.

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References:

[1] RYUFUKU H, SASAKI K, WATANABE T. Phys Rev A, 1980, **21**: 745.
[2] BÁRÁNY A, ASTNER G, CEDERQUIST H, *et al.* Nucl Instr Meth B, 1985, **9**: 397.
[3] NIEHAUS A. J Phys B, 1986, **19**: 2925.
[4] JANEV R K, WINTER H. Phys Rep, 1985, **117**: 265.
[5] FRITSCH W, LIN C D. Phys Rep, 1991, **202**: 1.
[6] KRONEISEN O J, LÜDDE H J, KIRCHNER T, *et al.* J Phys A, 1999, **32**: 2141.
[7] STOLTERFOHT N, HAVENER C C, PHANEUF R A, *et al.* Phys Rev Lett, 1986, **57**: 74.
[8] MACK M, NIJLAND J H, STRATEN P V D, *et al.* Phys Rev A, 1989, **39**: 3846.
[9] STOLTERFOHT N, SOMMER K, SWENSON J K, *et al.* Phys Rev A, 1990, **42**: 5396.
[10] HOLT R A, PRIOR M H, RANDALL K L, *et al.* Phys Rev A, 1991, **43**: 607.
[11] FREMONT F, SOMMER K, LECLER D, *et al.* Phys Rev A, 1992, **46**: 222.
[12] PRIOR M H, HOLT R A, SCHNEIDER D, *et al.* Phys Rev A, 1993, **48**: 1964.
[13] FREMONT F, MERABET H, CHESNEL J Y, *et al.* Phys Rev A, 1994, **50**: 3117.
[14] CHESNEL J Y, MERABET H, FR MONT F, *et al.* Phys Rev A, 1996, **53**: 4198.
[15] CHESNEL J Y, MERABET H, SULIK B, *et al.* Phys Rev A, 1998, **58**: 2935.
[16] BLIMAN S, BRUCH R, CORNILLE M, *et al.* Phys Rev A, 2002, **66**: 052707.
[17] BODUCH P, CHANTEPIE M, HENNECART D, *et al.* J Phys B, 1989, **22**: L377.
[18] MARTIN S, BERNARD J, CHEN L, *et al.* Phys Rev A, 1995, **52**: 1218.

[19] LANGEREIS A, NORDGREN J, BLIMAN S, *et al.* Phys Rev A, 1999, **60**: 2917.
[20] YU D, CAI X, LU R, *et al.* Chin Phys Lett, 2005, **22**: 1398.
[21] YU D, CAI X, LU R, *et al.* Phys Rev A, 2007, **76**: 022710.
[22] SAKAUE H A, DANJO A, HOSAKA K, *et al.* J Phys B, 2004, **37**: 403.
[23] LÜ Y, CHEN X, CAO Z, *et al.* Act Phys Sin, 2010, **59**(06): 3892. (in Chinese)
(吕瑛，陈熙萌，曹柱荣，等. 物理学报，2010，**59**(06)：3892)
[24] KROK F, TOLSTIKHINA I Y, SAKAUE H A, *et al.* Phys Rev A, 1997, **56**: 4692.
[25] LIN C D. Phys Rev Lett, 1983, **51**: 1348.
[26] LIN C D. Adv At Mol Phys, 1986, **22**: 77.
[27] LIN C D, WATANABE S. Phys Rev A, 1987, **35**: 4499.
[28] BACHAU H, RONCIN P, HAREL C. J Phys B, 1992, **25**: L109.
[29] RONCIN P, GABORIAUD M N, BARAT M, *et al.* J Phys B, 1993, **26**: 4181.
[30] SANCHEZ I, BACHAU H. J Phys B, 1995, **28**: 795.
[31] CAO Z, YU D, YANG W, *et al.* J At Mol Phys, 2004(Suppl): 0135–04. (in Chinese)
(曹柱荣, 于得洋, 扬威, 等. 原子与分子物理学报, 2004(增刊)：0135–04.)
[32] CEDERQUIST H. Z Phys D, 1991, **21**: 6.
[33] CEDERQUIST H, ANDERSSON H, BEEBE E, *et al.* Phys Rev A, 1992, **46**: 2592.
[34] LU R, YU D, SHAO C, *et al.* Nucl Instr Meth B, 2010, **268**: 2592.

慢速高电荷态离子与氦原子碰撞中双俘获稳定比的势能参量

杜 凡[1, 2]，卢荣春[1]，于得洋[1]

(1. 中国科学院近代物理研究所，兰州 730000；
2. 中国科学院大学，北京 100049)

摘要： 在慢速高电荷态离子与氦原子碰撞的双电子转移过程中，借用虚态图像来描绘转移电子间的强关联特性；根据分子库仑过垒模型纳入反应 Q 值，定义势能参量 ω 来区分碰撞系统并度量双电子转移过程。对照之前的实验数据，清晰地显示当 $\omega \leqslant 1$ 和 $\omega \geqslant 2$ 时，纯双电子俘获或自电离双俘获分别占优。澄清了碰撞系统的本质区别在于散射离子上两个转移电子的平均激发能和平均束缚能的相对比率。

关键词： 双电子转移；纯双俘获；自电离双俘获；双俘获稳定比

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通信作者： 于得洋，E-mail: d.yu@impcas.ac.cn。