Transfer excitation processes in ion-atom collisions at high energies

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A theory of ion-atom and ion-molecular collisions at high energies is formulated in which the projectile ions undergo simultaneous electron transfer and excitation (TE). A unified description of both resonant and nonresonant processes is presented. The resonant mode (RTE) is mediated by one of the target electrons, which excites the projectile and at the same time is captured by the projectile ion, thus forming a doubly excited intermediate state of the projectile ion. In the impulse approximation, this is related to the dielectronic recombination process in electron-ion collisions. The same doubly excited states can also be formed by one of the target electrons and the target core, interacting with the projectile ion in which the target core does the exciting and the electron is simply transferred. This is a nonresonant process (NTE), although the projectile is again left in a doubly excited state. We propose here still another mechanism for the formation of doubly excited states, UTE. The new process involves two target electrons in a nonresonant way, just as in the NTE, such that the electron that excites the projectile is left in the continuum, as viewed in the projectile rest frame. Some of the experimental evidence for these reactions is discussed.

I. INTRODUCTION

Much experimental effort has been expended[1-3] in recent years to understand the transfer excitation (TE) processes in high-energy ion-atom and ion-molecular collisions in which the projectile ions (A^{z+}) (i) are excited while one of the target electrons is transferred to the projectile to form a doubly excited state (d) of the projectile $(A^{(z-1)+})^{**}$. Schematically for a target atom (or molecule) B, TE is described as

$$\begin{aligned} &A^{Z+}+B\rightarrow(A^{(Z-1)+})^{**}+B^{+}, \quad \text{TE} \\ &(A^{(Z-1)+})^{**}\rightarrow(A^{(Z-1)+})^{*}+\gamma, \quad \text{TEX} \\ &\qquad\rightarrow(A^{Z+})+e', \quad \text{TEA} . \end{aligned} \tag{1.1}$$

where TEX represents TE with emission of one or more photons and TEA represents TE with one or more Auger electron emissions. Analogous definitions apply for similar labels used later. In particular, the resonant component of (1.1), RTE, is compared[4] with the dielectronic recombination (DR) process in electron-ion collisions,[5] as

$$\begin{aligned} &e+A^{Z+}\rightarrow(A^{(Z-1)+})^{**}, \quad \text{RE} \\ &(A^{(z-1)+})^{**}\rightarrow(A^{(Z-1)+})^{**}+\gamma, \quad \text{DR} \\ &\qquad\rightarrow(A^{Z+})+e', \quad \text{RES} \end{aligned} \tag{1.2}$$

where RE denotes resonant excitation and RES for RE scattering. That is, in the projectile rest frame in (1.1), the target B simply provides a beam of free electrons (and the core b) for the process (1.2). Thus the analysis of RTE has been carried out rather successfully in impulse approximation by folding the DR cross sections over the target Compton profile. The DR process (1.2) has received much attention recently because of its importance in the study of high-temperature laboratory and astrophysical plasmas. Direct measurement of the DR cross sections has proved difficult, because of their small magnitude. Nevertheless, several careful experimental measurements using the electron-ion crossed and merged beams have been reported recently,[6-10] all of which involved intrashell excitations. On the other hand, most of the reported DR measurements involving intershell excitations have been of the RTE type, and the agreements between experiments and theory, with allowance for the possible field effect, have been excellent in all cases.

The nonresonant modes of (1.1), NTE, can also create doubly excited states (d), where one of the target electrons is simply transferred to an excited state of the projectile, while core b excites the projectile. A couple of precise NTE data[1-3] have been available for some time, but detailed theoretical study is lacking. This process manifests itself as a broad peak at relatively low energy, as a result of convolution of the capture probability which decreases with energy and the excitation probability which rapidly increases with energy and levels off.

In the course of analysis of RTE,[5,11] especially for the systems S^{13+}, Ca^{17+}, and Nb^{31+} on He and H_2 targets, it was noted[1,5] that the high-energy end of the RTE cross sections was unusually high and unexplainable by any available physical mechanisms. A detailed analysis was then carried out to determine whether the field of the target core b may affect the cross section in this energy region.[11] The effect was too small to explain the discrepancy, because of the presence of a fast Auger decay channel which was independent of the high Rydberg states (HRS) formed during the capture. A new mechanism, the uncorrelated transfer excitation (UTE), involving at least two electrons of He, was[12] then proposed to explain this anomaly. In UTE, two target electrons are actively involved in the creation of doubly excited projectile states; one electron excites the projectile and is left in the continuum, as viewed in the projectile rest frame, while the second electron is simply captured, as in NTE, to form a

doubly excited state of the projectile. It has the correct threshold energies. Some additional evidence for the presence of UTE is reported,[13] but a detailed theoretical analysis is needed.

In view of increasing experimental activities in recent years, it is of interest to formulate the TE problem once more and provide a calculationally tractable procedure for the analysis of the existing data. Since TE is a higher-order charge exchange process involving at least two or more electrons, the calculations are difficult to perform, and the theory has thus far been unable to provide a quantitative understanding of the experiments, except in the case of RTE, where the precise DR cross sections and impulse approximation are used to analyze the data, with surprisingly successful result. On the other hand, an initial attempt by Feagin *et al.*[14] and a more heuristic approach of Brandt[15] are the only available theory of NTE. We present here a general theoretical framework for the treatment for all three phenomena, RTE, NTE, and UTE, and cast the theory in a form suitable for applications. The theory sorts out in a unified way the three different modes of TE and facilitates their comparison. Proliferation of different channels present in this many-particle collision system warrants a systematic development of the theory. The principal result is contained in Eq. (3.1), with the individual cross sections given by Eqs. (3.6), (3.22), and (3.25). Details of the application of (3.6) for RTE have already been reported, while (3.22) and (3.25) for the NTE and UTE are being applied in the study of the reactions for the specific systems (Si^{11+} + He and $Ca^{17+}+H_2$, He).

II. BASIC FORMALISM: ELECTRON TRANSFER COLLISIONS

In order to simplify the discussion of the direct and excitation transfer reactions and still to include all the processes discussed in Sec. I, we consider a simple three-electron collision system $A+B$ (see Fig. 1)

$$(a+e_1)+(b+e_2+e_3)\rightarrow \begin{cases} (a+e_1)+(b+e_3)+e_2 & \text{(2.1a)} \\ (a+e_1+e_2)+(b+e_3)+\gamma & \text{(2.1b)} \\ (a+e_1+e_2)^{**}+(b+e_3)\ , & \text{(2.1c)} \end{cases}$$

$$(a+e_1+e_2)^{**}\rightarrow A'+\gamma \rightarrow A+e_2\ , \quad \text{(2.1d)}$$

$A=(a+e_1)$, $B=(b+e_2+e_3)$, $A'=(a+e_1+e_2)^{**}$, $B'=(b+e_3)$, where a and b denote the ion cores of A and B, with all the spectator electrons included implicitly in a and b. The target system B can be either an atom (such as He, Ne, Ar, Kr, etc.) or a molecule (such as H_2), but we simply refer it as atom in the following. In actual applications, the effect of the spectator electrons as well as their Pauli exchange must be correctly included. The Hamiltonian of the system is given by[16]

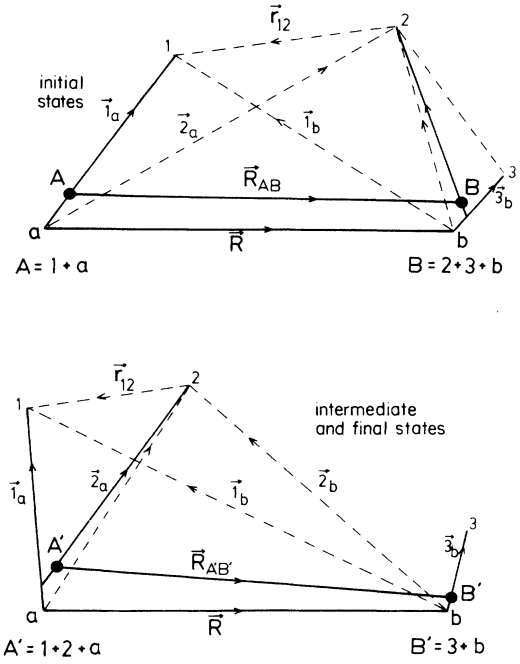

FIG. 1. Coordinate system used for the reactions described in (2.1). The initial state, and the intermediate and final states, respectively, require two different sets of orthogonal coordinates because of the electron rearrangement. The center of masses of B, A', and B' are exaggerated in the figure; their effect on the bound states of the respective electrons is small.

$$H_{\rm tot}=H_M+H_R+D=H+D,\quad H_M=K+V$$
$$(E-H_{\rm tot})\Psi^{\rm tot}_{i,f}=0\ , \qquad \text{(2.2)}$$

where the matter and radiation field Hamiltonians are defined as

$$K=K_{AB}+K_{a1}+K_{b2}+K_{b3}=K_{A'B'}+K_{a1}+K_{a2}+K_{b3}\ , \qquad \text{(2.3)}$$
$$V=\sum_{i=1}^{3}(V_{ai}+V_{bi})+\sum_{i>j=1}^{3}V_{ij}+V_{ab}\ ,$$
$$H_R=\sum_{\mathbf{k}}\sum_{\alpha}\tfrac{1}{2}\hbar\omega_{\mathbf{k}}(a^{\dagger}_{k\alpha}a_{k\alpha}+a_{k\alpha}a^{\dagger}_{k\alpha})\ , \qquad \text{(2.4)}$$

and

$$D=-\sum_{\mathbf{k}\alpha}\frac{e}{m}\left[\frac{2\pi\hbar}{\omega\mathbf{k}}\right]^{1/2}\times\sum_{i=1}^{3}(\mathbf{p}_i\cdot\epsilon_{\alpha}a^{\dagger}_{k\alpha}e^{-i\mathbf{k}\cdot\mathbf{r}_i}+\text{H.c.})\ ,$$
$$[a_{k\alpha},a^{\dagger}_{k'\alpha'}]=\delta_{\mathbf{k}\mathbf{k}'}\delta_{\alpha\alpha'}\ . \qquad \text{(2.5)}$$

In (2.3)–(2.5), we have K_{AB} equal to relative kinetic energy for the systems A and B, $K_{a1}=$ kinetic energy for electron 1 in the center of mass c.m. of A; K_{b2}, K_{a2}, and $K_{A'B'}$ are similarly defined. For the bound states, the difference between the c.m. of $(b+3)$ and b for electron 2, for example, is negligible, but such difference may be

important for continuum orbitals where it can generate a translation factor. In addition, H_R is the radiation field Hamiltonian and D represents the electron-radiation field coupling. In the actual calculation, the electric dipole coupling in the position representation will be sufficient. (The quantized radiation field Hamiltonian H_R and electron-radiation coupling D are convenient in correctly treating the radiative emission, radiative widths, and radiative cascades. A completely consistent theory cannot be formulated without them.) The effect of the radiation channel becomes very large when highly charged ions are involved.

For the TE process, we set

$$H=H_c+V_c, \quad c=i \text{ or } f \tag{2.6}$$

with, for the initial state,

$$\begin{aligned} H_i&=K+V_{a1}+V_{b2}+V_{b3}+V_{23}+U_i+H_R \ , \\ V_i&=V_{12}+V_{b1}+V_{13}+(V_{a2}+V_{a3}+V_{ab}-U_i) \ , \end{aligned} \tag{2.6a}$$

and, for the final state,

$$\begin{aligned} H_f&=K+V_{a1}+V_{a2}+V_{12}+V_{b3}+U_f+H_R \ , \\ V_f&=V_{13}+V_{23}+V_{a3}+V_{b1}+V_{b2}+V_{ab}-U_f \ . \end{aligned} \tag{2.6b}$$

Since projectile A is usually highly stripped, its Coulomb effect on the electronic orbitals of B should be properly taken into account. We incorporate this distortion by including the distortion potentials U_c in H_c. In Eq. (2.6), K is the total kinetic energy operator of the system. The channel wave functions for (2.1b) and (2.1d), for example, are defined, for each channel Hamiltonian H_c with effective distortion potentials U_c, by

$$(H_c-E)\Phi_{cX}=0 \ , \tag{2.7}$$

where, for example, we have the product functions for the electronic, ionic core, and radiation parts for each channel $c=i$ or f as

$$\begin{aligned} \Phi_{iX}&=\psi_A(\mathbf{1}_a)\psi_B(\mathbf{2}_b,\mathbf{3}_b)u_i(\mathbf{R}_{AB},\mathbf{K}_i)\varphi(a,b)|\mathbf{0}\rangle \ , \\ \Phi_{fX}&=\psi_{A'}(\mathbf{1}_a,\mathbf{2}_a)\psi_{B'}(\mathbf{3}_b)u_f(\mathbf{R}_{A'B'},\mathbf{K}_f)\varphi(a,b)|\mathbf{k}_\alpha\rangle \ , \end{aligned} \tag{2.8}$$

and $\varphi(a,b)$ is the internal wave functions of the cores a and b. In (2.8), $|\mathbf{0}\rangle$ and $|\mathbf{k}_\alpha\rangle$ denote the zero and one-photon states, respectively, with $a_{\mathbf{k}\alpha}|\mathbf{0}\rangle=0$ and $|\mathbf{k}_\alpha\rangle=a^\dagger_{\mathbf{k}\alpha}|\mathbf{0}\rangle$. The index X denotes the presence of one or more photons in the channel. Similarly, in the following, the presence of one or more Auger electrons will be denoted by subscript A.

The amplitude for the process (2.1) is given in the distorted wave approximation (DWA) and in the post form by

$$\begin{aligned} T^X_{fX-i}&=\langle\Phi_{fX}|D|\Psi^{\rm tot}_i\rangle \ , \\ T^A_{fA-i}&=\langle\Phi_{fA}|V_f|\Psi^{\rm tot}_i\rangle \ , \end{aligned} \tag{2.9}$$

where $\Psi^{\rm tot}_i$ is the solution for the full Hamiltonian $H_{\rm tot}$. In terms of the projection operators for the initial projectile state P_i and its complement Q_i, we have,[16] with $P_i+Q_i=1_i$,

$$\begin{aligned} \Psi^{\rm tot}_i&=P_i\Psi^P_i-(Q_iF_{\rm tot}Q_i)^{-1}F_{\rm tot}P_i\Psi^{\rm tot}_i \\ &=P_i\Psi^P_i-G^{{\rm tot},Q}F_{\rm tot}P_i\Psi^P_i \ , \end{aligned} \tag{2.10}$$

where $F_{\rm tot}\equiv E-H_{\rm tot}$ and $P_iF_{\rm tot}P_i\Psi^P_i=0$. It was shown previously[16] that the full Green's function $G^{{\rm tot},Q}$ may be expanded as

$$\begin{aligned} G^{{\rm tot},Q}&\equiv Q_i(F_{\rm tot})^{-1}Q_i \\ &=G^\Gamma+G^\Gamma WG^\Gamma+\cdots \ , \end{aligned} \tag{2.11}$$

where

$$G^\Gamma=[Q_i(F+i\Gamma^{\rm op}_a/2+i\Gamma^{\rm op}_r/2)Q_i]^{-1} \ , \tag{2.12}$$

and where W is the residual interactions not contained in G^Γ, and $F\equiv E-H$. In Eq. (2.12), $\Gamma^{\rm op}_a$ and $\Gamma^{\rm op}_r$ are the Auger and radiative widths operators.[16] Note that $(Q_iF_{\rm tot}Q_i)^{-1}\neq Q_i(F^{-1}_{\rm tot})Q_i$. Thus T^X_{fX-i} of (2.9) may be rewritten as

$$\begin{aligned} T^X_{fX-i}&=\langle P_f\Psi^P_{fX}|D|P_i\Psi^P_i\rangle+\langle P_f\Psi^P_{fX}|DG^\Gamma V_i|P_i\Psi^P_i\rangle \\ &\quad+\langle P_f\Psi^P_{fX}|DG^\Gamma WG^\Gamma V_i|P_i\Psi^P_i\rangle+\cdots \\ &\equiv T^{\rm REC}_{fX-i}+T^{\rm TEX}_{fX-i}+T^{\rm cascade}_{fX-i} \ . \end{aligned} \tag{2.13}$$

[The algebra involved in the derivation of Eqs. (2.10)–(2.13) is straightforward and we simply refer to Ref. 16 for the details.] The first term in Eq. (2.13) corresponds to the direct radiative capture without excitation (REC stands for radiative electron capture), while the second term provides the TE amplitudes of interest here. All the other higher-order terms represent cascade contributions. The third term in (2.13) will be important in the discussion of NTE and UTE amplitudes given in Sec. III.

Obviously a similar description can be given for T^A_{fA-i} by replacing the operator D in (2.13) by V_f; thus we have

$$\begin{aligned} T^A_{fA-i}&=\langle P_f\Psi^P_{fA}|V_f|P_i\Psi^P_i\rangle+\langle P_{fA}\Psi^P_{fA}|V_fG^\Gamma V_i|P_i\Psi^P_i\rangle \\ &\quad+\langle P_f\Psi^P_{fA}|V_fG^\Gamma WG^\Gamma V_i|P_i\Psi^P_i\rangle+\cdots \\ &=T^{\rm ioniz}_{fA-i}+T^{\rm TEA}_{fA-i}+T^{\rm Cascade}_{fA-i} \ . \end{aligned} \tag{2.14}$$

The first term describes the collisional ionization of the target B without electron transfer, and the second term gives the TEA amplitude of interest here. In the next section, we will analyze these two amplitudes TEX and TEA in detail.

It should be noted that in (2.14), both the initial and final state interactions V_i and V_f appear, except in the first term. In particular, the V_i term is essential in correctly describing the three different TE processes in a consistent way. In Ref. 14, however, the interaction V_f appeared on the right with P_i, which does not contain the RTE component corresponding to the interaction V_{12}. The same difficulty occurs with T^X of (2.13), where one then has to put a portion of V_{12} T^X *ad hoc*. This is not consistent and difficult to implement.

III. TRANSFER EXCITATION PROCESSES

The TEX and TEA amplitudes given by Eqs. (2.13) and (2.14) will now be analyzed, with special attention paid to

the resonant mode associated with the Green's function G^{Γ}, in which case these two amplitudes can be treated by an identical procedure. Therefore, in the following, we will derive the result first for TEX, and later convert it to TEA. We denote the initial and final distorted wave functions $P_i\Psi_i^P$ and $P_f\Psi_f^P$ simply by Φ_i and Φ_f. Noting that

$$V_i = V_{12} + V_{b1} + V_{13} + (V_{a2} + V_{a3} + V_{ab} - U_i)$$

from (2.6), we have

$$\begin{aligned} T_{fX-i}^{\mathrm{TEX}} &= \langle \Phi_{fX} | DG^{\Gamma} V_i | \Phi_i \rangle \\ &= T^{\mathrm{RTEX}}(V_{12}) + T^{\mathrm{NTEX}}(V_{b1}) \\ &\quad + T^{\mathrm{UTEX}}(V_{13}) + \cdots . \end{aligned} \tag{3.1}$$

We analyze below in some detail the amplitudes for the three processes, RTE, NTE, and UTE. In order to bring out clearly the difference between RTE and UTE, we explicitly assumed in (3.1) that electron 2 is transferred from B to A, while electron 1 in A is excited. Therefore the potentials in the brackets in (3.1) denote the interactions that cause the initial excitations.

A. Resonant transfer excitation

We first analyze the resonant mode of the TE amplitude mediated by V_{12} in V_i,

$$T_{fX-i}^{\mathrm{RTEX}} = \langle \Phi_{fX} | DG^{\Gamma} V_{12} | \Phi_i \rangle \tag{3.2}$$

where Φ_i and Φ_{fX} are given by Eq. (2.8). The Green's function G^{Γ} of Eq. (2.12) may be separated into two parts by convolution[16]

$$G^{\Gamma} = \frac{i}{\pi} \int g_{A'B'}(E-\eta) G_{12}^{\Gamma}(\eta) d\eta , \tag{3.3}$$

where

$$\begin{aligned} g_{A'B'}(E-\eta) = (E - \eta - K_{A'B'} - K_{b3} - V_{a3} - V_{13} - V_{23} \\ - V_{ab} - V_{b1} - V_{b2} - V_{b3})^{-1} \end{aligned}$$

and

$$\begin{aligned} G_{12}^{\Gamma} = (\eta - K_{a1} - K_{a2} - H_R - V_{a1} - V_{a2} - V_{12} \\ + i\Gamma_a^{\mathrm{op}}/2 + i\Gamma_r^{\mathrm{op}}/2)^{-1} . \end{aligned}$$

This particular separation of G into the purely electronic part corresponding to the system A' and the rest of the ionic part is convenient for the discussion of the RTE amplitude, where the ionic core b and electron 3 assume the spectator role. Note also that we chose the Hamiltonian H of the form $H_{\mathrm{tot}} = H_f + V_f + D$ for the intermediate states d, since electron 2 is transferred to the core a by V_{12} during the excitation transition $i \to d$. A slightly different separation of G^{Γ} will be introduced for the NTE and UTE amplitudes, because the nuclear core b and electron 3 play a more crucial role there. The final projection in (3.1) puts the ionic core states of G^{Γ} on energy shell, so that we have effectively

$$G^{\Gamma} \sim G_{12}^{\Gamma}(E_e')\delta , \tag{3.4}$$

where

$$\delta(E' - K_{A'B'} - U_f) = \sum_{f'} |u_{f'}\rangle\langle u_{f'}| ,$$

and $E \equiv E' + E_e'$ for the ions and the electrons, respectively. Finally, we then have

$$\begin{aligned} T_{fX-i}^{\mathrm{RTEX}} \approx \sum_d \langle \psi_{A'}; \mathbf{k} | D | \varphi_{A'}; \mathbf{0} \rangle \frac{1}{E_e' - E_d' + i\Gamma/2} \\ \times \langle \varphi_{A'} | V_{12} | \psi_a u_c \rangle . \end{aligned} \tag{3.5}$$

This amplitude describes the process in which one of the target electrons excites the projectile and at the same time the same electron is captured by the projectile, thus forming an intermediate state of doubly excited resonance state. Subsequently, this state will decay by emitting radiation (or Auger electrons.)

Following Brandt,[15] the RTE cross section in impulse approximation is given by

$$\sigma_i^{\mathrm{RTEX}} \equiv \sum_f \sigma_{fX-i}^{\mathrm{RTEX}} \cong \sum_d W_B(p_z) \bar{\sigma}^{DR}(i \to d) \frac{\Delta e_c}{K_i} , \tag{3.6}$$

where the target Compton profile W_B is defined by

$$W_B(p_z) \equiv \int dp_{\perp} |\tilde{\psi}_B(\mathbf{p})|^2 . \tag{3.7}$$

In Eq. (3.6) the RTE cross section is defined in terms of the DR cross section which is given in the form

$$\sigma^{\mathrm{DR}}(i \to d) = \frac{4\pi}{e_c(\mathcal{R})} V_a(i \to d) \omega(d) \tilde{\delta}(e_c)(\pi a_0^2) , \tag{3.8}$$

where V_a and $\omega(d)$ are the excitation-capture probabilities and fluorescence yields, respectively;

$$\begin{aligned} &V_a(i \to d) = (g_d/2g_i) A_a(d \to i) \quad \text{by detailed balance} \\ &\omega(d) = \Gamma_r'(d)/[\Gamma_a(d) + \Gamma_r(d)] \end{aligned} \tag{3.9}$$

for the statistical weights g_d and g_i, A_a is the Auger transition probability for the intermediate state d decaying to the particular final state f, and Γ_r and Γ_a are the radiative and Auger widths of the level d. The resonance profile $\tilde{\delta}$ is given by

$$\tilde{\delta} = \frac{\Gamma/(2\pi)}{(E_e' - E_d')^2 + \Gamma^2/4}, \quad \int \tilde{\delta}\, de_c' = 1 . \tag{3.10}$$

Here $E_e' = e_{a1} + e_c$ for the initial state binding energy of electron 1 and the kinetic energy of electron 2 in the projectile rest frame.

Usually, there are many intermediate resonance states (d) which are available for the TE processes. In the isolated resonance approximation,[16] we can simply group them together in small energy bins as[17]

$$\bar{\sigma}^{\mathrm{DR}}(i \to d) = \frac{1}{\Delta e_c} \int_{e_c - \Delta e_c/2}^{e_c + \Delta e_c/2} \sigma^{\mathrm{DR}}(i \to d)\, de_c' . \tag{3.11}$$

Here, Δe_c is a small energy bin chosen arbitrarily. We note that the projectile energies E_L in the laboratory frame can be very large, ~ 100 MeV, such that the electron energies of the target system in the projectile rest frame match the kinetic energies e_c involved in DR. The actual E_L near the resonances can have a large spread

due to the Compton profile.

In exactly analogous way, we have the amplitude for the resonant TEA process in which the resonant state (d), formed as in RTEX of (3.5), now decays by an Auger electron emission. The cross section is then simply given by

$$\sigma_i^{\mathrm{RTEA}} \cong \sum_d W_B(p_z)\bar{\sigma}^{\mathrm{REA}}(i \to d)\frac{\Delta e_c}{K_i} \tag{3.12}$$

where $\bar{\sigma}^{\mathrm{REA}}(i \to d)$ is the energy-averaged resonant excitation cross section

$$\sigma^{\mathrm{REA}}(i \to d) = \frac{4\pi}{e_c(\mathcal{R})} V_a(i \to d)\xi(d)\tilde{\delta}(E_e' - E_d)(\pi a_0^2) ,$$

with the Auger yield ξ defined by

$$\xi(d) \cong 1 - \omega(d) = \Gamma_a'(d)/\Gamma(d) .$$

The form (3.13) was used earlier[18] in the analysis of the O^{5+} data.[19]

B. Nonresonant transfer excitation.

Unlike in the RTE process where one single electron does the exciting as well as the transfer, an alternate mode which can produce the same intermediate state is possible; that is, the target core b can excite the projectile, while one of the target electrons can be transferred. This mode is termed NTE. From Eq. (3.1), the NTE amplitude is given by

$$T_{fX-i}^{\mathrm{NTEX}} = \langle \Phi_{fX} | DG^{\Gamma} V_{b1} | \Phi_i \rangle . \tag{3.14}$$

Obviously, core b plays a crucial role in exciting electrons in the projectile A, so that the separation of G^{Γ} into two parts as was done in Eq. (3.3) is not convenient for the present purpose. For NTE (and later for UTE), we do not have the usual resonance energy constraint of the type present in RTE. Instead, the NTE amplitude may be analyzed in terms of G^{Γ} as[16]

$$G^{\Gamma} \cong \frac{i}{\pi}\int g_3(E-\eta)G_{b1}^{\Gamma}(\eta)d\eta , \tag{3.15}$$

where

$$g_3 = (E - \eta - K_{b3} - V_{b3} - V_{a3} - V_{13} - V_{23} - V_{2b} - V_{ab})^{-1} ,$$

$$G_{b1}^{\Gamma} = (\eta - K_{A'b} - K_{a1} - K_{a2} - V_{a1} - V_{a2} - V_{12} - V_{b1} - H_R + i\Gamma^{\mathrm{op}}/2)^{-1} .$$

The difference between (3.16) and (3.3) is mainly in the kinetic energy term in G_{b1}^{Γ}. With the final state projection by Φ_{fX}, we have

$$G^{\Gamma} \sim G_{b1}^{\Gamma}\delta' . \tag{3.16}$$

Further reduction of $G_{b1}^{\Gamma}(E)$ is given by

$$G_{b1}^{\Gamma} \approx (2\pi)^{-3/2}\int e^{-i\mathbf{K}'\cdot(\mathbf{R}_{A'b}' - \mathbf{R}_{A'b})}d\mathbf{K}'G_{12}^{\Gamma} , \tag{3.17}$$

which essentially contains the same G_{12}^{Γ} used in RTE. We finally have

$$T_{fX-i}^{\mathrm{NTEX}} \approx \langle \Phi_{fX} | DG_{b1}^{\Gamma} V_{b1} | \Phi_i \rangle . \tag{3.18}$$

Thus

$$T_{fX-i}^{\mathrm{NTEX}} \approx \sum_d \int d\mathbf{p}\,\tilde{\psi}_B(\mathbf{p})\langle \psi_{A'};\mathbf{k}_\alpha | D | \varphi_{A'};\mathbf{0}\rangle \frac{1}{E_e' - E_d' + i\Gamma/2}\cdot\langle \varphi_{A'} e^{i\mathbf{K}_f\cdot\mathbf{R}_{A'b}} | V_{b1} | \psi_A e^{i\mathbf{p}\cdot\mathbf{r}_{b2}} e^{i\mathbf{K}_i\cdot\mathbf{R}_{AB}}\rangle , \tag{3.19}$$

where the crucial term is the one with V_{b1}. It contains both the excitation and transfer; that is, the excitation via V_{b1} and the capture by the overlap of $\psi_{A'2}$ in $\varphi_{A'}$ and the continuum electron wave function contained in $\exp(i\mathbf{K}_i\cdot\mathbf{R}_{AB})$. Since the projectile ion is charged, its effect on the electronic wave functions for electron 2 in B in the initial state cannot be ignored; we set

$$e^{i\mathbf{K}_i\cdot\mathbf{R}_{AB}} = e^{i\mathbf{K}_i\cdot\mathbf{R}_{A'b} + i\mathbf{k}_i\cdot\mathbf{r}_{2a}} \to e^{i\mathbf{K}_i\cdot\mathbf{R}_{A'b}} u_c(\mathbf{r}_{2a})$$

where u_c is the distorted continuum function. [The same procedure was followed in the case of RTE in Eq. (3.6) when we replaced the RTE amplitude in terms of the corresponding DR amplitude.] Using a product form of the wave function, the V_{b1} dependent part of the T^{NTEX} can be written as

$$\langle \psi_{A'2} | e^{i\mathbf{p}\cdot\mathbf{r}_{2a}} | u_c \rangle \cdot \langle \psi_{A'1} | \tilde{V}_{b1}(\mathbf{Q}-\mathbf{p},\mathbf{r}_{1a}) | \psi_{A1}\rangle \equiv C_e \cdot F_N , \tag{3.20}$$

where

$$\tilde{V}_{b1} \equiv \int d\mathbf{R}_{A'b} e^{i(\mathbf{Q}-\mathbf{p})\cdot\mathbf{R}_{A'b}}(-e^2 Z_b)|\mathbf{r}_{1a} - \mathbf{R}_{A'b}|^{-1} .$$

The NTEX cross section is then given by

$$\sigma^{\mathrm{NTEX}} = \left[\frac{\mathcal{M}}{2\pi}\right]^2 \frac{2\pi}{K_i^2}\int_{Q_{\min}}^{Q_{\max}} |T^{\mathrm{NTEX}}|^2 Q\,dQ \quad (\text{a.u.}) , \tag{3.21}$$

where

$$\mathbf{Q} = \mathbf{K}_i - \mathbf{K}_f, \quad \mathcal{M} = M_A M_B/(M_A + M_B) ,$$

$$Q_{\min} \cong \frac{\Delta}{2E_i}K_i, \quad \Delta = e_{a1}' - e_{a1} - e_{b2}$$

$$Q_{\max} \cong \infty ,$$

and thus

$$|T^{\mathrm{NTEX}}|^2 \approx 4\sum_d \omega(d)\int_0^{\infty} W_B(p)|C_e(p)|^2|F_N(Q,p)|^2 dp . \tag{3.22}$$

In general, for a neutral target B, $Z_b \gtrsim 1$. Preliminary calculation for the Si^{11+} + He case indicated that the cross section given by (3.21) is of right order of magnitude, with only a few low-lying states included.[20] A similar result was obtained earlier for the S^{13+} + He system.[21] A more detailed calculation is in progress. The NTE cross sections are generally peaked at low E_L and decreases as E_L is increased, because the capture probability decreases with increasing energy while the excitation probability increases sharply at threshold and then levels off at higher energies. The NTE contribution can be sizable in the energy region where RTE is dominant and the RTE-NTE interference effect can also be studied.

In most cases, the C_e factor in (3.20) turned out to be very sensitive to the orthogonality of $\psi_{A'2}$ and u_c, especially for p very small. To avoid this problem, we have rewritten C_e as

$$\langle \psi_{A'2}|e^{i\mathbf{p}\cdot\mathbf{r}_{2a}}|u_c\rangle \rightarrow \sum_{c'}\left\langle \psi_{A'2}\left|\frac{z'}{r_{2a}}\right|c'\right\rangle \frac{1}{E_{A'2}-E_{c'}} \times\langle c'|e^{i\mathbf{p}\cdot\mathbf{r}2a}|c\rangle$$

$$\approx\left\langle \psi_{A'2}\left|\frac{Z'}{r_{2a}}e^{i\mathbf{p}\cdot\mathbf{r}_{2a}}\right|c\right\rangle \times\frac{1}{E_{A'2}-\bar{E}_c}\equiv C_e' ,$$

where the Schrödinger equation for the bound state is used, as

$$|\psi_{A'2}\rangle \equiv G_{A'2}\left[\frac{Z'}{r_{2a}}\right]|\psi_{A'2}\rangle$$

and where the closure approximation was introduced for the Green's function $G_{A'2}$. This expression for C_e' is much less sensitive to the distortion of u_c. It is important to note here that the change C_e to C_e' in (3.19) is also obtained by going to one higher-order term in (2.13); the term with two G^Γ's in (2.13) gives the same C_e' when appropriate approximations are introduced in G^Γ and W.

The excitation probability F_N can be calculated using Born approximation for the nuclear motion of core b relative to core a. However, at low energies where the relative velocity v_c is lower than that of a typical orbital velocity of the electrons v_e in A (or more appropriately $e_c < \Delta_{fi}$ = transition energy for inelastic scattering, where e_c is the relative kinetic energy of an electron in B) the adiabatic correction has to be introduced; no excitations are possible if the perturber a moves too slowly. This is similar to corrections to impulse approximations. We thus have

$$F_N \rightarrow F_N' \approx F_N \exp(-\Delta_{fi}/e_c) .$$

This correction turned out to be important in getting the NTE peak at low energies to come out correctly. Details of the calculation are planned to be given elsewhere.

C. Uncorrelated transfer excitation

Since there are two electrons (e_2 and e_3) present in our model (2.1), it is also possible to have these two electrons to create the same intermediate state as in RTE and NTE; here e_3 assumes the role of core b in the NTE process and may excite the projectile A, while e_2 can be transferred. Thus the physical picture involved here is very much like that in NTE. However, the excitation by e_3 now requires a minimum incoming kinetic energy, as in any other excitation process, unless there is a strong correlation between e_3 and b. This in turn dictates the threshold energy for this mode to occur at energies just above the RTE peak. The UTE amplitude may be written, from Eq. (2.8), in an analogous way to the NTE amplitude, as

$$T^{\mathrm{UTEX}} = \langle \Phi_{fX}|DG^\Gamma V_{13}|\Phi_i\rangle , \tag{3.23}$$

where

$$G^\Gamma \approx \frac{i}{\pi}\int g_{ab}(E-\eta)G^\Gamma_{123}(\eta)d\eta , \tag{3.24}$$

with

$$g_{ab} = (E-\eta-K_{A'b}-V_{b1}-V_{b2}-V_{b3}-V_{ab}-V_{23}-V_{a3})^{-1}$$

and

$$G^\Gamma_{123} = (\eta-K_{a1}-K_{a2}-K_{a3}-V_{a1}-V_{a2}-V_{12} -V_{13}-H_R+i\Gamma^{\mathrm{op}}/2)^{-1} .$$

This can further be simplified as

$$G^\Gamma \approx G^\Gamma_{123}\delta'' \approx G^\Gamma_{12}g_3 ,$$

where

$$g_3 \approx (e_c-K_{a3}-\bar{V}_{A3}+i\epsilon)^{-1}, \quad \bar{V}_{A3} = \langle V_{a3}+V_{13}\rangle .$$

The corresponding cross section is then given by

$$\sigma^{\mathrm{UTEX}} \approx \frac{1}{2\pi k_i^2}g\int_{q_{\min}}^{q_{\max}}|T^{\mathrm{UTEX}}|^2 q\,dq(a_0^2) , \tag{3.25}$$

where

$$q_{\min} = k_i - k_f \quad \text{(for electron 3)} ,$$

$$q_{\max} \cong \infty ,$$

and

$$|T^{\mathrm{UTEX}}|^2 \approx 4\sum_d \omega(d)\int_0^\infty W_B(p)W_B(q,p)|C_e(p)|^2 \times|F_e(q,p)|^2dp , \tag{3.26}$$

where we assumed again that q is nearly perpendicular to $\mathbf{p}_z$ ($=p$ here). F_e is the collisional excitation amplitude, analogous to F_N in Eq. (3.20). The capture part C_e is the same as that used in NTE, and may be replaced again by C_e'. As noted above, from energy conservation, the UTE process should have the threshold at the ionization limit ($n=\infty$) of the RTE process, provided electrons 2 and 3 are not correlated and if we neglect their binding energies initially in B. (For the correlated case, however, we ex-

pect an enhancement of the RTE-type cross sections by the contribution of the UTE mode at lower energies.)

In actual applications, the distortion effect of the two electrons in B by the projectile field of a is very important, and we may conveniently replace (3.25) by

$$\sigma_{i\to d}^{\mathrm{UTE}} \approx \frac{4\pi}{k_c^2}\frac{g_d}{2g_i}\tau_0 \int dp\, W_B\, A_e(d'\to i)\omega(d)|C_e'|^2(\pi a_0^2)\ , \tag{3.27}$$

where the capture probability $|C_e'|^2$ is identical to that in the NTE case, while A_e is an analytic continuation of the Auger probability A_a, in which one of the bound state electrons is placed in the continuum with energy e_c', thus the excitation probability A_e. This is the same as the quantum defect theory procedure, and our MATRIX code easily handles its evaluation. The intermediate state d finally formed involves the excited state d' of A plus one of the electrons in B captured to A in order to form A'. Another electron 3 in B is "in the continuum" as seen in the A' rest frame; this electron 3 may still be bound to b or may be free.

IV. APPLICATIONS

We briefly summarize the current status of the TE measurements and theoretical analyses which have been carried out.

(i) RTE. For the latest experimental review, we refer to Tanis paper[1] on RTEX, where the states (d) formed in RTE decay by x-ray emissions. The following ions have been studied: Si^{11+}, S^{13+}, Ca^{10-19+}, and V^{19-22+} in which the $1s$ electron excitation was involved, and Nb^{31+} in which the L-shell electron excitation of the Ne-like system was measured. The theoretical interpretation of these systems in terms of DR was given in a series of publications.[5,16] More recently, some additional ionic systems were studied; $Ge^{29,31+}$, S^{15+}, and $F^{6,8+}$. In all cases, the agreement between theory and experiments were excellent, all at the level of $\pm 10\%$ or better. In addition, a state-by-state RTE was also studied[19] in which the Auger electrons emitted during the stabilizing stage of the states d were detected (RTEA). The theoretical analysis[18] provided reasonable ratios for the various resonance peaks corresponding to different term-split states of d, but improved measurements as well as more refined theoretical calculations of the Auger transition probabilities are needed to bring the RTEA process under control. Very recently, an additional way of measuring the RTE was proposed,[20] in which two x rays emitted during the decay of the states d were detected in coincidence. Theoretical analysis of this process requires however somewhat different cascade sequences than that for the RTEX or DR type, so that RTEX provided a new insight into the DR-like cascade process.[21] Considering the difficulty of measuring such double coincidence x rays, the agreement was excellent in the energy dependence of the cross section peaks as well as their overall magnitudes.

(ii) NTE. There are two explicit experiments reported on the NTEX, for the projectile systems Si^{11+} and S^{13+}, on the He and H_2 targets.[2,3] Preliminary analysis was reported,[12,22,23] which gave the correct energy dependence of the cross section but not its magnitude. The NTE process is dominant for lighter projectile ions, such as He,[24] where the NTE and RTE peaks often overlap, and their interference effect can be sizable. An attempt is being made to provide a more realistic theoretical estimate of this process at low energies using a coupled-channel approach,[25] but it would be more difficult to carry out such calculations for complex systems with many electrons and at high energies. Preliminary result of our calculation gives a cross section maximum of the order of 10^{-21} cm^2, which is consistent with the observed data. A more detailed analysis is in progress.[22,23]

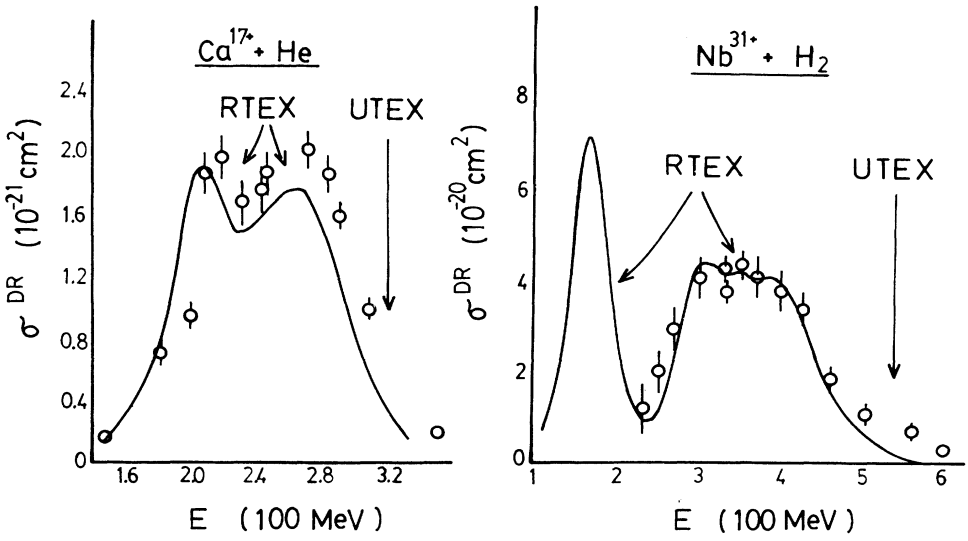

FIG. 2. Evidence for the presence of the UTE process is indicated. The experimental points are from Refs. 1 and 2, while the theoretical curves are taken from Ref. 5.

(iii) UTE. As noted in Sec. I, in the course of the analysis of the RTE process in S^{13+}, Ca^{17+} and Nb^{31+}, it was found that[1,11] the experimental data consistently showed a large shoulder on the high-energy side of the RTEX peak corresponding to the *KLM*, *KLN*, etc., transitions, where there were no apparent resonance contributions expected (Fig. 2). As a possible explanation of this anomaly, the effect of the core field of *B* on the RTEX cross section was estimated,[11] with negative result. The reason for this was due to the presence of an additional strong Auger channel of the type *KLL* involving the original 2*s* spectator electron in the Li-like projectile. The *KMM* and *KMN* excitation modes also contribute in the high-energy tail region, but again because of the additional cascade Auger channels present, which are of the types *LMM*, *LMN*, etc., their effect is expected to be small, even with possible field enhancement. Subsequently, a new process UTE was proposed to explain this phenomena.[26] More recently, the experimental group at Oak Ridge National Laboratory (ORNL) has seen a similar phenomenon[13] in the F^{6+} + He and F^{8+} He systems. Theoretical effort to treat this process in detail is underway, along with the NTE work.

In all three modes considered above, the actual calculation requires extensive numerical work, because of a large number of intermediate states which contribute to the total cross section. For RTE, we have already set up a detailed DR-type code plus a folding subroutine for the Compton profile for different target systems. Recently, we have modified this code to handle the problems specific to the NTE and UTE cases. Some preliminary results have already been obtained for the Si and S projectiles on He and H_2, for which earlier experimental data are available. A detailed report of this result is planned to be given later.[23]

V. DISCUSSION

Ion-atom and ion-molecular collisions at high energies leading to RTE, NTE, and UTE are not only of intrinsic interest as the first multistep charge exchange process, but can also provide valuable information on the DR and other related processes where often the cross sections are too small for direct measurements. The relationship between the ion-atom and electron-ion collisions in a unified treatment[16] can be useful in correlating various scattering data. Thus RTEA versus resonant scattering, RTEX versus DR, and inner-shell excitation Auger decay (ISEA) versus excitation-Auger ionization in electron-ion collisions, are some of the examples.[16] Many of these processes can be analyzed using the same Green's functions and the same folding procedure. In particular, the UTE amplitude is closely related to that for the NTE. We are dealing here essentially with a five-body problem and focusing on a complicated set of processes requiring second- and third-order amplitudes; the theory is very complicated and requires many drastic approximations. The final form of the theory presented here seems to correctly reflect the basic physics involved and describe the all three modes of TE in a unified way.

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