# Influence of Nuclear Reactions on Electron Transfer in Energetic Ion-Atom Collisions

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The influence of inelastic nuclear scattering on atomic charge transfer in asymmetric ion-atom collisions is described within a new theory, combining a two-channel model for the nuclear reaction with the impulse approximation for electron capture by the projectile. Test calculations of the capture probability during the reaction $^{18}O(p,\alpha)^{15}N$ indicate that inelastic nuclear reactions are a more transparent probe for the atomic transition amplitudes than elastic resonances.

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The interplay between nuclear reactions and atomic excitation or rearrangement manifests itself in an interference structure of the atomic transition probabilities, because the transiently formed compound nucleus causes a time delay between the atomic amplitudes for the incoming and the outgoing parts of the collision. The investigation of atomic transitions during resonant nuclear scattering can therefore serve as an atomic clock for nuclear reaction times, but also as a stringent test for atomic models due to the sensitivity to phase differences, provided the energy $\Delta E$ transferred to the active electron is comparable with the nuclear decay width $\Gamma$.

Investigations concerning the influence of an elastic nuclear resonance on inner-shell ionization[1-5] and electron capture[6,7] have established the existence of pronounced interference structures. Inelastic nuclear resonances, with their additional wealth of possibilities to probe half-trajectory transition amplitudes and isotope or recoil effects, have the advantage, compared to elastic resonances, that the absence of the Coulomb contribution to the scattering amplitude reduces the number of nuclear interference terms, and hence allows for a much clearer display of the interference effects from the atomic partial amplitudes. An extension of the theoretical models to allow for nuclear reactions has been attempted[8] in the case of ionization by means of a simple generalization of the Blair-Anholt formula,[1] followed by a more rigorous formulation of the first Born theory within a two-channel approach for the nuclear reaction.[9]

Electron transfer is a more promising candidate than ionization to be probed during nuclear reactions in energetic ion-atom collisions, since the transferred energy $\Delta E$ is larger than that for ionization, such that shorter nuclear lifetimes become accessible. Also, for ionization the interference effects are weakened by the energy distribution of the ejected electrons, whereas $\Delta E$ is sharp in the case of capture. On the other hand, there is a need for a sensitive test of the current atomic capture theories. For large-angle scattering in asymmetric collisions, the most advanced theory is the strong-potential Born (SPB) approximation,[10,11] which is, however, only tractable in combination with a rather restrictive peaking approximation.[7] This so-called full-peaking approximation, where the momentum transfer is kept fixed during the collision, is in some cases in severe disagreement with experimental data at backward angles.[12]

The on-shell limit of the SPB theory, the impulse approximation (IA), is more readily accessible to less restrictive peaking approximations.[11] While it is commonly considered inferior to the SPB theory, it has recently been shown[13] that, at least for small scattering angles, a correct incorporation of the channel distortion by the second collision partner brings the SPB theory into close agreement with the IA. In its fully peaked version, the IA has already been applied to capture at large scattering angles in the absence of a resonance.[14]

In this Letter, we improve upon the description of electron transfer by evaluating the IA in the less restrictive transverse-peaking approximation which allows for a variation of the momentum transfer along the direction of the ejectile. The transverse-peaked IA provides a much better representation[15] of the angular and energy dependence of experimental capture cross sections than the fully peaked SPB. For inclusion of reactive scattering, the impulse approximation is combined with the two-channel formalism[9] for nuclear reactions in a version which is adapted to the combination with a higher-order atomic theory. Basically, the two-channel model relies on the assumption that the transiently formed compound nucleus decays into two channels, an elastic channel $a$ and an inelastic channel $b$. Correspondingly, the nuclear scattering state with incident momentum $\mathbf{K}_a$ (indices $a$ refer to channel $a$, indices $b$ to channel $b$) is, at asymptotic internuclear distances $R$, represented by

$$\psi_{\mathbf{K}}^{(\pm)\infty}(\mathbf{R}) = \left( e^{i\mathbf{K}_a\cdot\mathbf{R}_a} + A_{aa}^{(\pm)}(K_a,\theta_a)\frac{e^{\pm iK_aR_a}}{R_a} \right)\phi_a + A_{ba}^{(\pm)}(K_a,\theta_b)\frac{e^{\pm iK_bR_b}}{R_b}\phi_b , \quad (1)$$

where $A_{aa}$ is the elastic-scattering amplitude (including the Coulomb amplitude) and $A_{ba}$ is the reaction amplitude.[16]

For each channel, the angle between $\mathbf{K}$ and $\mathbf{R}$ is denoted by $\theta$, and $\phi$ refers to the internal state of the projectile and target nuclei. Assuming orthogonality and completeness of the two-channel functions $\phi_a$ and $\phi_b$, the transition amplitude for capture of a target electron by a light projectile is readily obtained from the generalization of the one-channel case,[7]

$$W_{fi}^{ba}=\int d\mathbf{K}\,d\mathbf{q}\sum_{\lambda=a,b}\langle\tilde{\psi}_f^{(-)}|\psi_{\lambda\mathbf{K}}^{(\sigma)}(\mathbf{R})e^{-\iota\beta\mathbf{K}\cdot\mathbf{r}_T}\mathbf{q}(\mathbf{r}_T)\rangle \times\{\langle\psi_{\lambda\mathbf{K}}^{(\sigma)}(\mathbf{R})e^{-\iota\beta\mathbf{K}\cdot\mathbf{r}_T}\varphi_{\mathbf{q}}(\mathbf{r}_T)|V_P|\tilde{\psi}_i^{(+)}\rangle+\langle\psi_{\lambda\mathbf{K}}^{(\sigma)}(\mathbf{R})e^{-\iota\beta\mathbf{K}\cdot\mathbf{r}_T}\varphi_{\mathbf{q}}(\mathbf{r}_T)|V_N|\tilde{\phi}_i\rangle\}\,, \tag{2}$$

where $\sigma=+$ for $\lambda=a$ and $\sigma=-$ for $\lambda=b$, and $\beta=m/(m+M_T)$ denotes the ratio of electron mass to target mass. The function

$$\tilde{\psi}_i^{(+)}=\psi_{a\mathbf{K}_i}^{(+)}(\mathbf{R})\exp(-\beta\mathbf{K}_{ia}\cdot\mathbf{r}_T)\varphi_i(\mathbf{r}_T)$$

represents the initial state with the internuclear potential $V_N$ included, while

$$\tilde{\phi}_i=\phi_a\exp(i\mathbf{K}_{ia}\cdot\mathbf{R}_a-i\beta\mathbf{K}_{ia}\cdot\mathbf{r}_T)\varphi_i(\mathbf{r}_T)$$

is the initial state without $V_N$. Correspondingly, the final state is given by

$$\tilde{\psi}_f^{(-)}=\psi_{b\mathbf{K}_f}^{(-)}(\mathbf{R})\exp(i\alpha\mathbf{K}_{fb}\cdot\mathbf{r}_P)\varphi_f(\mathbf{r}_P)$$

with $\alpha=m/(m+M_P)$ and $M_P$ the the projectile mass. According to (2), the electron transfer proceeds via ionization from the initial electronic target state $\varphi_i(\mathbf{r}_T)$ to an intermediate target continuum state $\varphi_{\mathbf{q}}(\mathbf{r}_T)$ with momentum $\mathbf{q}$, induced either by the electron-projectile interaction $V_P$ or by nuclear recoil (i.e., $V_N$). The subsequent capture into the bound projectile state $\varphi_f(\mathbf{r}_P)$ is described in terms of an overlap between the free electronic state $\mathbf{q}(\mathbf{r}_T)$ and the final state.

The large differences in the length scales of the nuclear and atomic wave functions allow for the replacement of the nuclear functions by their asymptotic form (1) in the region outside the nuclear interaction radius, $R\gg R_N$ where the $\mathbf{R}$-dependent coupling operators $\hat{A}(\mathbf{R})$ (i.e., the electronic transition matrix elements) collect their dominant contributions. In the interior of the nuclei ($R\lesssim R_N$), on the other hand, $R$ can be set equal to zero in the electronic matrix elements. As a consequence, the nuclear matrix elements are approximated in the following way:

$$\langle\psi_{\lambda\mathbf{K}}^{(\sigma)}(\mathbf{R})|\hat{A}(\mathbf{R})|\psi_{a\mathbf{K}_i}^{(+)}(\mathbf{R})\rangle \approx\langle\psi_{\lambda\mathbf{K}}^{(\sigma)\infty}(\mathbf{R})|\hat{A}(\mathbf{R})-\hat{A}(0)|\psi_{a\mathbf{K}_i}^{(+)\infty}(\mathbf{R})\rangle +\langle\psi_{\lambda\mathbf{K}}^{(\sigma)}(\mathbf{R})|\hat{A}(0)|\psi_{a\mathbf{K}_i}^{(+)}(\mathbf{R})\rangle\,. \tag{3}$$

The electronic transition operators entering into $\hat{A}(R)$ are channel specific when they are related to the asymptotic nuclear states, e.g.,

$$V_P(\mathbf{r}_P)=V_{Pa}(\mathbf{r}_P)\hat{P}_a+V_{Pb}(\mathbf{r}_P)\hat{P}_b\,, \tag{4}$$

where $V_{P\lambda}$ is the electron-projectile interaction in channel $\lambda$ and $\hat{P}_\lambda$ the projection operator onto that channel ($\lambda=a,b$). In the last term of (3) we make the additional assumption that $\hat{A}(0)$ is independent of the nuclear functions such that it can be taken outside the matrix element as in the one-channel case. The remaining overlap $\langle\psi_{\mathbf{K}}^{(\sigma)}|\psi_{a\mathbf{K}_i}^{(+)}\rangle$ is easily evaluated with the help of standard scattering theory.[7,17] The recoil matrix element involving the coupling by $V_N$ can be calculated without the approximation (3) in its on-shell limit which is accurate to the order of $(\Delta K_\lambda/K_\lambda)^2$ (where $\Delta K_\lambda$ is the channel-specific momentum transferred to the electron), and is expressible in terms of $A_{ba}$. As a result, the transition amplitude $W_{fi}^{ba}$ is uniquely determined by the nuclear reaction amplitudes in combination with the electronic matrix elements, without knowledge of the nuclear wave functions inside the nuclear interaction region. For large-angle scattering, only terms linear in the reaction amplitudes need be retained, and the transition amplitude for electron capture during reactive nuclear scattering takes the form (in atomic units, $\hbar=m=e=1$)

$$W_{fi}^{ba}=\frac{1}{(2\pi)^2\mu_b}\left[A_{ba}^{(+)}(K_{fa},\theta)a_{fi}^{(a)}+\int d\mathbf{q}\,a_{fq}^{(b)}A_{ba}^{(+)}(K_{qa},\theta)a_{qi}^{(a)}+a_{fi}^{(b)}A_{ba}^{(+)}(K_{ia},\theta)\right]+W_{fi}^{S}\,, \tag{5}$$

where $\theta$ is the scattering angle (between $\mathbf{K}_i$ and $\mathbf{K}_f$) and $\mu_b$ the reduced mass in channel $b$. Up to minor quantum-mechanical corrections and a common negative sign, $a_{fi}^{(a)}$ and $a_{fi}^{(b)}$ are equal to the semiclassical electron transfer amplitudes in channels $a$ and $b$, respectively, while $a_{qi}^{(a)}$ and $a_{fq}^{(b)}$ are the electronic amplitudes for ionization in channel $a$ and subsequent capture in channel $b$, respectively. Hence, the contributions to $W_{fi}^{ba}$ arise from the following processes: (i) nuclear scattering at the initial energy $E_{ia}$, followed by electron transfer in channel $b$; (ii) ionization in channel $a$ to an intermediate continuum state, subsequent nuclear scattering with the momentum $K_{qa}$ (corresponding to an energy $E_{ia}-\Delta\varepsilon_{fi}+v_b^2/2-\mathbf{q}\cdot\mathbf{v}_b$, where $\Delta\varepsilon_{fi}$ is the difference in the electronic binding energies and $\mathbf{v}_b$ the ejectile velocity), and eventually capture in channel $b$; (iii) electron transfer in channel $a$ and afterwards nuclear scattering at the final momentum $K_{fa}$ (i.e., at the energy $E_{ia}-\Delta E$, where $\Delta E=\Delta\varepsilon_{fi}+v_b^2/2$); and (iv) electron transfer during nuclear contact, denoted by $W_{fi}^S$. This so-called sticking term collects the terms with $\hat{A}(0)$ and is proportional to the difference of the reaction amplitudes. Details of the evaluation will be presented elsewhere.[15] If in Eq. (5)

the indices $b$ are formally replaced by $a$, the one-channel transition amplitude[7] is recovered.

From $W_{fi}^{ba}$, the capture probability as a function of scattering angle is obtained by means of

$$P(\theta)=\frac{(2\pi)^4\mu_b^2(v_b/v_a)N_0|W_{fi}^{ba}|^2}{|A_{ba}^{(+)}(K_{ia},\theta)|^2}, \tag{6}$$

where $v_a$ is the projectile velocity, $N_0$ is the degeneracy of the initial electronic state, and spin summations have been suppressed. The numerator of (6) is equal to the differential capture cross section during the reaction, while $|A_{ba}|^2$ is the nuclear reaction cross section.

As a test case, we have studied electron transfer during the reaction $^{18}O(p,\alpha)^{15}N$ near the isolated $s_{1/2}$ resonance at a proton energy of $E_p=2.363$ MeV.[18] For unpolarized particles, the scattering amplitude for this reaction can be approximated by the Breit-Wigner form[16,17]

$$A_{ba}^{(+)}(K_{ia},\theta)=-\frac{1}{2K_{ia}}(2l_a+1)^{1/2}e^{i(\sigma_a+\sigma_b)}\times\frac{\Gamma_b}{E_{ia}-E_R^{(a)}+i\Gamma/2} \tag{7}$$

if background phases are neglected. In this expression, $l$ is the channel angular momentum, $\sigma$ the corresponding Coulomb phase shift, $\Gamma=\Gamma_a+\Gamma_b$ the total width, and $E_R^{(a)}$ the c.m. resonance energy. As the channel velocities $v_a,v_b$ exceed the target $K$-shell orbiting velocity, electron capture proceeds mainly from the $K$ shell of the target to the $K$ shell of the projectile.

Since the partial widths in channel $a$ and channel $b$ are nearly equal ($\Gamma_a=2.7$ keV, $\Gamma_b=1.6$ keV), we have compared in Fig. 1 the capture cross section at $\theta=150°$ with the result from the elastic channel $^{18}O(p,p)^{18}O$. For both channels, the energy dependence of the capture cross section follows closely to that for the respective nuclear cross section which in the case of the $\alpha$-particle production has a Breit-Wigner shape.

Interference structures emerge only when the ratio of these cross sections, i.e., the capture probability, is calculated. For our test case, the requirement of $\Gamma\sim\Delta E$ is well satisfied ($\Delta E=1.8$ keV for the elastic and 1.6 keV for the inelastic channels), and clear structures are seen in $P(\theta)$. The angular variation of these structures is shown in Fig. 2, and there is a basic difference between the channels $a$ and $b$: For capture in the inelastic channel, $P(\theta)$ has a maximum near the resonance energy which is more pronounced the smaller the scattering angle. In contrast, for channel-$a$ capture the shape of $P(\theta)$ varies strongly with $\theta$ and the excursion of $P(\theta)$ is largest for backward angles. This shape variation in the elastic channel is caused by the interference of the Breit-Wigner scattering amplitude with the Coulomb scattering amplitude which dominates at small $\theta$ and suppresses the effect of the energy dependence of the Breit-Wigner

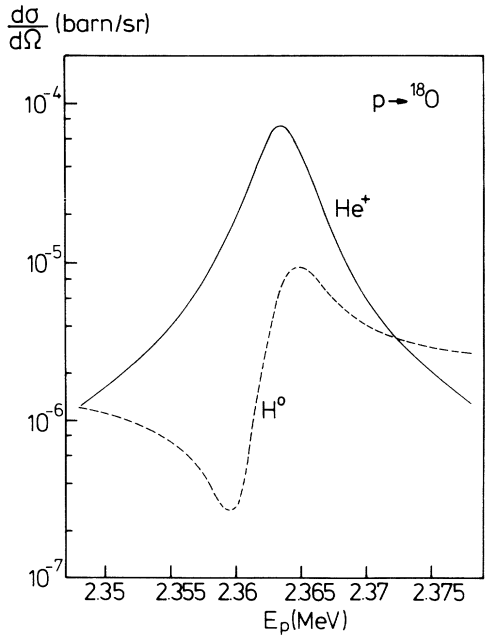


FIG. 1. Cross sections for $K$-shell capture by $He^{++}$ from the $^{18}O(p,\alpha)^{15}N$ reaction and by $H^+$ in the elastic $^{18}O(p,p)$ collision as a function of the proton energy $E_p$ at the scattering angle $\theta=150°$.

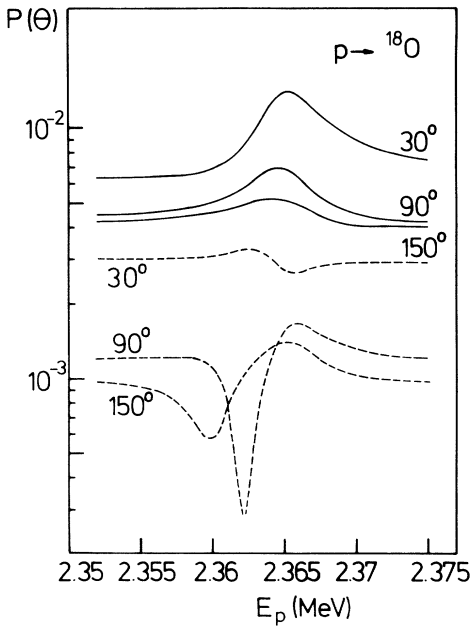


FIG. 2. $K$-shell capture probabilities by $He^{++}$ from the $^{18}O(p,\alpha)^{15}N$ reaction (solid curves) and by $H^+$ in the elastic $^{18}O(p,p)$ collision (dashed curves, multiplied by a factor of 10) across the resonance at 2.363 MeV at three scattering angles, $\theta=30°$, 90°, and 150°. The solid curves are normalized to the inelastic nuclear scattering cross section.

term. The smooth angular dependence of $P(\theta)$ in the inelastic channel is due to the absence of the Coulomb scattering amplitude. The average capture probability by $He^{++}$ lies a factor of 50 above the average $P(\theta)$ for capture by $H^+$, which confirms the approximate scaling of $P(\theta)$ with the fifth power of the nuclear charge.[11]

A pilot investigation of measuring electron capture during a nucleon transfer reaction has been performed by Horsdal Pedersen.[19] The experiment aimed at measuring the angular dependence of the capture probability by the $\alpha$ particles produced in the $^{19}F(p,\alpha\gamma)^{16}O$ reaction. As the resonance energy is as low as 0.873 MeV, the captured electrons originate from all target shells, and to judge from the investigations of elastic resonances,[7] the summation of all shell contributions will reduce the interference structures considerably. In fact, only a rather weak variation of $P(\theta)$ with scattering angle and energy was found, which tentatively was interpreted as being due to the fact that only a single partial amplitude of $W_{fi}^{ba}$ (the one describing electron transfer after the nuclear scattering) gives a large contribution, such that interference effects are suppressed. From the investigation of the reaction $^{18}O(p,\alpha)^{15}N$ we conjecture that this simple interpretation of $P(\theta)$ in terms of a half-trajectory transition probability cannot be supported; in fact, at all scattering angles, the partial amplitudes for electron transfer after the nuclear scattering and for electron transfer before the nuclear scattering are of comparable magnitude. This leads to a considerable dependence of the capture probability on the scattering angle for angles below 90°.

In conclusion, the investigation of electron capture in the $^{18}O(p,\alpha)^{15}N$ reaction (where the criterion $\Delta E \sim \Gamma$ for interference to occur is satisfied) has demonstrated that excursions of the capture probability up to a factor of 2 are found when the projectile energy is varied across the resonance. A more detailed study concerning the influence of the nuclear reaction parameters will be given in a forthcoming paper.[15]

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