Charge Transfer to a Fast Projectile in the Presence of a Nuclear Resonance

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We have developed a distorted-wave strong-potential Born approximation for charge transfer at large scattering angles in asymmetric ion-atom collisions, and applied it to the calculation of electron capture in resonant nuclear collisions. A strong variation of the capture probability across the resonance is predicted.

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During the last few years measurements of atomic ionization probabilities in coincidence with resonant nuclear scattering in asymmetric ion-atom collisions has proved the feasibility of extracting data on nuclear scattering amplitudes from atomic physics experiments,[1-3] and the theoretical understanding of such processes appears to be satisfactory.[4-6] In this Letter we propose an alternative method for studying atomic-nuclear interference phenomena in similar collision systems, namely the measurement of the variation of the electron capture probability across a nuclear resonance. As in the case of ionization, the sensitivity of the process to a nuclear delay time is due to the development of an extra energy phase difference between the capture amplitudes for the incoming and the outgoing parts of the collision, although the details of the capture mechanism are somewhat more involved. Both mechanisms are basically sensitive to nuclear widths Γ which are comparable to the atomic energy transfer ΔE (atomic units $\hbar = e = m_e = 1$ are used throughout),

$$\Delta E \approx \Gamma. \tag{1}$$

However, the energy transfer for a given collision velocity v is different for ionization (I) and capture (C)

$$\Delta E^I = |E_i^T| + E_f, \quad \Delta E^C = |E_i^T| - |E_f^P| + v^2/2, \tag{2}$$

where for definiteness we consider capture from the inner shell of the target, which is taken as the heavy collision partner. E_i^T and E_f^P are the energies of the initial target and the final projectile bound states, respectively. E_f is the energy of the emitted electron. If this electron is not detected, the resonance structure of the ionization probability will be smeared out by the energy distribution of the δ electrons, while the energy transfer for the capture process is well defined. Furthermore, measurements of total ionization probabilities are restricted to $\Gamma \approx |E_i^T|$ according to Eq. (1), while for capture the additional $v^2/2$ allows broader resonances, which are more likely to occur, to be investigated.

The theory for electron capture which corresponds to the first-order perturbation theory for ionization in asymmetric collisions is the strong-potential Born approximation (SPB),[7] or approximations based upon it. This theory has been very successful in explaining experimental results on inner-shell capture by light particles.[8,9] Recently we have shown,[10] using a semiclassical version of the SPB approach, that also for capture at large scattering angles the agreement between theory and experiment[11] is good. But although nuclear resonant scattering has a natural interpretation as a time-delay effect, an appropriate theoretical description should be based on a fully quantal description of the internuclear motion.[1] We have therefore generalized the quantal formulation of the SPB[9] to include distorted waves for the nuclear motion.

As in the plane-wave case, the SPB capture amplitude can be written in terms of an excitation amplitude of the electron in the target system, times an overlap with a moving projectile state:

$$W_{fi} = \int d\vec{K}\, d\vec{q}\, \langle \chi^{(-)}_{\vec{K}_f} \psi_f^P | \chi^{(-)}_{\vec{K}} \vec{q} \rangle \langle \chi^{(-)}_{\vec{K}} \psi^T_{\vec{q}}(\omega) | V_P + V_R | \chi^{(+)}_{\vec{K}_i} \psi_i^T \rangle . \tag{3}$$

Here, V_P is the projectile potential, ψ_i^T is the electronic initial state, $\psi^T_{\vec{q}}(\omega)$ is an off-shell target continuum state of energy $\omega = K_i^2/2\mu + E_i^T - K^2/2\mu$, $\vec{K}_i$, $\vec{K}$, and $\vec{K}_f$ are initial, intermediate, and final relative nuclear

momenta, $\chi_{\vec{K}}^{(+)}$ ingoing and outgoing nuclear scattering states (eigenstates of the internuclear Hamiltonian H_N), $|\vec{q}\rangle$ is an electronic plane wave, and $\mu^{-1}=M_P^{-1}+M_T^{-1}$ with M_P (M_T) the projectile (target) mass. Equation (3) is different from the corresponding plane-wave result[9] in three respects: Firstly, the final electronic projectile state ψ_f^P must incorporate in a nonperturbative way the strong influence of the nuclear collision on an electron bound to the weak potential (projectile recoil). In practice, this can be done by shifting the argument of the projectile momentum-space wave function by the outgoing velocity $(\vec{K}_f/\mu)$ even during the incoming part of the collision.[10,12] Secondly, the recoil of the target atom induces the effective potential $V_R=M_T^{-1}\vec{r}\cdot\nabla_{\vec{R}}V_N$, where V_N is the internuclear potential.[13] Thirdly, the exact inclusion of V_N requires the intermediate states $\chi_{\vec{K}}^{(-)}$ to be *eigenstates* of H_N, reflecting the possibility of nuclear scattering *between* excitation and capture. A more detailed discussion of the derivation of Eq. (3) and its evaluation will be presented elsewhere.[14]

An important simplification in the present situation is that the length scales of the nuclear and the atomic effects are very different. Thus we can assume that there exists a cutoff radius R_N, outside of which the nuclear wave functions have reached their asymptotic values, and where the main contribution to the atomic matrix elements arises.[4,5] In this region we have

$$\chi_{\vec{K}}^{(+)}(\vec{R}) \approx \chi_{\vec{K}}^{as}(\vec{R})=e^{i\vec{K}\cdot\vec{R}}+f(\vec{K},\theta_{\hat{K},\hat{R}})e^{iKR}/R, \quad R>R_N \tag{4}$$

[and $\chi_{\vec{K}(-)}(\vec{R})+\chi_{-\vec{K}}^{(+)*}(\vec{R})$]. Here f is the nuclear scattering amplitude (we use the notation $\hat{a}$ for the direction of $\vec{a}$). Strictly speaking, an additional phase $\sim\ln KR$ should appear in the outgoing wave in Eq. (4), but the effect of such a term is negligible in situations of practical interest.

For resonant nuclear scattering, the projectile will have a large amplitude for being found inside the target nucleus. When $R<R_N$, Eq. (4) cannot be used. However, since $V_P(\vec{r}-\vec{R})$ is a slowly varying function of $\vec{R}$ for $R<R_N$ for all values of $\vec{r}$ that contribute significantly to the electronic matrix elements, one can exploit the orthogonality of $\chi_{\vec{K}'}^{(-)}$ and $\chi_{\vec{K}}^{(+)}$ for $K\neq K'$ to find

$$\langle\chi_{\vec{K}'}^{(-)}|V_P(\vec{r}-\vec{R})|\chi_{\vec{K}}^{(+)}\rangle \approx\langle\chi_{-\vec{K}'}^{as*}|V_P(\vec{r}-\vec{R})-V_P(\vec{r})|\chi_{\vec{K}}^{as}\rangle. \tag{5}$$

The last term of the right-hand side of Eq. (5) is the so-called sticking term,[4,5] which describes the electronic excitation during nuclear contact. The recoil matrix element can be evaluated in a similar manner, by first using the identities $\nabla_{\vec{R}}V_N=[\nabla_{\vec{R}},H_N]=\mu[[\vec{R},H_N],H_N]$. The sticking term is negligible in this case.

With Eqs. (4) and (5), W_{fi} can be evaluated. For large-angle scattering it is sufficient to retain the terms linear in f, corresponding to a single nuclear scattering. Terms involving $\exp[i(K+K')R]$, which describe the projectile backscattering on the *electron,* can also be dropped. The capture amplitude can then be written in the form

$$W_{fi}=W_{fi}^P+W_{fi}^S+W_{fi}^R+R_{fi}. \tag{6}$$

Here the term W_{fi}^P is the contribution arising from $V_P(\vec{r}-\vec{R})$ in Eq. (3), while W_{fi}^R and W_{fi}^S come from the recoil term (involving V_R) and the sticking term, respectively, as in the case of ionization. R_{fi} is a sticking correction to the transfer amplitude, which can generally be neglected. Explicit expressions for W_{fi} when V_P is a Coulomb potential will be given elsewhere.[14] These expressions are still not very well suited for numerical evaluation, however. By virtue of the fact that the electronic momenta (e.g, q) will be small compared to K, K_i, and K_f, the latter can be replaced by K_i unless differences $K-K'$ are involved. In the limit where f is constant on the energy scale of E_i^T, one then finds $W_{fi}^S=R_{fi}=0$, and

$$W_{fi}=-f(K_i,\theta_{\hat{K}_i,\hat{K}_f})a_{fi}/4\pi^2\mu,$$

where a_{fi} is the *semiclassical* capture amplitude in the zero–impact-parameter approximation.[10] At asymptotically large velocities its structure can even be understood classically.[15]

Even if f is not constant, W_{fi} can be evaluated by use of the same approximations as in the semiclassical case, namely replacing the off-shell wave function $\psi_{\vec{q}}^T(\omega)$ by a renormalized Coulomb wave[7-9] and using Briggs peaking approximation, which exploits the fact that ψ_f^P is strongly peaked in momentum space, so that $\vec{q}\approx\vec{K}_f/\mu$. In this approximation the expression for W_{fi}^P can be written as

$$W_{fi}^P\approx a_{ii}f(K_f,\theta)+a_{if}f(K_f',\theta)+a_{ff}f(K_i,\theta). \tag{7}$$

Again, in close analogy to the semiclassical results, the term involving a_{ii} can be identified as the partial amplitude for both excitation of the target and capture before the nuclear scattering, while the terms involving a_{if} and a_{ff} describe the contributions where the excitation takes place before, but capture

after, and both processes after the nuclear scattering, respectively. Accordingly, K_f' corresponds to the final energy reduced by $|E_f^P|$. Thus, while for ionization the time-delay effect is caused by the interference between two amplitudes, corresponding to ionization either before or after the nuclear scattering, in capture we have three, thus enhancing the possibility of seeing interference effects. To these amplitudes we must, as for ionization, add W_{fi}^R and W_{fi}^S which are easily evaluated, while $R_{fi}=0$. If should be noted that the general structure of W_{fi}^P in Eq. (7) can actually be found from the results indicated in Eq. (6), without further approximations.

We have evaluated the transfer probability $P(\theta)=2(2\pi)^4\mu^2|W_{fi}|^2/|f(K_i,\theta)|^2$ $(\cos\theta=\hat{K}_i\hat{K}_f)$ for K-K capture by proton impact in the simplest case of an s-wave resonance, with $f(K,\theta)$ taken to be a Breit-Wigner resonance plus a Coulomb amplitude. As a first test case we have chosen the "classical" resonance in ^{58}Ni at a projectile energy $E_p=3.151$ MeV of width $\Gamma=5.6$ keV. The results for $\theta=90°$ are shown in Fig. 1. $P(\theta)$ increases almost by a factor of 3 at the resonance, compared to about (40–50)% for ionization.[1] Far away from the resonance the present rules are identical to our previous semiclassical ones. Furthermore, our calculations show that the capture process is more sensitive to time-delay effects than total ionization probabilities. To illustrate this increased sensitivity when condition (1) is not well fulfilled, we also made calculations for the hypothetical widths $\Gamma=56$ and 0.56 keV. It is seen that even for the very wide resonance ($\Gamma/\Delta E\approx 5.6$), the time-delay effect is clearly visible on $P(\theta)$. Perhaps more interestingly, for the very long-lived resonance, the effect is as big as for $\Delta E\approx\Gamma$, although it is much narrower in energy. Such a narrow signal would be completely washed out by the width of the δ-electron distribution in a measurement of total ionization probabilities.

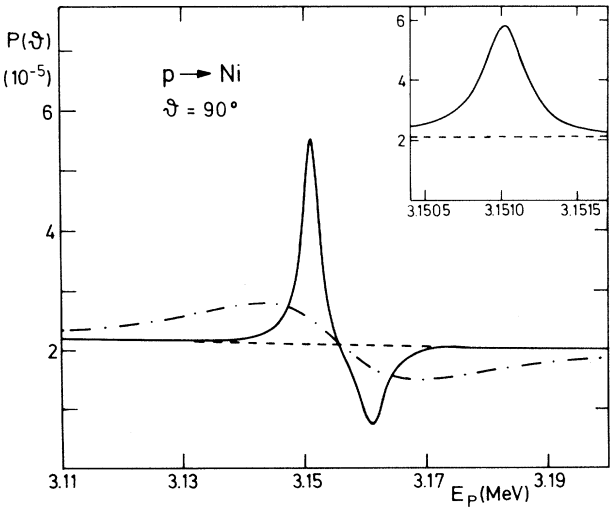

FIG. 1. Capture probability as a function of projectile energy. The resonance width is taken to be 5.6 keV (full curve), 56 keV (dash-dotted curve) and 0.56 keV (inset). Dashed curves denote a semiclassical calculation (without a resonance).

Actually, capture measurements may be difficult with a Ni target. However, calculations on lighter target elements with $s_{1/2}$ resonances (e.g., ^{22}Ne, ^{28}Si) predict signals at least as strong as shown in Fig. 1 for $\theta\gtrsim 90°$ where the Breit-Wigner part in f dominates the Coulomb background. In order to avoid the additional capture from other shells which would involve a smearing out of the signal due to different values of ΔE^C, one has either to do coincidence experiments or to measure systems at a sufficiently high collision energy, where K capture will dominate.[11] As an example of the latter possibility we show in Fig. 2 results for the resonance in ^{12}C at $E_P=462$ keV ($\Gamma=35$ keV). Here, a careful remeasurement found no effect for ionization, in agreement with the theoretical expectations.,[16] In contrast, for capture we predict a distinct signal, although the strong variation of the background may make experimental detection hard. The signal is far from strong enough to explain the reported large effect in an x-ray detection experiment,[17] but it clearly illustrates the increased sensitivity of capture measurements over ionization for time-delay effects.

In the first experiments reporting K-capture probabilities arising from ^{12}C at large scattering angles,[11] also an attempt was made to measure the

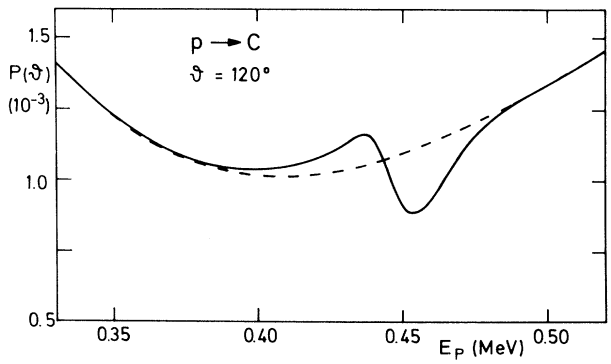

FIG. 2. Capture probability as a function of projectile energy. The full curve implies $\Gamma=35$ keV, the dashed curve a semiclassical calculation (without a resonance).

time-delay effect at the $p_{3/2}$ and $d_{5/2}$ resonances at $E_P \approx 1.7$ MeV with $\Gamma \approx 60$ keV for $\theta = 15°$. However, no effect was seen at this small scattering angle. If we disregard the angular momentum of the resonance, which is not crucial for the qualitative features of the effect, the present theory gives the same results as in the absence of a resonance, since the nuclear scattering amplitude is completely dominated by Coulomb scattering in this case, and is in good agreement with experiment (within 10%).

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