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A time-dependent analysis of transfer ionization in one-dimensional kinematics

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Synopsis We analyze a transfer ionization (TI) reaction in the fast proton-helium collision $H^+ + He \to H^0 + He^{2+} + e^-$ by solving a time-dependent Schrödinger equation (TDSE) under the classical projectile motion approximation in one-dimensional kinematics. By comparing results of the TDSE and various perturbative Born series calculations, we conclude that the recent discrepancies of experimental and theoretical data may be attributed to deficiency of the Born models used by other authors. We demonstrate that the correct Born series for TI should include the momentum space overlap between the double ionization amplitude and the wave function of the transferred electron.

In a recent work [1], we reported calculations of transfer ionization in a fast proton scattering on the helium atom

$$H^+ + He \to H^0 + He^{2+} + e^-$$

for the paramenters of experiments [2, 3]. Our approach is based on the classical approximation for both a nucleus and a projectile and a solution of a time-dependent Schrödinger equation (TDSE) for two electrons in one-dimensional (1D) kinematics. The classical projectile motion approximation (CPA) is very accurate for the present problem because the proton wavelength $\lambda_p \sim 10^{-3}$ a.u. is much smaller than the atom size.

To gain a deeper physical insight into specific mechanisms of the TI reaction, we also performed perturbative 1D calculations which mimicked the plane-wave first Born calculations (PWFBA) performed by other authors [2, 3, 4]. We identified a strong effect of the non-orthogonality of the initial and final states which lead to a spurious unphysical term. This term may be responsible for poor performance of the PWFBA. The authors of Ref. [2, 3, 4] interpreted this term as a first-Born description of the second-Born binary encounter process.

Among various approximate perturbative TI schemes, the results that are closest to the non-perturbative CPA calculations are obtained by the overlap

$$A(k) = \sqrt{2}\int_{-\infty}^{\infty} u_{\rm H}^*(k_1 - v_H) A_{\rm DI1B}(k_1, k) dk_1$$

of the first-Born double ionization amplitude $A_{\rm DI1B}(k_1, k_2)$ with the momentum profile of the final state wave function $u_{\rm H}(k)$ of a fast hydrogen atom. This indicates that the most probable scenario of TI involves double ionization (TIDI) and subsequent capture of those of the ejected electrons which falls into the attractive potential well of the proton by matching its velocity.

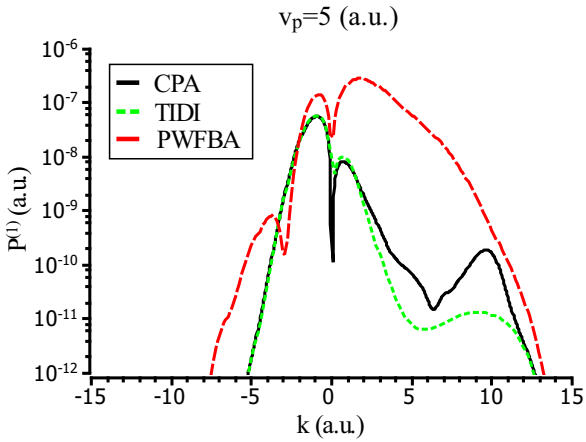

Figure 1. The TI probability density $P^{(1)}(k)$ as a function of the ejected electron momentum for the proton energy $E_p = 630$ keV. Various calculations are displayed with the following line styles: the CPA (black solid line), the PWFBA (red dashed line) and the TIDI (green dotted line).

References

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