Wave-packet continuum-discretisation approach to helium single ionisation by energetic protons

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Synopsis We have developed a wave-packet continuum-discretisation approach for the description of helium structure in the frozen-core approximation. The approach has been applied to calculate helium single ionisation by energetic protons using the convergent close-close coupling method.

We consider differential ionisation of helium by protons. This is a four-body collision problem where the electron-electron correlation of the target can have an effect on the scattering dynamics. We have calculated the fully differential ionisation cross sections (FDCS). The measurements of FDCS have become feasible due to advances in the cold-target recoil-ion momentum spectroscopy (COLTRIMS) technique. From theoretical point of view it is important to develop a model which is accurate and effective in the calculations of differential cross sections. To this end we have developed an approach to the description of the frozen-core helium based on wave-packets. The He wave packets are constructed from the integrals of continuum functions representing the active electron. The continuum functions are obtained by solving the Schrödinger equation for the helium atom numerically. In addition to being orthonormal and applicable to scattering calculations, the wave packets constructed this way provide a flexibility in creating states with arbitrary energies. This greatly simplifies calculations of differential ionisation. A similar wave-packet based description of atomic hydrogen applied for calculations of antiproton-impact ionisation of hydrogen produced excellent results for various differential cross sections in a wide projectile energy range [1].

To test the wave-packet based model of helium target in practice we have incorporated it into the one-centre semiclassical convergent close-coupling (SC-CCC) approach [1] and applied to scattering of energetic protons from helium at incident energies where the electron-capture channel is negligible. In Fig 1 and 2 we show the electron angular dependence of the FDCS for single ionisation of He by 1 MeV protons in the coplanar and azimuthal planes, where the energy of the ejected electrons $E_e = 6.5$ eV and the momentum transfer of the projectile $q = 0.75$ a.u. The present results are compared with the recent experimental data and the first Born approximation (FBA) calculations [2]. Overall good agreement with experiment has been obtained for both geometries considered, except for a slight overestimation of the coplanar plane FDCS above 60° and a slight underestimation of the azimuthal plane FDCS at ejection angles closer to the backward scattering direction.

![Figure 1](image1.png)

**Figure 1.** The FDCS for proton-impact single ionisation of He in the coplanar plane. The experiment and the first Born calculations are due to [2].

![Figure 2](image2.png)

**Figure 2.** The same as in Figure 1, but for the azimuthal plane.

References


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