Distorted-wave impulse approximation for symmetric $(e,2e)$ measurements on helium

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The factorized distorted-wave impulse approximation (DWIA) is used to analyze the momentum profiles of the noncoplanar symmetric $(e,2e)$ transitions from the helium-atom ground state to the He^+ $n=1$ and $n=2$ states. The overlap function used for the calculation of the DWIA cross section is derived from a very accurate configuration-interaction wave function of the helium-atom ground state. The DWIA cross sections provide a better fit to the experimental data than the equivalent plane-wave impulse-approximation cross sections, although when the $n=1$ to (summed) $n=2$ cross-section ratio is depicted, this does not seem to be the case.

The factorized distorted-wave impulse approximation (DWIA) has been successful in calculating relative cross sections for noncoplanar symmetric $(e,2e)$ experiments on argon[1] and xenon.[2] It has been equally successful for a similar experiment on helium,[3] leaving the ion in the $1s$ ground state. The amplitude for all these reactions is dominated by the appropriate target Hartree-Fock (HF) orbital for all the observed ion states, including those fragments of the valence s orbital split by final-state-configuration interaction.

For the $(e,2e)$ reaction on helium, the $n=2$ and $n=3$ ion states have also been observed. The population of these excited states is due to a combination of initial-state-configuration interaction and the nonorthogonality of the helium-atom HF $1s$ orbital and the helium-ion wave functions. A converged configuration-interaction (CI) wave function (in natural orbital form) for the helium-atom ground state[4] was used with the plane-wave impulse approximation (PWIA) to calculate the ratio of the (summed) $n=2$ and $n=1$ cross sections as a function of the recoil momentum q. In this report we examine the use of this wave function in conjunction with the DWIA to compute the $n=1$ and the (summed) $n=2$ cross sections.

The following form for the DWIA was used in the calculation of the triple differential cross section:

$$\frac{d^5\sigma}{d\Omega_1 d\Omega_2 dE_1} = (2\pi)^4 \frac{k_1 k_2}{k_0} f_{ee} \times \Sigma_{\rm av} \, |\langle \chi^{(-)}(\mathbf{k}_1)\chi^{(-)}(\mathbf{k}_2)|\, G_{nl}\chi^{(+)}(\mathbf{k}_0)\rangle|^2 \,. \tag{1}$$

The spin-averaged Mott scattering factor for the two electrons (half off-shell) is denoted by f_{ee}. The incident and outgoing electron momenta are denoted by k_0, k_1, and k_2, respectively, while $\Sigma_{\rm av}$ denotes a sum over final state and an average over initial-state degeneracies. The entrance channel distorted wave, $\chi^{(+)}(\mathbf{k}_0)$ was calculated in the static (plus equivalent local exchange) potential of the helium HF ground state. The distorted waves for the exit channels $[\chi^{(-)}(\mathbf{k}_1), \chi^{(-)}(\mathbf{k}_2)]$ were calculated in the static exchange potentials appropriate to the $1s$, $2s$, and $2p$ ion states. The overlap of the helium and helium-ion wave functions $G_{nl}(r)$ was determined from a very accurate CI expansion[4] (giving 98.6% of the correlation energy) of the helium-atom ground state. The systematic nature of this calculation (within the scope of the PWIA) clearly demonstrated that the overlap functions had converged to within 1% (for recoil momentum, q, less than 3.0 a.u.) and could not be the source of any discrepancy of the PWIA with experiment.

Results of the calculations for the $n=1$ and summed $n=2$ momentum profiles are shown in Fig. 1. The DWIA result for the transition to the ion ground state [Fig. 19(a)] is clearly an improvement over the corresponding PWIA result. These results for the momentum profiles are almost identical to those obtained using the helium-atom HF wave function to compute the overlap

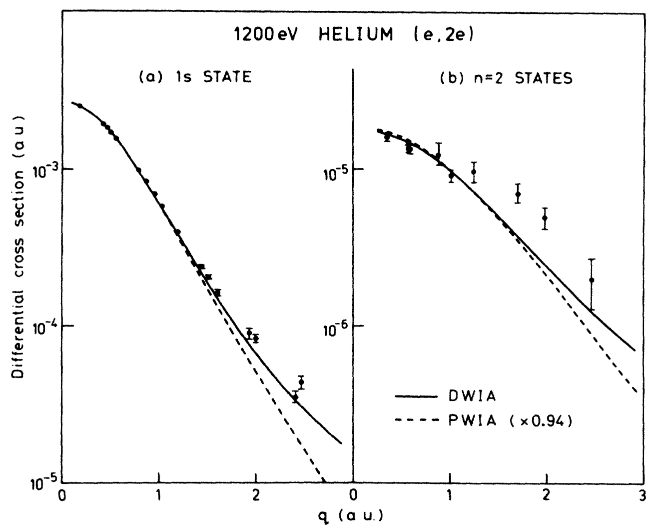

FIG. 1. The momentum profiles for (a) the $n=1$ and (b) the total $n=2$ transitions are plotted as a function of the recoil momentum q, for both the PWIA and DWIA calculations. The data for the $n=1$ transition have been normalized to the DWIA curve at small q. The experimental data for $n=2$ did not have to be normalized since the relative strength of the $n=2$ transitions to the $n=1$ transition is known.

function. The summed $n=2$ DWIA cross sections [Fig. 1(b)] are also an improvement over the PWIA calculation. In this instance it is vital that the CI determined overlap function is used in the computation of the DWIA matrix element. The helium HF $1s^2$ configuration provides a very poor representation of the He^+ $2s$ overlap function and cannot leave the ion in the $2p$ state.

Previous papers[3,4] have displayed the $\sigma(n=2)/\sigma(n=1)$ ratio since the distinctions between the He^+ $(n=2)$ and He^+ $(n=1)$ overlap functions become immediately apparent. In Fig. 2 this ratio is depicted for both the PWIA and DWIA calculations. Although the DWIA is an improvement over the PWIA for the individual $n=1$ and $n=2$ cross sections, this is not the case for the $\sigma(n=2)/\sigma(n=1)$ ratio. The DWIA value for the ratio does not agree with experimental data at large recoil momenta.

Finally we summarize our present understanding of the symmetric $(e,2e)$ reaction on helium. The differential cross section is sensitive to details of correlated wave functions for the helium ground state.[3] This was shown by the PWIA, but the conclusion is not altered by the DWIA. Different correlated wave functions give cross sections that differ more widely at higher momenta. The DWIA and PWIA for the same wave function also differ more widely at higher momenta. Thus the effects of improvements to the reaction and structure parts of the calculation can be similar. It is therefore important that we have used a converged CI expansion[4] for the structure. Discrepancies must be due to the reaction theory. Since the DWIA using static exchange potentials is adequate to describe $(e,2e)$ on argon[1] and xenon[2] there must be an aspect of the helium case for which the distorted-wave description of the initial or final state is less adequate than for larger atoms. A possibility is the fact that coupling between the degenerate $2s$ and $2p$ states of He^+ is ignored in this approximation. Further refinements to the calculation would be justified only if more-accurate experimental data are available.

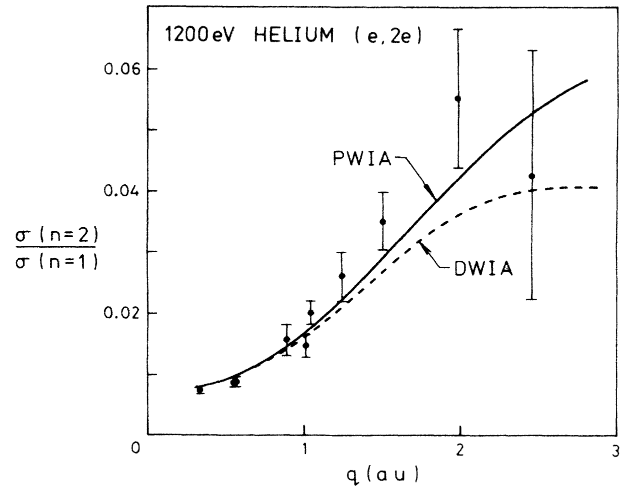

FIG. 2. The $n=2$ to $n=1$ cross-section ratio, $(\sigma_{2s}+\sigma_{2p})/\sigma_{1s}$, is plotted as a function of the recoil momentum q, and is compared with the experimental data. Results for both the PWIA and DWIA calculations are depicted.

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