An electron momentum spectroscopy study for elucidating the range of the validity of the plane wave impulse approximation

Isao Nakajima [1], **Masakazu Yamazaki, Noboru Watanabe, Masahiko Takahashi** [2]

Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai 980-8577, Japan

Synopsis We have examined the range of the validity of the plane wave impulse approximation (PWIA) by making comparisons with binary (e,2e) cross sections measured for several rare gases at various incident electron energies (E_0). The comparisons clearly show that the PWIA reproduces the experimental results up to larger momenta at higher E_0 value. These findings strongly indicate that a wider range of spatial distributions of molecular orbitals (MOs) could be assessed with binary (e,2e) spectroscopy.

Electron momentum spectroscopy (EMS) [1,2], also known as binary (e, 2e) spectroscopy, is a kinematically-complete electron-impact ionization experiment performed under the so-called high-energy Bethe ridge conditions where electron-induced Compton scattering occurs. For predicting this reaction, widely used is the PWIA which assumes energies of the continuum electrons are high enough to neglect their interaction with the residual ion. The triple differential cross section (TDCS) of PWIA is then directly connected to the electron momentum distribution of a molecular orbital (MO) of choice. Thus, the knowledge about the range of the validity of PWIA is the key for promoting molecular science with EMS. However, such experimental studies are scarce as yet and the detailed knowledge is among the issues to be further explored. In the present work, we have conducted a series of EMS experiments on rare gases at various E_0 in order to examine the range of the validity of the PWIA closely.

The experiments were performed at an E_0 range from 1.2 keV to 10 keV by using our symmetric-noncoplanar (e,2e) spectrometer [3]. Briefly, electron impact ionization occurred where an incident electron beam collided with a rare gas atom from a gas nozzle. Two outgoing electrons having equal energies and making the scattering angle of 45 degrees were dispersed by a spherical analyzer and detected by a position-sensitive detector. In this kinematics, the momentum of the target electron, before ionization, can then be determined only from the azimuthal angle differences between the two outgoing electrons.

Fig. 1 shows one of the experimental results thus obtained, which are the TDCSs for the ionization of the Ne 2p orbital measured at E_0 of 1.2 and 4.0 keV. Also included are associated PWIA calculations as well as distorted wave impulse approximation (DWIA) calculations that consider distortion of electron waves due to the static Coulomb field of the residual ion. Normalization of the experimental and PWIA TDCSs are made by fitting their maximum values to that of the corresponding DWIA one and the normalization factor (NF) values used for the PWIA results are given in the figure. It is evident that the momentum value q_{th}, at which PWIA begins to deviate from the experiment, for 4.0 keV is noticeably larger than that for 1.2 keV. Also evident is that the NF value for PWIA approaches to unity with increase in E_0. In addition, both of the q_{th} and NF values for 2.0 keV were found to lie in between those of 1.2 keV and 4.0 keV (not shown). These observations mean that the range of the validity of the PWIA becomes broader at higher E_0 value, indicating that a wider range of spatial distributions of MOs could be assessed with EMS.

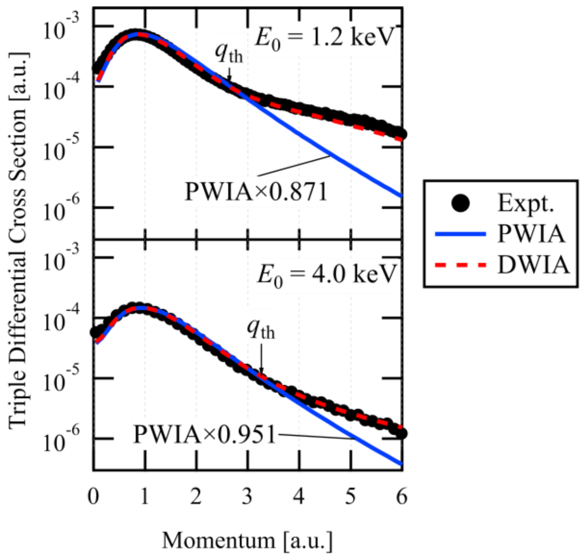

Figure 1. Experimental and theoretical TDCSs of the Ne 2p atomic orbital.

[1] E-mail: inaka@mail.tagen.tohoku.ac.jp
[2] E-mail: masahiko@tagen.tohoku.ac.jp

References

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