Photoionization of H\textsubscript{2} using the molecular R-matrix with time approach

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Synopsis We present results of the first calculations using the variational ab initio molecular R-matrix with time approach. We have calculated two and four-photon ionization cross sections for H\textsubscript{2} and studied the effects of electron correlation and choice of the Gaussian atomic basis sets. Our results are compared with earlier calculations.

The atomic R-matrix with time dependence (RMT) \cite{1} approach has been applied successfully to the study of the interaction of atoms with ultrashort laser pulses. The approach is based on the R-matrix method that divides space into an inner and an outer region. RMT uses highly accurate wavefunctions in the inner region that describe multi-electronic interactions precisely. In the outer region, the ionized electron becomes distinguishable; here the single-electron time-dependent Schrödinger equation is solved, with the electron subject to the long-range potential of the molecule and the laser field.

Recently, we have extended the original atomic R-matrix software \cite{2} to treat interaction of laser fields with molecules in the fixed-nuclei approximation. The molecular, inner-region data required (transition dipole moments, etc.) are generated using the UKRmol+ suite \cite{3}, a highly accurate set of (time-independent) programs initially designed to treat electron and positron scattering from polyatomic molecules.

The RMT approach is very general and allows the study of a range of processes from the perturbative to highly non-linear regimes. Detailed understanding of the molecular RMT models for multiphoton ionization is a prerequisite for its application to processes such as strong-field ionization and high-harmonic generation.

In order to gain this understanding and validate the molecular RMT calculations, we have studied two- and four-photon ionization of H\textsubscript{2} for which earlier results are available. Figure 1 shows our simplest results produced using a Gaussian basis set for the bound orbitals and B-splines for the description of the continuum. Our cross sections are in good agreement with those obtained with the diatomic R-matrix Floquet approach \cite{4} but less so with other calculations. We have studied the effect of the modelling of electron correlation for multiphoton ionization and will compare the results of our close-coupling models with similar results obtained using other approaches.

Figure 1. Cross section for two-photon ionization of H\textsubscript{2}. Our initial results show good agreement with earlier Floquet calculations.

References

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