

An effective eigenchannel R-matrix calculation of electron-ion scattering processes with spectroscopic precision

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Synopsis Using our eigenchannel R-matrix method, the scattering matrices in the whole energy regions can be directly calculated with spectroscopic precision. From the short range scattering matrices, various scattering cross sections, such as total excitation cross sections, differential cross sections and so on, can be obtained. The $e+Kr^+$ system is used as an illustration example, the degree of accuracies of scattering matrices is calculated within about 6%, which should be much more accurate than state-of-the-art scattering experiments.

Understanding the detailed dynamics of electron-atom interactions is of fundamental importance in theoretical atomic physics as well as for basic needs in the fields of astrophysics, fusion energy researches and so on. Theoretical computations should play indispensable role to satisfy such needs. The eigenchannel R-matrix method developed recently [1] can directly calculate the short range scattering matrices with spectroscopic precision (i.e., the electron correlations can be adequately taken into accounts). From the short range scattering matrices, various scattering cross sections, such as total excitation cross sections, differential cross sections and so on, can be calculated with the precision of experimental spectroscopic accuracies. Such theoretical precisions should be more accurate than state-of-the-art scattering experiments.

To demonstrate the validity of the method, we use the $e+Kr^+$ system (i.e., the energy levels of Kr as well as the collision processes of electron and Kr^+) as an illustration example. By comparisons between the calculated energy level positions and the accurate spectroscopic measurements, degree of accuracy of scattering matrices of various partial waves can be determined readily to within about 6%. The calculated low energy electron scattering cross sections with the same accuracy are compared with the available experimental measurements [2].

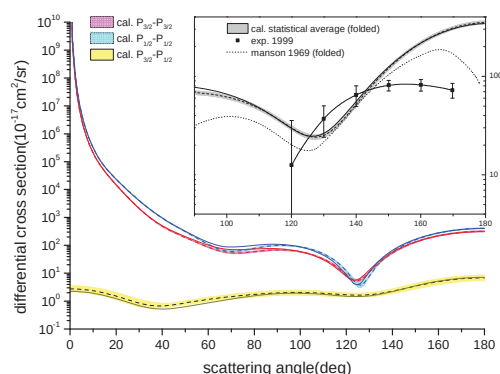


Figure 1. Differential cross section of $e+Kr^+$ at 3.3eV. The color areas in the figure indicated our calculation precision determined by spectroscopic experiments.

Our calculated differential cross section is in agreement with experimental one at low angles, the deviations at large angles are discussed, which can show the indispensable role of theoretical calculations.

References

- [1] X Gao *et al* 2012 *Chin. Phys. Lett.* **29** 033101
- [2] I Williams *et al* 1999 *Phil. Trans. R. Soc. Lond. A* **357** 1297

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