Differential cross sections of an electron scattering by two-centre Coulomb potentials

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Synopsis We have developed an efficient numerical method for calculating the differential cross sections (DCSs) of an electron scattering by two nuclei fixed in the space based on the R-matrix propagation technique in the prolate spheroidal coordinates. The DCSs of H_2^+ and HeH^{2+} are demonstrated.

Collisions between an electron with two nuclei fixed in the space are the most fundamental processes expressing the electron-molecular interactions. We have developed an efficient numerical procedure based on the R-matrix propagation method in the prolate spheroidal coordinates, and calculated the differential cross sections (DCSs) of H_2^+ and HeH^{2+}. In the calculations, two positive charges $(Z_1, Z_2) = (1, 1)$ and $(2, 1)$ for H_2^+ and HeH^{2+} are located at $z = -R/2$ and $R/2$ respectively, on the z axis [1].

In general, the DCSs for modified Coulomb potentials are calculated by decomposing the scattering amplitude into two parts [2], i.e.,

$$f(\boldsymbol{k}_\mathrm{s}, \boldsymbol{k}_\mathrm{i}) = f_0^c(\boldsymbol{k}_\mathrm{s}, \boldsymbol{k}_\mathrm{i}) + f_0'(\boldsymbol{k}_\mathrm{s}, \boldsymbol{k}_\mathrm{i}), \qquad (1)$$

where $f_0^c(\boldsymbol{k}_\mathrm{s}, \boldsymbol{k}_\mathrm{i})$ is the Coulomb scattering amplitude for the net charge at the origin and $f_0'(\boldsymbol{k}_\mathrm{s}, \boldsymbol{k}_\mathrm{i})$ is attributed to the short range potential. $\boldsymbol{k}_\mathrm{i}$ and $\boldsymbol{k}_\mathrm{s}$ are the wave vectors of the incident and scattering electron, respectively. The above decomposition works well for H_2^+, but not for HeH^{2+} due to the dipole nature. Indeed, the partial wave expansion does not converge for the latter case. To overcome this computational difficulty, we introduce another form of the decomposition of the scattering amplitude

$$f(\boldsymbol{k}_\mathrm{s}, \boldsymbol{k}_\mathrm{i}) = f_{12}^c(\boldsymbol{k}_\mathrm{s}, \boldsymbol{k}_\mathrm{i}) + f_{12}'(\boldsymbol{k}_\mathrm{s}, \boldsymbol{k}_\mathrm{i}), \qquad (2)$$

where

$$f_{12}^c(\boldsymbol{k}_\mathrm{s}, \boldsymbol{k}_\mathrm{i}) = \frac{Z_1 f_1^c(\boldsymbol{k}_\mathrm{s}, \boldsymbol{k}_\mathrm{i})}{Z_1 + Z_2} + \frac{Z_2 f_2^c(\boldsymbol{k}_\mathrm{s}, \boldsymbol{k}_\mathrm{i})}{Z_1 + Z_2}. \qquad (3)$$

Here, $f_1^c(\boldsymbol{k}_\mathrm{s}, \boldsymbol{k}_\mathrm{i})$ and $f_2^c(\boldsymbol{k}_\mathrm{s}, \boldsymbol{k}_\mathrm{i})$ are the Coulomb amplitudes shifted in the directions $z = -R/2$ and $R/2$, respectively. Thus, the amplitude $f_{12}'(\boldsymbol{k}_\mathrm{s}, \boldsymbol{k}_\mathrm{i})$ contains neither the long-range Coulomb effect nor the dipole effect, so that the partial wave expansion of $f_{12}'(\boldsymbol{k}_\mathrm{s}, \boldsymbol{k}_\mathrm{i})$ is converged rapidly as shown in figure 1.

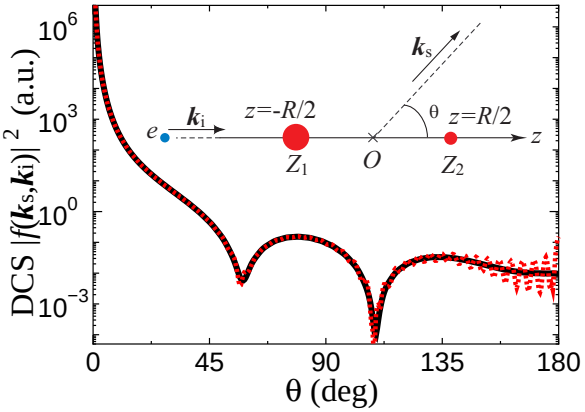

Figure 1. The electron scattering DCSs of the system HeH^{2+} ($Z_1 = 2$, $Z_2 = 1$, and $R = 2.0$ a.u.) for electron energy 150 eV. The inset indicates the geometry of the collision system. Solid black curve: the DCS calculated by using the new method [equation (2)], doted red curve: the DCS by the standard decomposition [equation (1)]. The same number of partial waves are used in both calculations. Oscillating behavior in the doted red curve is due to lack of the number of partial waves.

References

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