§25. Calculation of Electron Impact Excitation Cross Section of Atomic Hydrogen Based on the Time-dependent Schrödinger Equation

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For spectroscopic diagnostic of fusion plasmas, we have developed an atomic hydrogen collisional-radiative model [1], in which levels are distinguished by the principal quantum number n. The statistical population distribution is assumed for different orbital quantum number l in the same n. However, in fusion plasmas, in many cases, this assumption may not be valid under the radiation trapping of the Lyman lines of atomic hydrogen. In order to construct a code which distinguishes l levels, electron impact excitation cross section between each (n, l) level should be calculated; We have developed a code which is based on the time-dependent Schrödinger equation.

The Hamiltonian for this system is

$$i\hbar\frac{\partial\Psi}{\partial t} = H\Psi, \tag{1}$$

$$\begin{aligned} H &= -\frac{\hbar^2}{2\mu}({\nabla_1}^2 + {\nabla_2}^2) - \frac{Ze^2}{4\pi\epsilon_0}\left(\frac{1}{r_1} + \frac{1}{r_2}\right) + \frac{e^2}{4\pi\epsilon_0 r_{12}} \\ &= H_1 - \frac{\hbar^2}{2\mu}{\nabla_2}^2 - \frac{Ze^2}{4\pi\epsilon_0 r_2} + \frac{e^2}{4\pi\epsilon_0 r_{12}}. \end{aligned}$$

Here "1" and "2" denote the incident electron and the electron of the target atom, respectively. μ is the reduced mass.

The total wave function is expanded in terms of eigenfunctions of the atom

$$\Psi(\vec{r_1}, \vec{r_2}, t) = \sum_\beta F_\beta(\vec{r_2}, t)\psi_\beta(\vec{r_1})e^{-i\frac{E_\beta}{\hbar}t}. \tag{2}$$

The expansion coefficient F_β, which gives the cross section is obtained by the next differential equation, which is derived from the time-dependent Schrrödinger equation,

$$\begin{aligned} &\frac{\partial F_\alpha(\vec{r_2}, t)}{\partial t} \\ =\ & -\frac{1}{i\hbar}\frac{\hbar^2}{2\mu}{\nabla_2}^2 F_\alpha(\vec{r_2}, t) - \frac{1}{i\hbar}\frac{Ze^2}{4\pi\epsilon_0}\frac{F_\alpha(\vec{r_2}, t)}{r_2} \\ +\ & \frac{1}{i\hbar}\frac{e^2}{4\pi\epsilon_0}\sum_\beta F_\beta(\vec{r_2}, t)e^{-i\frac{(E_\beta - E_\alpha)t}{\hbar}}\int \psi_\alpha^*(\vec{r_1})\frac{1}{r_{12}}\psi_\beta(\vec{r_1})d\vec{r_1}. \end{aligned} \tag{3}$$

By separating the real and imaginary parts,

$$F_\alpha(x_2, y_2, z_2, t) = F_\alpha^R(x_2, y_2, z_2, t) + iF_\alpha^I(x_2, y_2, z_2, t), \tag{4}$$

eq.(3) can be numerically solved,

$$\frac{\partial F_\alpha^R}{\partial t} = -\frac{\hbar}{2\mu}{\nabla_2}^2 F_\alpha^I + \frac{1}{\hbar}\sum_\beta (V_{\alpha\beta}^R F_\beta^I + V_{\alpha\beta}^I F_\beta^R), \tag{5}$$

$$\frac{\partial F_\alpha^I}{\partial t} = \frac{\hbar}{2\mu}{\nabla_2}^2 F_\alpha^R - \frac{1}{\hbar}\sum_\beta (V_{\alpha\beta}^R F_\beta^R - V_{\alpha\beta}^I F_\beta^I), \tag{6}$$

$$V_{\alpha\beta} = -\delta_{\alpha\beta}\frac{Ze^2}{4\pi\epsilon_0}\frac{1}{r_2} + \frac{e^2}{4\pi\epsilon_0}e^{-i\frac{(E_\beta - E_\alpha)t}{\hbar}}\int \psi_\alpha^*(\vec{r_1})\frac{1}{r_{12}}\psi_\beta(\vec{r_1})d\vec{r_1}.$$

The real and imaginary parts are defined at leapfrog different time steps [2]. Runge-Kutta method is adopted for solving eqs.(5) and (6). Spatially, the finite difference method is applied.

Figure 1 shows an example of the calculation. Initial state of atom is 2s. Wave function of an incident electron is a plane wave function multiplied by Gaussian, whose energy is approximately 0.5 ± 0.05 eV. In this study, five levels up to n=2 are considered. Figure 1 shows snapshots of the squared values of the expansion coefficients for 2s, 2p magnetic sublevels in eq.(2). Conservation of the total probability of the scattered electron is confirmed. Obtained excitation cross section from 2s to 2p is 1.3×10^{-14}cm^2. We will calculate cross sections in the wide range of the incident electron energy by including higher lying levels of the atom.

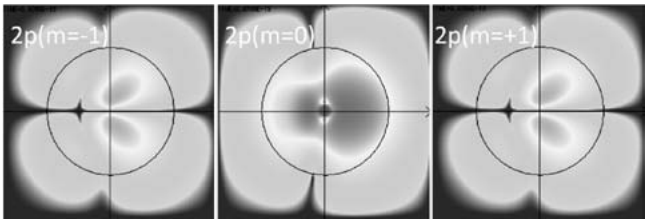

Fig. 1: Squared values of the expansion coefficients in eq.(2), 2s, 2p (m=± 1) and 2p (m=0). The horizontal axis is taken in the direction of the incident electron. Atom is located at the origin. Region of $-25a_0 \sim 25a_0$ is shown.

1) K.Sawada, J. Plasma Physics 72, 1025 (2006).

2) A.Askar, A.S.Cakmak, J. Chem. Phys. 68, 2794 (1977).