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Weak correlation theory of electron hydrogen atom ionization collisions

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Abstract. A hyperspherical partial wave method of Das to calculate cross sections for ionization of hydrogen atoms by electrons has been applied for low energies. Here effect of coupling among different partial waves is neglected.

Keywords. Electron; hydrogen; ionization; partial waves.

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1. Introduction

During the last few years considerable effort has been made in quest of a suitable theoretical method capable of giving accurate cross section results for atomic ionization problems over wide kinematic conditions. Distorted wave Born approximation (DWBA, Jones *et al* [1]), three-body distorted wave Born approximation (3DWBA, Jones *et al* [2]), dynamic screening of three two-body Coulomb interaction method (DS3C, Berakdar and Briggs [3]), BBK theory (Brauner *et al* [4]), convergent close coupling calculation (CCC, Bray *et al* [5]), multiple scattering theory (MST, Das and Seal [6, 7]), are some, which may be mentioned in this context. Although most of these calculations give excellent cross section results for intermediate and high energies, none of these methods works well for low energies (Konovalov [8], Rösel *et al* [9]). At low energies, correlation in the final three particle state is so strong that any perturbation in the potentials in the final channel leads to unacceptable cross section results under many circumstances. Keeping this in view Das [10, 11], treating all the particles on an equal footing, developed a formalism, using hyperspherical coordinates, for electron hydrogen atom ionization collisions. This theory gives accurate cross section results and is expected to be suitable particularly for low energies, for which a small number of partial waves in the final three-particle state are important. Here we perform a simplified version of the calculation in which effect of coupling is neglected (in view of Lin's observation (Lin [12])) to gain some initial experience for a more complicated calculation. We report here some of these preliminary results and informations which will be helpful in future for more accurate calculation along this line.

2. Theory

The (direct) T-matrix element for ionization of a hydrogen atom by an incident electron of energy E_i and momentum $\mathbf{p}_i$ when the two outgoing electrons have momentum $\mathbf{p}_1$ and $\mathbf{p}_2$ respectively is given by

$$T_d = \langle \Psi_f^{(-)} | V_i | \Phi_i \rangle, \tag{1}$$

where Φ_i is the initial unperturbed state corresponding to a decomposition of the total Hamiltonian H, say

$$H = H_i + V_i, \tag{2a}$$

where

$$V_i(\mathbf{r}_1, \mathbf{r}_2) = 1/r_{12} - 1/r_2, \tag{2b}$$

$\mathbf{r}_1, \mathbf{r}_2$ being position vectors of the atomic and the incident electron and $\Psi_f^{(-)}$ is the exact final three particle scattering state with converging wave boundary conditions. In hyperspherical coordinates $\Psi_f^{(-)}$ may be represented as (see Das [10, 11], particularly for notations)

$$\Psi_f^{(-)} = \sqrt{\frac{2}{\pi}} \sum_\lambda \left(\frac{F_\lambda(\rho)}{\rho^{5/2}} \right) \phi_\lambda^* \phi_\lambda(\alpha, \hat{r}_1, \hat{r}_2). \tag{3a}$$

Here $\rho = PR$, $R = \sqrt{r_1^2 + r_2^2}$, $P = \sqrt{p_1^2 + p_2^2}$, $\alpha = \tan^{-1}(r_2/r_1)$, $\alpha_0 = \tan^{-1}(p_2/p_1)$ and

$$\phi_\lambda(\alpha, r_1, r_2) = P_n^{l_1 l_2}(\alpha)\, Y_{l_1 l_2}^{lm}(\hat{r}_1, \hat{r}_2), \tag{3b}$$

$P_n^{l_1 l_2}(\alpha)$ being the Jacobi polynomial.

The radial waves F_λ's satisfy the coupled set of equations (see Das [10], Lin [12])

$$\left[\frac{d^2}{d\rho^2} + 1 - \frac{\nu_\lambda(\nu_\lambda + 1)}{\rho^2} \right] F_\lambda + \sum_{\lambda'} \frac{2\alpha_{\lambda\lambda'}}{\rho} F_{\lambda'} = 0. \tag{3c}$$

Here λ stands for the multiplet (n, l_1, l_2, l, m) or the eigenvalue $2n + l_1 + l_2$ depending on the context and $\nu_\lambda = \lambda + 3/2$ and

$$\alpha_{\lambda\lambda'} = \left\langle \phi_\lambda \left| \frac{1}{\cos\alpha} + \frac{1}{\sin\alpha} - \frac{1}{|\hat{r}_1 \cos\alpha - \hat{r}_2 \sin\alpha|} \right| \phi_{\lambda'} \right\rangle \Big/ P. \tag{3d}$$

When the off-diagonal matrix elements $\alpha_{\lambda\lambda'} (\lambda \neq \lambda')$ are neglected, the solution of eq. (3c) simply becomes Coulomb waves corresponding to charge parameter $\alpha_{\lambda\lambda} \equiv \alpha_\lambda$. In this approximation which we call *weak correlation approximation* the final three-particle scattering state becomes

$$\Psi_{f0}^{(-)} = \sum_\lambda 2(2\pi)^{5/2} i^\lambda e^{-i\eta_\lambda} \left(\frac{F_\lambda^{(0)}(\rho)}{\rho^{5/2}} \right) \phi_\lambda^*(\alpha_0, \hat{p}_1, \hat{p}_2) \times \phi_\lambda(\alpha, \hat{r}_1, \hat{r}_2). \tag{4}$$

$F_\lambda^{(0)}$ satisfies the boundary conditions

$$F_\lambda^{(0)}(\rho) \sim \rho^{\nu_\lambda + 1}, \quad \rho \to 0$$

$$\sim \sin(\rho - \nu_\lambda \pi/2 + \alpha_\lambda \ln 2\rho + \eta_\lambda), \quad \rho \to \infty,$$

where

$$\eta_\lambda = \arg\Gamma(\nu_\lambda + 1 - i\alpha_\lambda).$$

Explicitly $F_\lambda^{(0)}$ is given by

$$F_\lambda^{(0)}(\rho) = \mathrm{e}^{1/2\pi\alpha_\lambda}|\Gamma(\nu_\lambda + 1 + i\alpha_\lambda)|2^{\nu_\lambda}\rho^{\nu_\lambda+1}\mathrm{e}^{-i\rho}$$
$$\times {}_1F_1(i\alpha_\lambda + \nu_\lambda + 1, 2\nu_\lambda + 2, 2i\rho)/\Gamma(2\nu_\lambda + 2).$$

Asymptotically $\Psi_\mathrm{f}^{(-)}$ (and also $\Psi_{\mathrm{f}0}^{(-)}$) behaves as a superposition of a distorted plane wave and incoming converging waves only.

Exchange amplitude is obtained after the substitution $\alpha \to \pi/2 - \alpha$ and $\hat{r}_1 \rightleftarrows \hat{r}_2$. Differential cross section is then obtained as usual.

In our present calculation we included terms in the expansion (4) for n, l, l_1, l_2 taking values from zero to certain maximum values $n_{\max}, l_{\max}, l_{1\max}, l_{2\max}$ and set $m = 0$. For fixed values of other parameters, convergence is practically obtained with $n_{\max} = 5$ or 6 in all the calculations reported here. So we took $n_{\max} = 6$ in this calculation. We varied $l_{\max}$ from zero to a maximum value of six and for fixed $l_{1\max}$ we varied $l_{1\max}(= l_{2\max})$ from zero to seven only. With these values convergence is practically obtained in the results. Here we have calculated triple differential cross sections in a plane configuration for incident electron energies of 17·6 eV, 27·2 eV and 54·4 eV in the low energy range for which there are certain experimental results. Results are presented and discussed in the next section.

3. Results

Three sets of results for triple differential cross section are presented in figure 1 for three different incident energies corresponding to the parameters (a) $E_\mathrm{i} = 54{\cdot}4$ eV, $E_1 = 5$ eV, $\theta_2 = 4°$; (b) $E_\mathrm{i} = 27{\cdot}2$ eV, $E_1 = E_2 = 6{\cdot}8$ eV, $\theta_2 = 15°$; and (c) $E_\mathrm{i} = 17{\cdot}6$ eV, $E_1 = E_2 = 2$ eV, $\theta_2 = 140°$. Angles are measured positive or negative depending on if the direction is anticlockwise or clockwise with reference to the incident electron momentum direction.

In figure 1(a) we compare one set of our results for 54·4 eV energy with the theoretical results of convergent close coupling calculation (CCC, Bray *et al* [5]), BBK theory (Brauner *et al* [4]), three-body distorted wave Born approximation (3DWBA, Jones *et al* [2]) and with the experimental results of Ehrhardt *et al* [13] as normalized by Bray *et al.* The experimental results of Ehrhardt and associates are not absolute. For a fixed energy a single multiplicative factor normalizes the results for all scattering angles. Since CCC calculation gives a good total ionization cross section, Bray *et al* [5] normalized these experimental data for each energy by multiplying with a single factor which gives visually the best fit with all of their theoretical results. Thus in normalizing the data of Ehrhardt *et al* for 54·4 eV, they considered all the four sets of results corresponding to $\theta_2 = 4°$, 10°, 16° and 23° during the visual fit (see also figure 2 in ref. [5]). Now the comparison with our results show that our results are really good and are of the right order of magnitude. Inclusion of the effect of coupling are expected to give still better results.

In figures 1(b) and 1(c) we compare one set of our theoretical results for each of energies 27·2 eV and 17·6 eV with the experimental results of Ehrhardt *et al* [13], again

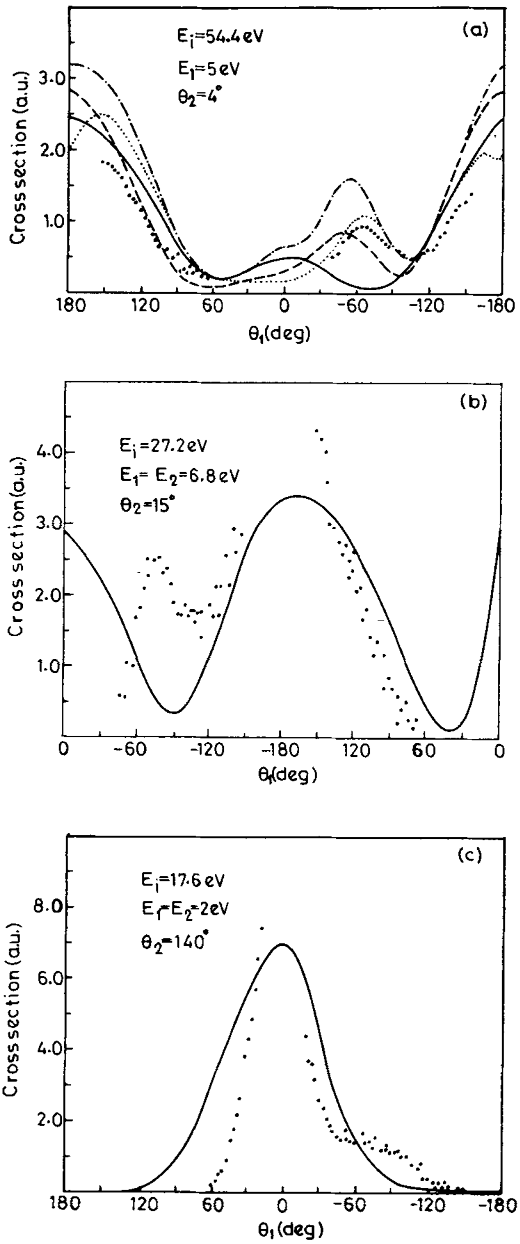

Figure 1a, b, c. Triple differential cross sections for ionization of hydrogen atoms by electrons in a plane for different scattering angles (θ_1) and for three different sets of kinematic conditions. Theory: continuous, present theory; dashed, BBK [4]; dash-dotted, 3DWBA [2]; dotted, CCC [5]. Experiment: points Ehrhardt *et al* [13] suitably normalized.

suitably normalizing their data, since these are not absolute. Here we did not present results of other theories such as BBK, since these are not of comparable accuracy. The comparison qualitatively shows that the present results are not bad. Inclusion of coupling effect may be expected to improve the results further. The results are also in conformity with the observations of Murray *et al* [14] regarding contributing partial waves.

The calculations presented here were done on a 486 PC with Linux as operating system. For a single point (i.e. for fixed energy and angles) it took about half an hour computer time for a double precision calculation.

4. Conclusion

The present weak correlation theory is capable of representing gross features of low energy cross section curves. For very low energies, effect of coupling among different partial waves is important and cannot be simply neglected. The calculation will then become much more complicated. Such a calculation is now in progress.

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