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ASYMPTOTIC FORM FOR THE CROSS SECTION FOR THE COULOMB INTERACTING REARRANGEMENT COLLISIONS

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It is shown that in a rearrangement collision leading to the formation of the highly excited hydrogenlike states the cross section in all orders of the Born approximation behaves as $1/n^2$, with n the principal quantum number, thus invalidating the Brinkman-Kramers approximation for large n. Similarly, in high energy inelastic electron-hydrogenlike atom collisions the exchange cross section for sufficiently large n dominates the direct excitation cross section.

We consider the collision of two like and one unlike charged particles 1, 2, 3 with masses m_1, m_2, m_3 and charges Z_1e, Z_2e, Z_3e, respectively, where e is the absolute value of the electronic charge. The collision is represented by $1 + (2 + 3) \to (1 + 3) + 2$ where (2 + 3) and (1 + 3) represent the hydrogenlike states of 2 and 3, and 1 and 3, respectively. We assume that (2 + 3) is in the ground state, but (1 + 3) is in an arbitrary state including the continuum. Examples would be capture of an electron by a proton incident on atomic hydrogen, and the exchange effect in scattering of electrons by atomic hydrogen.

The collision amplitude in the M^{th} order of the Born approximation is given by[1]

$$T_f^{(M+1)} = \langle \exp(i\mathbf{k}_2 \cdot \mathbf{r}_2)\,\Psi(f, \mathbf{r}_{13})\,|\,V_f(G_o V_i)^M\,|\,\exp(i\mathbf{k}_1 \cdot \mathbf{r}_1)\Psi(i, \mathbf{r}_{23})\rangle \qquad (1)$$

where the subscript f on the left hand side designates that the post interaction form has been used for the amplitude. $\Psi(i, \mathbf{r}_{23})$ and $\Psi(f, \mathbf{r}_{13})$ are the bound states of (2 + 3) and (1 + 3) where $\mathbf{r}_{23}$ and $\mathbf{r}_{13}$ are vectors connecting particles 2 and 1 respectively to particle 3. The vectors $\mathbf{r}_1$ and $\mathbf{r}_2$ connect the centers of masses of (2 + 3) and (1 + 3) to the particles 1 and 2, and vectors $\mathbf{k}_1$ and $\mathbf{k}_2$ are the propagation vectors of particles 1 and 2 with respect to the centers of masses of (2 + 3) and (1 + 3), respectively. $|\mathbf{k}_2|$ is related to $|\mathbf{k}_1|$ through

$$\frac{\hbar^2 k_2^2}{2\mu_2} = \frac{\hbar^2 k_1^2}{2\mu_1} + E(2,3) - E(1,3), \quad \mu_i = \frac{m_i(m_j + m_k)}{m_i + m_j + m_k} \qquad (2)$$

where E(2, 3) and E(1, 3) are the energies of (2 + 3) and (1 + 3) states. Finally, $V_f = V_{12} + V_{23}$, and $V_i = V_{12} + V_{13}$, where V_{ij} is the potential between i and j particles, and G_o is the three body Green's function for outgoing waves. It should be noted that V_{12} is repulsive, while V_{13} and V_{23} are attractive potentials. The rearrangement cross section is related to the rearrangement amplitude through the relationship

$$\sigma = \frac{\mu_1 \mu_2}{2\pi\hbar^4} \left(\frac{k_2}{k_1}\right) \int |T|^2 \, d(\hat{k}_1 \cdot \hat{k}_2) \tag{3}$$

We first consider the first Born approximation which corresponds to M = 0 in (1). The cross section when only V_{23} is taken into account, commonly called the Brinkman-Kramers cross section, was originally calculated by Brinkman and Kramers[2] taking the ground state as the final state. Calculations for the excited states as the final states have been carried out by May[3] and Omidvar[4]. These calculations indicate that at high relative incident energies the cross section behaves as n^{-3} with n the principal quantum number of the final excited state. This behavior has also been predicted by Oppenheimer[5].

We shall consider here the part of the amplitude coming from the V_{12} potential that can be written[6]

$$T_f^{(1)}(V_{12}) = 4\pi Z_1 Z_2 e^2 \int U^*(f, \mathbf{C} - \mathbf{p})\, U(i, \mathbf{B} - \mathbf{p}) \frac{d\mathbf{p}}{p^2},$$

$$\mathbf{C} = \mathbf{k}_1 - \frac{\mu_{13}}{m_3}\mathbf{k}_2, \quad \mathbf{B} = \frac{\mu_{23}}{m_3}\mathbf{k}_1 - \mathbf{k}_2, \quad \mu_{ij} = \frac{m_i m_j}{m_i + m_j} \tag{4}$$

where

$$U(j, \mathbf{q}) = (2\pi)^{-3/2} \int \exp(i\mathbf{q} \cdot \mathbf{r})\, \Psi(j, \mathbf{r})\, d\mathbf{r} \tag{5}$$

In this article this amplitude is evaluated for large n and it is shown that the asymptotic form of the cross section with respect to n is dominated by this amplitude.

When the bound states are expressed in parabolic coordinates we have[4]

$$U(nn_1m, \mathbf{q}) = \frac{\delta(m, o)\sqrt{n}}{\pi} \; \frac{(\alpha/2)^{5/2}}{|\omega|^4} \left(\frac{\omega^*}{\omega}\right)^{2n_1},$$

$$\alpha = \mu_{ij} Z_i Z_j/(m_e n a_o), \; \omega = \frac{1}{2}(\alpha - iq), \; \hat{z} = \hat{q}, \tag{6}$$

with n_1 and m the Stark and the absolute value of the magnetic quantum numbers, m_e the electronic mass, and a_o the Bohr radius. In (6) the spacial quantization axis is taken along **q**.

Taking the ground state as the initial state and designating the final state by $n\, n_1\, m$, through (6) Eq. (4) can be written

$$T_{nn_1m}^{(1)}(V_{12}) = \delta(m, 0)\; 32\pi^{-1} Z_1 Z_2 e^2 (\alpha_0 \alpha)^{5/2} \sqrt{n}\, \mathcal{J},$$

$$\alpha_0 = \mu_{23} Z_2 Z_3/(m_e a_0), \; \alpha = \mu_{13} Z_1 Z_3/(m_e n a_0), \tag{7}$$

$$\mathcal{J} = \int \frac{dp}{p^2\,[\alpha_0{}^2 + (\mathbf{B} - \mathbf{p})^2]^2\,[\alpha^2 + (\mathbf{C} - \mathbf{p})^2]^2} \left(\frac{\alpha - i\,|\mathbf{C} - \mathbf{p}|}{\alpha + i\,|\mathbf{C} - \mathbf{p}|}\right)^{2n_1} \qquad (8)$$

For $n_1 = 0$ and $n \to \infty$ the integration in (8) can be affected by a delta function integration. This leads to

$$T_{nom}{}^{(1)}\,(V_{12}) \approx \frac{\delta(m,0)\;32\pi Z_1 Z_2 e^2 \sqrt{n}\,\alpha_0{}^{5/2}\,\alpha^{3/2}}{C^2\,[\alpha_0{}^2 + (\mathbf{B} - \mathbf{C})^2]^2}\;,\;\alpha \to 0 \qquad (9)$$

For $n_1 \neq 0$ this method of integration is not applicable.

For evaluation of $\mathcal{J}$ for arbitrary n_1 we introduce in Eq. (8) $\mathbf{q} = \mathbf{C} - \mathbf{p}$ and make use of the Feynman's parametric integration method[7]. Then $\mathcal{J}$ can be written

$$\mathcal{J} = -\frac{\partial \mathcal{J}_1}{\partial(\alpha_0{}^2)}\;,\;\mathcal{J}_1 = 4\pi \int_0^1 dx\,(\mathcal{J}_2 + i\mathcal{J}_3)\,, \qquad (10)$$

$$\mathcal{J}_2 = \frac{1}{2}\int_{-\infty}^{+\infty} \frac{(\alpha - iq)^{2(n_1-1)}}{(\alpha + iq)^{2(n_1+1)}}\;\frac{q^2 dq}{(q^2 + \Delta)^2 - 4Q^2q^2}\;, \qquad (11)$$

$$\mathcal{J}_3 = -\int_0^{\infty} \frac{\sin(4n_1\phi)}{(\alpha^2+q^2)^2}\;\frac{q^2 dq}{(q^2 + \Delta)^2 - 4Q^2q^2}\;,\;\phi = \tan^{-1} q/\alpha \qquad (12a)$$

$$\mathcal{J}_3 = -\sum_{\nu=0}^{2n_1-1} \binom{4n_1}{2\nu + 1} (-)^{\nu}\,\alpha^{4n_1-1-2\nu} \int_0^{\infty} \frac{q^{2\nu+3}\,dq}{(\alpha^2+q^2)^{2(n_1+1)}\,[(q^2+\Delta)^2 - 4Q^2q^2]}\;, \qquad (12b)$$

$$\Delta = [\alpha_0^2 + (\mathbf{B} - \mathbf{C})^2]\ x + C^2\ (1 - x),\ \mathbf{Q} = -\mathbf{B}\ x + \mathbf{C} \tag{13}$$

$\mathcal{J}_2$ can be evaluated by a contour integration. The evaluation of $\mathcal{J}_2$ for $n_1 = 0$ and $\alpha \to 0$ gives $\mathcal{J}_2 \approx -\pi/(4\alpha\Delta^2)$. Substitution of this result in (10) leads to a result identical to (9). For $n_1 \neq 0$ and $\alpha \to 0$, $\mathcal{J}_2$ does not show any pole with respect to α, and remains finite as $n \to \infty$.

To evaluate $\mathcal{J}_3$ we use the form (12b). By an ordinary integration we find that

$$\mathcal{J}_3 \approx \frac{c_{n_1}}{2\alpha\Delta^2}\ ,\ c_{n_1} = \sum_{\nu=0}^{2n_1-1} \binom{4n_1}{2\nu+1} \sum_{\lambda=0}^{\nu+1} \frac{(-)^\lambda}{2n_1 + 1 - \lambda} \binom{\nu+1}{\lambda},\ \alpha \to 0 \tag{14}$$

Substitution of this result in (10) gives

$$T_{nn_1m}(V_{12}) \approx \frac{\delta(m,0)\, 32\pi\, Z_1 Z_2 e^2 \sqrt{n}\, \alpha_0^{5/2} \alpha^{3/2}}{C^2\ [\alpha_0^2 + (\mathbf{B} - \mathbf{C})^2]^2}\ \frac{2i\, c_{n_1}}{\pi}\ ,\ n_1 = 1, 2, 3, \cdots,\ \alpha \to 0 \tag{15}$$

By substituting from (9) and (15) into (3), neglecting contribution due to the V_{23} potential, and summing the right hand side of (3) with respect to n_1 and m, we find an expression for the total cross section for capture into an excited state n. This is given by

$$\frac{\sigma(n)}{\pi a_0^2} \approx 2^9 \left(\frac{\mu_1\mu_2}{m_e^2}\right) (Z_1 Z_2)^2\ \alpha_0^5\ n\alpha^3 \left[1 + \frac{4}{\pi^2} \sum_{n_1=1}^{n-1} c_{n_1}^2\right]$$

$$\times \frac{k_2}{k_1} \int \frac{d(\hat{k}_1 \cdot \hat{k}_2)}{C^4\ [\alpha_0^2 + (\mathbf{B} - \mathbf{C})^2]^4}\ ,\ n \to \infty \tag{16}$$

As $n_1 \to \infty$, c_{n_1} approaches zero. This can be shown if $\mathcal{J}_3$ is expressed through (12a) in its asymptotic form with respect to n_1:

$$\mathcal{J}_3 \approx -\frac{\pi}{\alpha} \int_0^{\pi/2} \frac{q^2 \phi\, \delta(\phi)\, d\phi}{(\alpha^2 + q^2)\, [(q^2 + \Delta)^2 - 4Q^2 q^2]}, \quad n_1 \to \infty \tag{17}$$

Comparison of (14) and (17) shows that $c_{n_1} \to 0$ as $n_1 \to \infty$. Using the explicit form of c_{n_1} as given by (14) it is found that

$$\sum_{n_1=1}^{\infty} c_{n_1}^2 \approx 0.616$$

(Cf. Eq. (16)).

The integrals $\mathcal{J}_2$ and $\mathcal{J}_3$ can also be evaluated analytically for arbitrary n, providing a ~~an easy~~ method ~~hitherto not given in the literature~~ for evaluation of the capture cross sections for the arbitrary excited states.

¶ We thus conclude from (16) that due to the repulsive potential the cross section at large n and high impact energies behaves as $1/n^2$. This has two implications: (1) The cross section according to the Brinkman-Kramers approximation, commonly assumed valid for high principal quantum numbers, is not valid. For the low lying levels this approximation gives too large a cross section. In the case of the symmetric charge exchange between protons and atomic hydrogens Jackson and Schiff[6] have shown that inclusion of the V_{12} potential reduces the BK cross sectional values in the energy range of interest by almost an order of magnitude, bringing them closer to the experimental results. Their assumption concerning the n dependence of the cross section for the excited state is not however correct, and their calculated cross sections should be renormalized before they can be compared with the measurements. Similarly, the assumption made by Bates and Dalgarno[8] that the ratio $\sigma(n\ell)/\sigma(1s)$ is the same for both the Born and the BK approximations is incorrect. $n\ell$ and 1s designate here the final excited or the ground states. (2) In high energy inelastic scattering of electrons by hydrogenlike atoms the exchange cross section behaving as $1/n^2$ dominates the direct cross section which behaves as $1/n^3$, a result of significance in plasma and astrophysical calculations.

Considering the second Born approximation, from (1) we find that

$$T^{(2)}_{nn_1m} = \frac{2e^4}{\pi}\iint \frac{dq\,dq'\,[Z_2Z_3U^*(nn_1m,\mathbf{A})+Z_1Z_2U^*(nn_1m,\mathbf{D})]\,[Z_1Z_3U(100,\mathbf{E})+Z_1Z_2U(100,\mathbf{F})]}{\left[\frac{\hbar^2k_2^2}{2\mu_2} + E(1,3) - \frac{\hbar^2q^2}{2\mu_2} - \frac{\hbar^2q'^2}{2\mu_{13}}\right](\mathbf{k}_2-\mathbf{q})^2(\mathbf{k}_1+\frac{\mu_{13}}{m_3}\mathbf{q}+\mathbf{q}')^2},$$

$$\mathbf{A} = -\mathbf{q}' + \frac{\mu_{13}}{m_3}(\mathbf{k}_2-\mathbf{q}),\quad \mathbf{D} = -\mathbf{q}' - \frac{\mu_{13}}{m_1}(\mathbf{k}_2-\mathbf{q})$$

$$\mathbf{E} = \frac{\mu_{23}}{m_3}\mathbf{k}_1 + \mathbf{q},\quad \mathbf{F} = -\frac{\mu_{23}}{m_2}\mathbf{k}_1 + \frac{\mu_{13}}{m_1}\mathbf{q} - \mathbf{q}' \tag{18}$$

where 100 and $n\,n_1m$ designate the initial and final states. Comparison of (18) with (4) shows that $T_{nn_1m}^{(2)}$ has similar n dependence as $T_{nn_1m}^{(1)}$. Therefore the cross section due to the second Born approximation at high n behaves similarly as $1/n^2$.

Regarding the higher orders in the Born series it is seen from (1) that the dependence of these orders on the final state is through the first squared bracket in the numerator of the integrand in (18). Then, provided the higher order amplitudes have well defined values, their dependence on n for large n is the same as for the second order amplitude.

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