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DIVERGENCE OF THE TOTAL CROSS SECTION FOR THREE BODY REARRANGEMENT COLLISIONS WITH COULOMB INTERACTIONS

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Abstract. Three charged particles 1, 2, 3 collide according to the reaction 1+(2+3)+(1+3)+2, where (2+3) and (1+3) are hydrogenlike bound states. It is shown that when (1+3) is in a highly excited state n, due to the repulsive potential, the cross section in the first Born approximation behaves as 1/n which makes the total cross section to diverge like ln n. The total cross sections in the higher orders of the Born approximation are similarly divergent logarithmically.

We consider the collision of three charged particles 1, 2, 3 with masses m_1, m_2, m_3 and charges Z_1 e, Z_2 e, Z_3 e, respectively, where e is the absolute value of the electronic charge. The collision is represented by 1+(2+3)+(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 N^{th} order of the Born approximation is given by

\[ T_f^{(M+1)} = \langle \exp(ik \cdot r) \psi(f, r_{12}) | V_f(G_{01}V_i)^M | \exp(ik \cdot r) \psi(i, r_{23}) \rangle \]  

where the subscript f on the left hand side designates that post interaction form has been used for the amplitude. \( \psi(i, r_{23}) \) and \( \psi(f, r_{12}) \) are the bound states of (2+3) and (1+3) with \( r_{23} \) and \( r_{12} \) vectors connecting particles 2 and 1 respectively to particle 3.
Vectors $\xi_1$ and $\xi_2$ connect the centers of masses of (2+3) and (1+3) to the particles 1 and 2, and vectors $k_1$ and $k_2$ are the propagation vectors of particles 1 and 2 with respect to the centers of masses of (2+3) and (1+3), respectively. $|k_2|$ is related to $|k_1|$ through

$$\frac{\hbar^2 k_1^2}{2\mu_1} = \frac{\hbar^2 k_2^2}{2\mu_2} + E(2,3) - E(1,3) , \quad \mu_1 = \frac{m_1(m_1+m_2)}{m_1+m_2+m_k}$$ (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 $V_{ij} = V_{12} + V_{13}$, where $V_{ij}$ is the potential between i and j particles, and $G_0$ 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

$$\sigma = \frac{\mu_1 \mu_2}{2\pi \hbar^2} \left( \frac{k_2}{k_1} \right) \int |T|^2 d(k_1 \cdot k_2)$$ (3)

We first consider the first Born approximation which corresponds to $M = 0$ in (1). The cross section in this approximation due to the $V_{23}$ potential, commonly called the Brinkman-Kramers cross section, has been calculated by Brinkman and Kramers using the ground state wave function as the final state. Calculations using the excited states as the final state have been carried out by May$^3$, and by a different method by 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$^5$. The amplitude due to the $V_{12}$ potential has been evaluated by
Jackson and Schiff\textsuperscript{6} using the ground state wave function as the final state. Similar calculations for the first few excited states as the final state has been performed by Mapleton\textsuperscript{7}. Here we derive a general expression for the amplitude due to the $V_{12}$ potential for all the excited final states, and find its limiting value as $n$ tends to infinity.

The amplitude due to the $V_{12}$ potential can be written

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

$$C = \frac{k - \frac{\mu_1}{m_1} k_2}{\frac{\mu_2}{m_2} k_1}, \quad B = \frac{\mu_2 k_1 - k_2}{\frac{\mu_1}{m_1} + \frac{\mu_2}{m_2}}, \quad \mu_{ij} = \frac{m_i m_j}{m_i + m_j} \quad (4)$$

where

$$U(j, q) = \frac{(2\pi)^{-1/2}}{\sqrt{n}} \exp \left( \frac{i q - r}{\sqrt{2n}} \right) \left( \frac{\omega}{\sqrt{n}} \right)^{n_1} \quad (5)$$

When the bound states are expressed in parabolic coordinates we have\textsuperscript{6}

$$U(n, m, q) = \frac{\delta(m, \omega) \sqrt{n}}{\pi} \left( \frac{\alpha - iq}{\omega} \right)^{n_1} \left( \frac{\omega}{\sqrt{n}} \right)^{2n_1},$$

$$\alpha = \mu_{ij} Z_1 Z_j/(m_e a_o), \quad \omega = \frac{1}{2} (\alpha - iq), \quad \hat{z} = \hat{q} \quad (6)$$

with $n_1$ and $m$ the parabolic and magnetic quantum numbers, $m_e$ the electronic mass, and $a_o$ the Bohr radius. In (6) the spacial quantization axis is taken along $q$. As $n$ tends to infinity, $\alpha \rightarrow 0$, and by the definition of the delta function (6) can be written

$$U(n, m, q) = \delta(m, \omega) \sqrt{n} (2\alpha)^{3/2} \delta(q), \quad \alpha \rightarrow 0, \quad \hat{z} = \hat{q} \quad (7)$$

When use is made of (7) in (4) we obtain
At high incident energies $|k|$ will be independent of $n$ (cf. Eq. (2)). Then (4) shows that $B$ and $C$ are also independent of $n$. In this case as $n$ becomes large $T_{nn_1m}^{n_1}$ becomes proportional to $n^{-1}$. When the squared modulus of $T_{nn_1m}^{n_1}$ is summed with respect to $n_1m$ and the result is substituted in (3) we find that the cross section for the repulsive potential $V_{12}$ for large quantum numbers behaves as $n^{-1}$, whereas the corresponding cross section for $V_{23}$ potential behaves as $n^{-3}$. This has two implications: (1) the cross section due to the repulsive potential or "core" potential at large $n$ dominates the Brinkman-Kramers cross section, (2) the total cross section which is a sum of the individual cross sections with respect to $n$ diverges as $kn$.

The capture into the continuum states of (1+3) can be considered by analytic continuation of the bound state cross section. The appropriate equation is given by

$$\frac{d\sigma}{d(\epsilon/R)} = \frac{\sqrt{\epsilon/R}}{2[1-\exp(-2\pi\beta)]} \left[ n^3\sigma(n) \right] , \quad \beta = \frac{\mu_{1\bar{3}Z_1Z_3}}{m_0^2\sqrt{\epsilon/R}}$$

(9)

where $\epsilon/R$ is the relative kinetic energy of the particles 1 and 3 in rydberg, and $d\sigma/d(\epsilon/R)$ is the continuum capture cross section per unit range of this energy. $\sigma(n)$ is the bound state capture cross section given by (3). From the foregoing discussion and (9) it can be seen that as $\epsilon/R \to 0$ the continuum cross section goes to infinity as $(\epsilon/R)^{-1}$. 
We now consider the divergence in the second Born approximation. Designating the initial state by 100 and the final state by \( \text{nn}_m \), by a straightforward substitution in (1) we find that

\[
\tau_{\text{nn}_m} = \frac{2\pi^4}{\hbar^2} \int dq dq' x \left[ \begin{array}{c}
\frac{\hbar^2 k_2^2}{2\mu_2} + E(1,3) - \frac{\hbar^2 q^2}{2\mu_1} - \frac{\hbar^2 q'^2}{2\mu_1} \\
(k_2 - q)^2(k_1 + \frac{\mu_1}{m_1} q + q')^2
\end{array} \right]
\]

\[
\times [Z U^*(\text{nn}_m, A) + Z U^*(\text{nn}_m, D)] [Z U(100, E) + Z U(100, F)]
\]

where

\[
A = -q' + \frac{\mu_1}{m_1} (k_2 - q), \quad D = -q' - \frac{\mu_1}{m_1} (k_2 - q)
\]

\[
E = \frac{\mu_1}{m_1} k_1 + q, \quad F = -\frac{\mu_1}{m_2} k_1 + \frac{\mu_1}{m_1} q - q'
\]

When \( n \) tends to infinity, Equation (7) can be used to evaluate the first squared bracket in the numerator in the integrand in (10). Then, similar to the first Born approximation, at high incident energies and large quantum numbers \( \tau_{\text{nn}_m} \) behaves as \( n^{-1} \), and the corresponding cross section for the \( n^{th} \) level will behave as \( n^{-1} \). It should be noted that in applying (7) to (10) assumption is made that once \( A \) and once \( B \) are the spacial quantization axis. In actual computation the states should be rotated to refer to a common \( z \)-axis. This transformation, will not however change the \( n \) dependence of the amplitude.

Regarding the higher order terms in the Born amplitude it is seen from (1) that the dependence of these terms on the final state is through the first squared bracket in the numerator of the integrand in (10). Then, provided the higher order
terms have well defined values, their dependence on \( n \) for large
\( n \) is the same as the second order term, and the corresponding

total cross section diverges as \( in n \).

It is then concluded that the sum of the Born series give
rise to a total cross section which as \( n \) increases diverges like
\( in n \). It is possible that a perturbation theory such as the
Born approximation cannot be applied for the final excited
states higher than a certain excited state. In this case a
criterion should be found for the validity of the Born approximation.

References

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