X-641-72-361

PREPRINT

NASA TM X- 66054

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K. OMIDVAR

SEPTEMBER 1972

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GODDARD SPACE FLIGHT CENTER
GREENBELT, MARYLAND

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K. Omidvar

NASA/Goddard Space Flight Center
Greenbelt, Maryland 20771

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 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.

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We consider the collision of three 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)→(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]

$$T_f^{(M+1)} = \langle \exp(i\underset{\sim}{k}_2 \cdot \underset{\sim}{r}_2)\Psi(f,\underset{\sim}{r}_{13})|V_f(G_oV_i)^M|\exp(i\underset{\sim}{k}_1 \cdot \underset{\sim}{r}_1)\Psi(i,\underset{\sim}{r}_{23})\rangle \quad (1)$$

where the subscript f on the left hand side designates that post interaction form has been used for the amplitude. $\Psi(i,\underset{\sim}{r}_{23})$ and $\Psi(f,\underset{\sim}{r}_{13})$ are the bound states of (2+3) and (1+3) with $\underset{\sim}{r}_{23}$ and $\underset{\sim}{r}_{13}$ vectors connecting particles 2 and 1 respectively to particle 3.

Vectors $\underset{\sim}{r}_1$ and $\underset{\sim}{r}_2$ connect the centers of masses of (2+3) and (1+3) to the particles 1 and 2, and vectors $\underset{\sim}{k}_1$ and $\underset{\sim}{k}_2$ are the propagation vectors of particles 1 and 2 with respect to the centers of masses of (2+3) and (1+3), respectively. $|\underset{\sim}{k}_2|$ is related to $|\underset{\sim}{k}_1|$ through

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

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 in this approximation due to the V_{23} potential, commonly called the Brinkman-Kramers cross section, has been calculated by Brinkman and Kramers[2] 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[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[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[6]

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

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

where

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

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

$$U(nn_1 m, \underset{\sim}{q}) = \frac{\delta(m,o)\sqrt{n}}{\pi} \ \frac{(\alpha/2)^{5/2}}{|\omega|^4} \left(\frac{\omega^*}{\omega}\right)^{2n_1} \quad ,$$

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

with n_1 and m the 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 $\underset{\sim}{q}$. As n tends to infinity, $\alpha \to o$, and by the definition of the delta function (6) can be written

$$U(nn_1 m, \underset{\sim}{q}) = \delta(m,o)\pi\sqrt{n}(2\alpha)^{3/2}\delta(\underset{\sim}{q}) \ , \ \alpha \to o \ , \ \hat{z} = \hat{q} \tag{7}$$

When use is made of (7) in (4) we obtain

$$T^{(1)}_{nn_1m}(V_{12}) = \frac{\delta(m,o)\,32\pi Z_1 Z_2 e^2 \sqrt{n}\,\alpha_o^{5/2}\alpha^{3/2}}{C^2[\alpha_o^2 + (\underset{\sim}{B} - \underset{\sim}{C})^2]^2} ,$$

$$\alpha_o = \mu_{23} Z_2 Z_3/(m_e a_o) \ , \ \alpha = \mu_{13} Z_1 Z_3/(m_e n a_o) \to o \qquad (8)$$

At high incident energies $|\underset{\sim}{k}_2|$ will be independent of n(cf. Eq.(2)). Then (4) shows that $\underset{\sim}{B}$ and $\underset{\sim}{C}$ are also independent of n. In this case as n becomes large $T^{(1)}_{nn_1m}$ becomes proportional to n^{-1}. When the squared modulus of $T^{(1)}_{nn_1m}$ is summed with respect to $n_1 m$ 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 $\ln n$.

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

$$\frac{d\sigma}{d(\varepsilon/R)} = \frac{\sqrt{\varepsilon/R}\,\beta}{2[1-\exp(-2\pi\beta)]}\left[n^3\sigma(n)\right]_{n\to i\sqrt{R/\varepsilon}} , \ \beta = \frac{\mu_{13} Z_1 Z_3}{m_e\sqrt{\varepsilon/R}} \qquad (9)$$

where ε/R is the relative kinetic energy of the particles 1 and 3 in rydberg, and $d\sigma/d(\varepsilon/R)$ 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 $\varepsilon/R \to 0$ the continuum cross section goes to infinity as $(\varepsilon/R)^{-1}$.

We now consider the divergence in the second Born approximation. Designating the initial state by 100 and the final state by nn_1m, by a straightforward substitution in (1) we find that

$$T^{(2)}_{nn_1m} = \frac{2e^4}{\pi}\iint \frac{d\underset{\sim}{q}\,d\underset{\sim}{q}'\,x}{\left[\frac{\hbar^2k_2^2}{2\mu_2} + E(1,3) - \frac{\hbar^2q^2}{2\mu_2} - \frac{\hbar^2q'^2}{2\mu_{13}}\right](\underset{\sim}{k}_2-\underset{\sim}{q})^2(\underset{\sim}{k}_1+\frac{\mu_{13}}{m_3}\underset{\sim}{q}+\underset{\sim}{q}')^2}$$

$$x[Z_2Z_3U^*(nn_1m,\underset{\sim}{A})+Z_1Z_2U^*(nn_1m,\underset{\sim}{D})][Z_1Z_3U(100,\underset{\sim}{E})+Z_1Z_2U(100,\underset{\sim}{F})] \qquad (10)$$

where

$$\underset{\sim}{A} = -\underset{\sim}{q}' + \frac{\mu_{13}}{m_3}(\underset{\sim}{k}_2 - \underset{\sim}{q}) \;,\; \underset{\sim}{D} = -\underset{\sim}{q}' - \frac{\mu_{13}}{m_1}(\underset{\sim}{k}_2 - \underset{\sim}{q})$$
$$\underset{\sim}{E} = \frac{\mu_{23}}{m_3}\underset{\sim}{k}_1 + \underset{\sim}{q} \;,\; \underset{\sim}{F} = -\frac{\mu_{23}}{m_2}\underset{\sim}{k}_1 + \frac{\mu_{13}}{m_1}\underset{\sim}{q} - \underset{\sim}{q}' \qquad (11)$$

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 $T^{(2)}_{nn_1m}$ 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 $\underset{\sim}{A}$ and once $\underset{\sim}{B}$ 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 ℓn 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 ℓn 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.

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