0.1 Collisions Influenced by Interatomic Forces (pgs. 10-11)

In the previous section, it was assumed that the collision between the incident and target atom was instantaneous. In general, this is not true and often the atoms interact via an interaction force $F(r)$ which depends on the distance r between the atoms. The force here is the derivative of a potential function $V(r)$:

$$F(r) = -\frac{\partial V(r)}{\partial r} \tag{1}$$

The collision between the incident and target particle is essentially a central force problem when considering the center of mass frame of reference. Conservation of angular momentum states that

$$Mr^2\dot{\theta} = p\sqrt{2ME_R} = \text{constant} \tag{2}$$

where E_R is the total energy given by

$$E_R = \frac{M}{2}\left(\dot{r}^2 + r^2\dot{\theta}^2\right) + V(r) \tag{3}$$

If we let $u = \frac{1}{r}$, then we can rewrite this equation as

$$\left(\frac{\partial u}{\partial \phi}\right)^2 + u^2 = \frac{1}{p^2}\left(1 - \frac{V(r)}{E_R}\right) \tag{4}$$

Following Lehman and Shapiro [3], we can write this solution in the form of an integral equation. First, noting that $\frac{d}{du}\left(\frac{\partial u}{\partial \phi}\right)^2 = 2\frac{\partial^2 u}{\partial \phi^2}$, we can differentiate equation (4) with respect to u:

$$\begin{aligned}\frac{\partial^2 u}{\partial \phi^2} + u^2 &= \frac{1}{2p^2E_R}\frac{\partial V}{\partial u}\\ u'' + u^2 &= -g\end{aligned}$$

where the first equation is of the form of the second equation. To solve this equation for u, we note that the solution must have the form $u = u_h + u_p$ where u_h and u_p are the homogeneous and particular solutions of the equation. To get u_h, we solve the homogeneous equation

$$u_h'' + u_h^2 = 0 \tag{5}$$

The general solution is $u_h = C\cos\phi + D\sin\phi$. The particular solution is

$$u_p = -\int_0^\theta \sin(\phi - \phi')\, g(u(\phi'))\, d\phi'$$

since $u_p'' + u_p^2 = -g$. Now, $\sin\phi \to \frac{p}{r} = bu$ or $u = \frac{\sin\phi}{p}$ as $\phi \to 0$. It can be seen that as $r \to \infty$ $(u \to 0)$, u_p goes to zero faster than $\sin\phi$. As a result, $C = 0$ and $D = \frac{1}{p}$ and so

$$u = \frac{\sin\phi}{p} - \int_0^\theta \sin(\phi - \phi')\, f(u(\phi'))\, d\phi'$$

Solving equation (2) for θ in terms of p and u yields

$$\theta = \pi - 2p\int_0^{u_0} \frac{du}{\left(1 - \frac{V(u)}{E_R} - p^2u^2\right)^{\frac{1}{2}}} \tag{6}$$

Here, u_0 is the value of u for when the denominator of the integrand vanishes and corresponds to the reciprical of the distance of closest approach.

Unfortunately, equation (6) can only be solved in closed form for a select few forms of $V(r)$:

$$V(r) = \begin{cases} \dfrac{Z_1 Z_2 e^2}{r} & \text{Coulomb Potential} \\ C/r^2 & \text{Inverse Square} \\ \begin{cases} 0 & r > R \\ \infty & r < R \end{cases} & \text{Hard Sphere} \end{cases}$$

For the Coulomb potential, the two atoms follow the trajectories as in Figure 1. The energy transfer T is

$$T_{coulomb} = E_0 \sin^2 \frac{\theta}{2} \tag{7}$$

The impact parameter p is

$$p = b \cot \frac{\theta}{2} \tag{8}$$

where b is the impact parameter for head-on collisions. The differential cross section $d\sigma$ is

$$\begin{aligned} d\sigma &= \frac{\pi b^2}{4} \csc^3 \frac{\theta}{2} \cos \frac{\theta}{2} d\theta \\ &\propto \frac{\pi b^2}{4} E_0 \frac{dT}{T^2} \end{aligned} \tag{9}$$

Here we see that the differential cross section is dominated by small-angle scattering, probably leading to the Coulomb logarithm when evaluating the total cross-section. For the inverse square potential,

$$d\sigma \propto E_R^{-\frac{1}{2}} T^{-\frac{3}{2}} dT$$

0.2 Comparison of the Real Collision with a Hard Sphere Collision (pgs. 11-12)

The scattering angle θ should be largely determined by the interaction potential at the distance of closest approach. Using equation (2), the potential at this distance is

$$V(r_0) = E_R \left(1 - \frac{p^2}{r_0^2}\right) \tag{10}$$

where r_0 is the distance of closest approach. This distance depends mainly on how "hard" the potential is and how high the incident particle energy E_R is. For small impact parameters, we can consider two hard spheres of radius $R = r_0/2$. In this case, the second term in (10) is approximately zero and so

$$V(r_0) = V(2R) \approx E_R \tag{11}$$

For equal masses,

$$V(2R) = \frac{E_0}{2} = \frac{T_{max}}{2} \tag{12}$$

We see that, in the center of mass frame, the kinetic energy of the incident particle is completely transferred to potential energy at the distance of closest approach r_0. Note that this is true *only* in the case of a pure two-body collision (no external forces from other atoms). We thus need to come up with a way to describe a more realistic potential that includes contributions from other atoms.

0.2.1 The Interatomic Potential (pgs. 12-13)

In atomic units, the potential due to a point charge $Z_1 e$ at a distance r is

$$V(r) = \frac{Z_1 e}{r} \tag{13}$$

For an atom with protons and electrons, the potential of the nucleus is shielded by the electrons that surround it:

$$V(r) = f\left(\frac{r}{a}\right) \frac{Z_1 e}{r} \tag{14}$$

where $f\left(\frac{r}{a}\right)$ is the screening function with screening length a. The form of the potential thus depends on the chosen form of f. Several forms of f have been proposed:

$$f\left(\frac{r}{a}\right)=\begin{cases} e^{-\frac{r}{a}} & \text{Bohr} \\ \frac{r}{a_1}e^{-\frac{C_1 r}{a_1}} & \text{Born-Mayer} \\ \psi\left(\frac{r}{a_2}\right)-\frac{C_2 a_2}{r} & \text{Thomas-Fermi} \end{cases} \tag{15}$$

where $\psi\left(\frac{r}{a_2}\right)$ is the solution of the differential equation

$$\psi''\left(\frac{r}{a_2}\right)=\left[\psi\left(\frac{r}{a_2}\right)\right]^{\frac{3}{2}}\cdot\left(\frac{r}{a_2}\right)^{-\frac{1}{2}}\cdot\psi\left(\frac{r}{a_2}\right) \tag{16}$$

Gombas modified the Thomas-Fermi function to have the same form for $f\left(\frac{r}{a}\right)$, but with $\psi\left(\frac{r}{a_3}\right)$ being the solution to

$$\psi''\left(\frac{r}{a_3}\right)=\frac{r}{a_3}\left[\frac{\left(\psi\left(\frac{r}{a_3}\right)\right)^{\frac{1}{2}}}{(r/a_3)}+\left(\frac{C_3 a_3}{2e}\right)^{\frac{1}{2}}\right]^3 \tag{17}$$

So long as we can define the potential due to one atom, we can use superposition to define the potential due to multiple atoms. Brinkman showed that the potential for a system of two atoms is [1]

$$V(r)=\frac{Z_1 Z_2 e^2}{r}\left[\frac{a_1^2\exp\left(-\frac{r}{a_B}\right)-a_2^2\exp\left(-\frac{r}{a_A}\right)^2}{ra_A^2-a_B^2}\right],\ a_A\neq a_B \tag{18}$$

where a_A and a_B are the screening lengths for the two atoms. If $a_A=a_B=a$ in the case of two identical atoms, then

$$V(r)=\frac{Z^2e^2}{r}\exp\left(-\frac{r}{a}\right)\left(1-\frac{r}{2a}\right) \tag{19}$$

As $r\to 0$, $V(r)$ resembles the Coulomb potential (not sure how though...seems blatantly inconsistent. Perhaps since $V\to\infty$ as $r\to 0$ for both potentials?). We see that V closely resembles the Bohr potential

$$V(r)=\frac{Z_1 Z_2 e^2}{r}\exp\left(-\frac{r}{a}\right) \tag{20}$$

The form of the screening length a was suggested by Bohr to be

$$a=a_0\left(Z_1^{\frac{2}{3}}+Z_2^{\frac{2}{3}}\right)^{-\frac{1}{2}} \tag{21}$$

where a_0 is the Bohr radius. For small impact parameters and large incident energy, the electron cloud has a negligible screening effect, corresponding to Rutherford scattering (clearly screening matters for small incident energies). For large impact parameters ($r\gg a$), V falls off rapidly, which corresponds to a large screening effect. Thus, there is a preference (higher probability) for small angle scattering with the Bohr potential.

0.2.2 The Form of the Scattering Law for a Realistic Potential (pgs. 13-14)

Using the form of the Bohr potential in equation (20), the scattering angle θ is given by equation (6)

$$\theta=\pi-2p\int_0^{u_0}\frac{du}{\left[1-\frac{Z_1 Z_2 e^2}{E_R}u\exp\left(-\frac{1}{au}\right)-p^2u^2\right]^{\frac{1}{2}}} \tag{22}$$

This integral equation can only be solved numerically and has been done by Everhart, Stone, and Carbone [2]. Starting from the differential cross-section for an arbitrary V

$$\sigma(\theta) = -\frac{p}{\sin\theta}\frac{dp}{d\theta} \tag{23}$$

we can rewrite equation (22) as

$$\begin{aligned} \theta &= \pi - \frac{2p}{a}\left[\int_0^Z y_0^{-\frac{1}{2}}dz - \int_0^Z \left(y_0^{-\frac{1}{2}} - y^{\frac{1}{2}}\right)dz\right] \\ y &= 1 - \left(\frac{p}{a}\right)^2 Z^2 - \left(\frac{b}{a}\right) Z\cdot\exp\left(-\frac{1}{Z}\right) \\ y_0 &= 1 - \left(\frac{p}{a}\right)^2 Z^2 - \left(\frac{b}{a}\right) Z\cdot\exp\left(-\frac{1}{Z_0}\right) \end{aligned} \tag{24}$$

where Z_0 is the root of the equation for y and b is the impact parameter for a head-on collision, as before, given by

$$b = \frac{Z_1 Z_2 e^2}{E_R} \tag{25}$$

In the limit of $\frac{b}{a} \to 0$, screening is negligible and the potential V is the Coulomb potential where the differential cross section becomes the Rutherford formula

$$\sigma(\theta) = \frac{b^2}{16}\csc^4\left(\frac{\theta}{2}\right) \tag{26}$$

which is true for high energies. But as the incident energy decreases, $\frac{b}{a}$ increases and thus screening must be taken into account. A plot of $\frac{\sigma(\theta)}{b^2}$ vs. θ was made for various values for $\frac{b}{a}$ and is shown below in Figure 1.

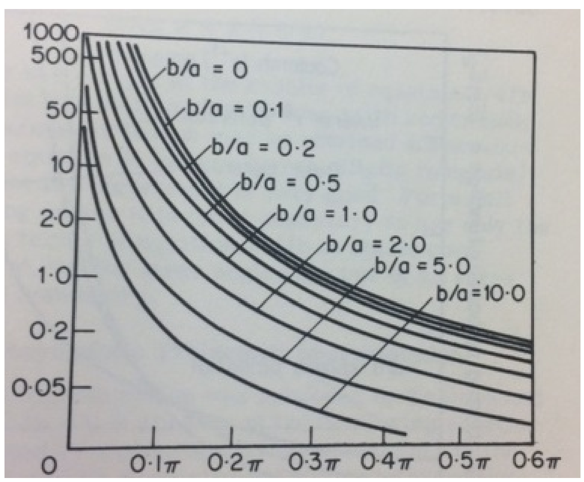

Figure 1: Plot of the differential scattering cross section $\frac{d\sigma(\theta)}{b^2}$ as a function of the scattering angle θ in the center of mass system.

Since the scattering angle θ is related to the energy transfer T through equations (11)-(13) and thus to the scattering probability function $g(E_1, E_2)$ from equation (19), we can plot g as a function relative energy retention E_2/E_1 for the case of Coulomb, inverse r^2, Bohr, and hard sphere potentials. In order to compare the Bohr potential with the hard sphere potential, since the first two can be solved in closed form, we use the relation $V(2R) = E_R$ as in equation (11) to rewrite the Bohr potential as

$$V(2R) = \frac{E_B}{2}\exp\left(-\frac{2R}{a_B}\right) / \left(\frac{2R}{a_B}\right) = \frac{A}{A+1}\frac{1}{2E_R} \tag{27}$$

where E_B is the Bohr energy

$$E_B = \frac{2Z_1 Z_2 e^2}{a_B}$$

The hard sphere radius was chosen so that $2R = 5.25a_B$, in the range where excessive screening can occur. Figure below shows the plot of g vs. θ.

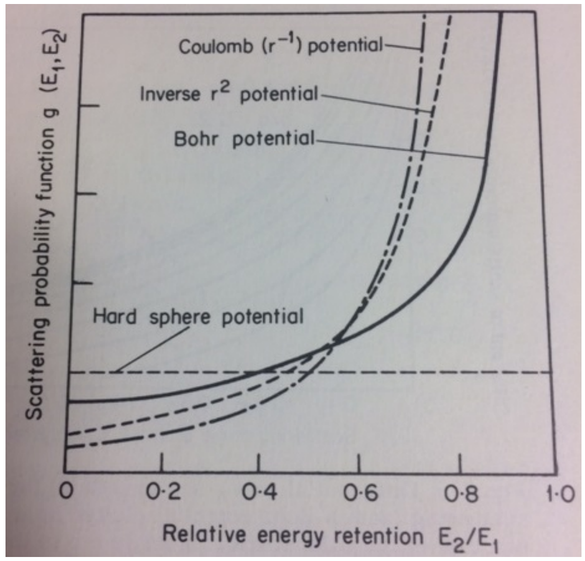

Figure 2: Plot of the scattering probability function g as a function of relative energy retention $\frac{E_2}{E_1}$

We see that, for the hard sphere potential, the scattering probability is constant, as we would expect from the results of the previous sections. However, for the other potentials, it is much more likely that the energy retention would be high (and thus small energy transfer T), corresponding to large impact parameters and grazing collisions. Even though the hard sphere potential may be a poor approximation comparatively, it has a well-defined total cross section, $\sigma = 4\pi R^2$ whereas the other potentials have infinite cross sections due to to small-angle scattering. Often the potential is cut off at a certain distance to ensure a finite cross-section, leading to the Coulomb logarithm.

References

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[3] Guy W. Lehman and Kenneth A. Shapiro. Approximate analytic approach to the classical scattering problem. *Physical Review*, 120(1):32–36, oct 1960.