SCATTERING OF IONS BY ATOMS

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The dependence of the impact parameter on energy of relative motion and scattering angle, and the transport cross section for atomic collisions are calculated using the interatomic potential previously found by the author from the Thomas-Fermi statistical theory of the atom.

INTRODUCTION

IF we treat the scattering of ions or atoms by atoms as elastic, and limit ourselves to scattering angles $\alpha > 10^{-2}$ (in the c.m. system), we find that, for energies of relative motion $E > 100$ ev/M (where M is the reduced mass in units of the mass of the hydrogen atom), the scattering is determined by the laws of classical mechanics. For very high energies, when the relative velocity of the colliding atoms exceeds $Z_1Z_2e^2/\hbar$, classical mechanics is not applicable, but the scattering is practically determined by the coulomb interaction, for which the results of quantum and classical mechanics coincide.

We may therefore assume that the scattering as calculated by the methods of classical mechanics gives the correct result for collision energies greater than 100 ev/M. The energy is limited from above only by relativistic velocities.

Actually, for energies exceeding ~ 1 kev, in addition to elastic scattering there is scattering accompanied by excitation, single or multiple ionization, and charge exchange of the colliding atoms.[1] As a result of this there is some uncertainty in the kinetic energy and interaction potential of the colliding atoms, which results in an additional smearing out of the wave packet which is not taken into account in deriving the condition for applicability of classical mechanics to elastic scattering.

However, for low collision velocities the probability of inelastic processes is small. For velocities exceeding 10^7 cm/sec the cross sections for elastic and inelastic scattering are of the same order, but appreciable scattering occurs only for strong overlapping of the electronic shells of the atoms. In this case the interaction potential is determined practically by the inner electrons alone, and they have velocities which are large compared to the velocity of the colliding atoms, and are weakly excited. Excitation of electrons in the outer shells of the atoms hardly changes the scattering potential. Finally, if the velocity of the colliding atoms is of the same order as, or greater than the velocity of the inner electrons, the scattering is practically coulombian. The change of kinetic energy in the collision process is also relatively slight,[2] not exceeding a few percent.

So, independently of the inelastic processes occurring during collision of the atoms, we can calculate approximately the dependence of the scattering angle on the impact parameter, using the potential for elastic interaction according to classical mechanics.

Such a calculation is needed for all sorts of problems; the depth of penetration of accelerated ions into matter; the disruption of the atomic lattice during penetration of ions into a solid (provided their velocity is so small that they lose energy mainly by elastic collision and not by ionization of the atoms; the determination of the energy which is given to the atoms of a gas during collisions with a beam of ions, and also the corresponding cross sections.

Here we treat only collisions with energies significantly greater than the ionization potential of the atoms (~ 1 kev or greater), where appreciable scattering is observed when there is a considerable overlap of the electronic shells of the atoms. It is only in this case that the scattering potential can be determined for any pair of colliding atoms on the basis of the statistical model.[3] When this is not the case, the interaction depends essentially on the outer electron shells of the atoms and must be determined individually for each colliding pair. In this latter case, the scattering itself is obviously isotropic (except for the region of very small angles), and has a weak energy dependence, while the cross section is of the order of gas-kinetic values.

DIMENSIONLESS ENERGY AND IMPACT PARAMETER

In a previous paper[4] it was found that, to an accuracy of 10%, the interaction potential for atoms, calculated on the basis of the statistical model for the electrons, can be represented as

$$U(r) = \frac{Z_1 Z_2 e^2}{r} \chi\left(\psi(Z_1, Z_2)\frac{r}{a}\right), \quad (1)$$

where $\chi(x)$ is the screening function in the Thomas-Fermi potential, Z_1 and Z_2 are the atomic numbers of the interacting atoms, r is the distance between the nuclei,

$$a = (9\pi^2/128)^{1/3}\hbar^2/me^2 = 4.7\cdot 10^{-9}\ \text{cm}, \quad (2)$$

$$\psi(Z_1, Z_2) = (Z_1^{1/2} + Z_2^{1/2})^{2/3} \quad (3)$$

for $0 < x < 15$, which describes the whole range of interactions, including $Z_1 = Z_2 = 100$.

The function (1) can be improved by using

$$\psi = 3[(Z_1 + Z_2)^{7/3} - Z_1^{7/3} - Z_2^{7/3}]/7Z_1Z_2, \quad (4)$$

for $0 < x < 2$, and

$$\psi = (Z_1^{3/3} + Z_2^{3/3})^{1/2}. \quad (5)$$

for $2 < x < 7$. Expressions (3), (4), and (5) coincide if Z_1/Z_2 is either large or small. For $Z_1 = Z_2$, the values of expressions (3), (4), and (5) are in the ratio 1:0.82:0.89. Possibly, such an improvement exceeds the accuracy of the theory.

The polar angle φ, which is related to the scattering angle α, is given in classical mechanics by the formula

$$\varphi = \frac{\pi - \alpha}{2} = \int_{r_0}^{\infty} \frac{p\,dr}{r^2\sqrt{1 - U(r)/E - (p/r)^2}}, \quad (6)$$

where p is the impact parameter, E is the kinetic energy of relative motion for $r \to \infty$, and

$$1 - U(r_0)/E - (p/r_0)^2 = 0. \quad (7)$$

If we introduce a new variable

$$x = \psi r/a, \quad (8)$$

then

$$U(r)/E = (Z_1Z_2\psi e^2/Ea)(\chi(x)/x) = V(x)/\mathcal{E}, \quad (9)$$

where $V(x) = \chi(x)/x$, and the dimensionless energy $\mathcal{E}$ is

$$\mathcal{E} = Ea/e^2Z_1Z_2\psi = E/30.5\,Z_1Z_2\psi, \quad (10)$$

where E is expressed in ev. If in addition we define a dimensionless impact parameter by

$$b = \psi p/a, \quad (11)$$

then (6) is expressed as

$$\alpha = \pi - 2\int_{x_0}^{\infty} \frac{b\,dx}{x^2\sqrt{1 - V(x)/\mathcal{E} - (b/x)^2}}, \quad (12)$$

where, in accordance with (7),

$$1 - V(x_0)/\mathcal{E} - (b/x_0)^2 = 0. \quad (13)$$

The solution of Eq. (12) for $b = b(\alpha, \mathcal{E})$ enables us, by calculating a single integral, to find the differential scattering cross section for any pair of colliding atoms, or for an atom and a singly charged ion:

$$\sigma(\alpha) = pdp/\sin\alpha d\alpha = a^2 b\,db/\sin\alpha d\alpha. \quad (14)$$

It is assumed that for strong interaction, when the electron shells of the atoms overlap, ionization of one of the atoms before collision is not very likely.

Frequently one is interested in the transport cross section

$$\sigma^* = \int_0^{\infty} (1 - \cos\alpha)\,2\pi pdp = \pi\int_0^{\pi} p^2 \sin\alpha\,d\alpha = a^2\sigma^{(*)}, \quad (15)$$

where

$$\sigma^{(*)} = \pi\int_0^{\pi} b^2 \sin\alpha\,d\alpha, \quad (16)$$

is the dimensionless transport cross section.

CALCULATION OF $b(\alpha, \mathcal{E})$ AND $\sigma^{(*)}(\mathcal{E})$

For the calculation of the polar angle, it is convenient to set $x = x_0/\cos\theta$ in (12), so that

$$\alpha = \pi - \frac{2b}{x_0}\int_0^{\pi/2} y(\theta)\,d\theta,$$

$$y(\theta) = \sin\theta\left[1 - \frac{V(x_0/\cos\theta)}{\mathcal{E}} - \left(\frac{b}{x_0}\right)^2\cos^2\theta\right]^{-1/2}. \quad (17)$$

The integrand in (17) has no singularities, is equal to 1 for $\theta = \pi/2$, while for $\theta \to 0$,

$$y(\theta) \to [(b/x_0)^2 - x_0V'(x_0)/2\mathcal{E}]^{-1/2}, \quad V'(x) < 0. \quad (18)$$

The derivative $y'(\theta)$ is equal to zero for $\theta = 0$ and $\theta = \pi/2$. If $V(x) \sim x^{-2}$, $y(\theta) \equiv 1$. It is also useful to introduce an "index" $n(x)$ according to the formula

$$n(x) = -xV'(x)/V(x).$$

The meaning of $n(x)$ is that, for values of x not too much greater than x_0,

$$V(x) \approx V(x_0)(x_0/x)^{n(x_0)} \quad (19)$$

$n(x)$ varies very slowly: from unity for $x = 0$ to $n \approx 3$ for $x = 15$. Using $n(x)$, the expression (18) is transformed to

$$\left[1-\left(1-\frac{1}{2}n(x_0)\right)V(x_0)/\mathcal{E}\right]^{-1/2}.$$

Since $V(x)$ is a monotonically decreasing function of x, and $V(x_0)$ is always less than $\mathcal{E}$, from our discussion, to an accuracy of 1%, the integral (17) is easily calculated for several points. However, when $\alpha = 0.3$, an error of 1% in the integral (17) gives an error of 10% in α. So for $\alpha < 0.3$, α is extrapolated using a power law: if $V(x)$ is written in the form of (19), then for small angles,

$$\alpha \approx -\frac{1}{\mathcal{E}}\int_b^\infty V'(x)\frac{b\,dx}{\sqrt{x^2-b^2}} \sim 1/\mathcal{E}b^{n(b)}. \qquad (20)$$

The results of the calculations for $\alpha \geq 0.3$ are given in the table.

The value of b for $\alpha < 0.3$ can be found by extrapolation using (20):

$$b = b(0.3;\ \mathcal{E})(0.3/\alpha)^{1/n}.$$

A good approximation for $\alpha \leq 1$ is

$$\alpha = V(b)\sqrt{\pi n(b)/2 - 0.57}/\mathcal{E},$$

for which $n(b)$ has the following values:

$b=$	0	0.3	0.5	1	2	3	4	6	8	12	20	∞
$n=$	1	1.3	1.5	1.7	2	2.2	2.4	2.6	2.8	2.9	3	4

where the value of b should be taken as the nearest greater value than that from $b(0.3, \mathcal{E})$.

In the interval $0.7 < x < 5$, $V(x)$ differs little from $0.45x^{-2}$. For $\alpha \geq 0.3$, there correspond to this range in x the values $0.05 < \mathcal{E} < 1$, where to sufficient accuracy we can replace $V(x)$ by $0.45x^{-2}$ and evaluate the integral (17) analytically. Finally, for $\mathcal{E} > 10$, $x \ll 1$, $\chi(x) \approx 1$, $V(x) \approx 1/x$ and

$$b = 1/2\mathcal{E}\tan\frac{\alpha}{2}. \qquad (21)$$

In intermediate cases, $b(\alpha, \mathcal{E})$ is found by standard interpolation in α and $\mathcal{E}$.

The transport cross section was also calculated using (15). The results of the calculation using the table are described to good accuracy by the formula (for $\mathcal{E} \geq 0.02$)

$$\sigma^{(*)} = (\pi/\mathcal{E})\ln(1+0.7\mathcal{E}), \qquad (22)$$

or

$$\sigma^* = \pi(Z_1Z_2e^4/E^2)\ln(1+0.7E/30.5Z_1Z_2\psi),\ (E \text{ Bev}).$$

The dependence of $p(\alpha, \mathcal{E})$ for collision of argon ions and argon atoms with relative energy 37.5 ev was determined in the work of Kaminker and Federenko[5] from the formula

$$p^2 = 2\int_\alpha^\pi \frac{d\sigma}{d\Omega}\sin\alpha\,d\alpha, \qquad (23)$$

Values of $b(\alpha, \mathcal{E})$

$\mathcal{E}$ \ α	0.3	0.5	0.7	1	1.5	2	2.5	$2.5 < \alpha < \pi$
0.02	8.8	6.7	5.6	4.2	2.8	1.8	1.0	
0.03	7.4	5.8	4.6	3.5	2.3	1.5	0.8	$1.3(\pi-\alpha)$
0.05	6.0	4.6	3.8	2.9	1.9	1.2	0.65	$1.0(\pi-\alpha)$
$0.05 < \mathcal{E} < 1$	$b \approx (\pi-\alpha)[0.45/(2\pi-\alpha)\alpha\mathcal{E}]^{1/2}$							
1	1.45	1.00	0.76	0.55	0.34	0.21	0.11	$0.18(\pi-\alpha)$
1.5	1.10	0.78	0.58	0.41	0.25	0.15	0.08	$0.12(\pi-\alpha)$
2	1.90	0.63	0.47	0.33	0.19	0.12	0.06	$0.09(\pi-\alpha)$
3	0.72	0.47	0.33	0.23	0.15	0.090	0.045	$0.07(\pi-\alpha)$
4	0.60	0.37	0.26	0.18	0.11	0.070	0.035	$0.053(\pi-\alpha)$
5	0.50	0.30	0.23	0.15	0.093	0.060	0.030	$0.045(\pi-\alpha)$
7	0.36	0.23	0.17	0.12	0.070	0.042	0.022	$0.033(\pi-\alpha)$
10	0.28	0.18	0.11	0.087	0.050	0.029	0.046	$0.024(\pi-\alpha)$

where $d\sigma/d\Omega$ is the "total differential cross section," i.e., the sum of all the differential cross sections for elastic and inelastic scattering as well as charge exchange. Actually the measurements were done only over the angular range $1° \leq \alpha \leq 22°$. The authors then extrapolated $d\sigma/d\Omega$ up to $\alpha = \pi$. So actually (23) was calculated using the formula

$$p^2 = 2\int_\alpha^{22°}\frac{d\sigma}{d\Omega}\sin\alpha d\alpha + p_0^2, \qquad (24)$$

where

$$\rho_0^2 = 2\int_{24°}^{\pi}\frac{d\sigma}{d\Omega}\sin\alpha\,d\alpha$$

was largely determined by quite arbitrary extrapolation of $d\sigma/d\Omega$. As a result of this extrapolation, they found a marked change in the behavior of $p(\alpha)$ in going from $\alpha = 16°$ to $\alpha = 24°$. We have recomputed their results, choosing p_0 so that the smooth variation of $p(\alpha)$ is not spoiled. Instead

of $p_0 = 5 \times 10^{-10}$ cm we used $p_0 = 1.26 \times 10^{-9}$ cm, after which the comparison of experimental and theoretically calculated values of $p(\alpha)$ looks as follows (in the lowest line, the uncorrected values of $p(\alpha)$ are given in parentheses):

α,°	2	4	6	8	10	12	16	20	24
$10^9 p_{\text{theor.}}$	5.6	4.1	3.3	2.9	2.5	2.3	1.9	1.7	1.54
$10^9 p_{\text{exp.}}$	7.8	5.5	4.1	3.1	2.5	2.1	1.6	1.4	1.26
	(7.7)	(5.3)	(3.9)	(2.8)	(2.3)	(1.8)	(1.2)	(0.8)	(0.5)

The calculated values of $p(\alpha)$ correspond approximately to a potential $\sim 1/r^2$. The experimental values for $\alpha > 6°$ are closer to a Coulomb law with $Z_1Z_2 = 114$ (fitted at $\alpha = 10°$). Thus according to experiment[5] the scattering proceeds as if right at the start of interaction all the outer shells of both of the colliding atoms flew off, or at least were "swollen" considerably (i.e., excited), while the inner (neon-like) shells were left complete.

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