Theoretical description of collisions in plasma : classical methods

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Abstract. — In the paper a general idea of deterministic (classical) approach to atomic collision phenomena is presented. The key points of the theory, which has the concept of a point electron carrying a point mass and a point charge as a basis, are briefly explained. The binary encounter approximation (b.e.a.) and the unperturbed collective field approximation (u.c.f.a.), the two fundamental ways of approximate analysis of the many body atomic collision problem are described and application of the both to calculation elementary processes in a plasma is shown. Possibility of precise estimation the value of the Coulomb logarithm is analysed and new point of view on the concept of the screening radius is presented. Perspectives of the deterministic approach are discussed.

1. **Introduction.** — The huge variety of phenomena that are observed in ionized gases has the origin in a relatively small number of atomic processes. The collisional ionization, which is the main source of free charges in a plasma, is one of the most important among them. Slowing down of charged particles is the other important process, which along with the collisional ionization plays the decisive role in electrical break-downs. Current flow and heat transport are almost in whole determined by electron scattering properties of atoms and molecules. Atomic scattering cross section is involved in any calculation considering the transport properties of ionized gases. Capture and excitation are the other two quantities which must be taken into account in most of the plasma calculations.

These and many other processes can be relatively easily described on the grounds of the assumption that the atom can be considered as a collection of point particles, the behaviour of which is *in the first instance* governed by the Newtonian dynamics and the Coulomb interaction.

Here the main points of the theory which has the above assumptions as a basis, and in fact was initiated at the beginning of the twentieth century with a famous work of Rutherford [1] and with eliminated by quantum mechanics works of Thomson [2], Thomas [3] and Williams [4], will be briefly described and applicability of the theory to analysis of processes in ionized gases will be discussed.

2. **Mathematical formulation of the atomic collision problem.** — With the assumption that electrons and nuclei can be considered as point particles carrying a point charge (q) and a point mass (m) the whole collision problem becomes reduced to analysis of the following set of equations

$$m_i \frac{\mathrm{d}^2\mathbf{r}_i}{\mathrm{d}t^2} + \sum_{i \neq j}^{n} q_i\, q_j\, \nabla_i\left(\frac{1}{r_{ij}}\right) = 0 \qquad i = 1, 2, \ldots, n\,, \tag{1}$$

where the number of equations is equal to the total number of particles involved in the collision. For solving the problem $2\,n$ constants defining initial conditions must be specified. In atomic collision problem those are : two sets of constants C_ξ^A and C_ξ^B describing the internal motion of electrons in isolated atoms, A and B, and data describing the initial motion of the whole atoms in space. Among the latter are : the relative velocity of atoms — v_{rel}, and two coordinates, the impact parameter D and the angle Θ, which in the plane perpendicular to the vector of relative velocity localise initial atomic trajectories in space (see Fig. 1). All C_ξ, which describe the behaviour of all electrons of the colliding atoms before collision, change in result of collision to C'_ξ. The all C'_ξ become known with solving the whole system of eq. (1). If relations between C_ξ and C'_ξ are known, that is the following relation is known

$$C'_\xi = f_\xi(D, \Theta\,; C_1, C_2, \ldots, C_\xi, \ldots, C_{2(n-2)})\,, \tag{2}$$

the cross section, which determines probability of definite change in $C_\xi (C_\xi \to C'_\xi)$ that is the probability of definite change in the state of colliding atoms can be

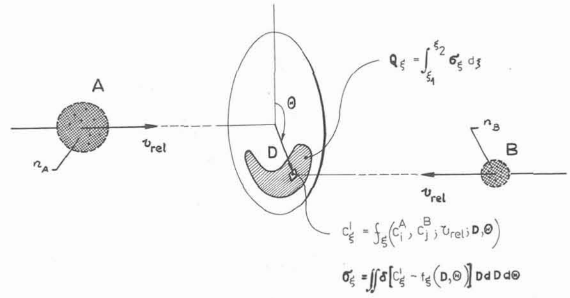

Fig. 1. — The collision between two sets of charged particles A and B is defined by internal motion of their components (by n_A and n_B constants C_i^A and C_j^B), the initial relative velocity v_{rel}, the impact parameter D and the azimuthal orientation of the shot line Θ. Cross section represents the sum of surface elements $D\,\mathrm{d}D\,\mathrm{d}\Theta$ for which the considered change ξ in the motion of the whole system or its components is observed.

calculated. Cross section which is formally defined in the following way [5]

$$\sigma_\xi = \int_0^{2\pi} \int_0^{\infty} \delta[C'_\xi - f_\xi(D, \Theta)] \, D \, \mathrm{d}D \, \mathrm{d}\Theta \,, \quad (3)$$

represents thus the sum of surface elements $D \, \mathrm{d}D \, \mathrm{d}\Theta$ for which relation (2) is fulfilled (see Fig. 1).

This formally trivial problem encounters great mathematical difficulties [6, 7]. Isolated collision between two elementary particles, that is the binary encounter, is the only case for which the exact analytical solution is known. Collisions in which three elementary particles are involved represents in fact the limit of exact numerical analysis. Practically, the only way of describing the collision processes which in ionized gases play the important role are approximate methods.

The well known binary encounter approximation (b.e.a.) is one of them [5-10]. In this approximation the collision between two systems of charged particles (atoms, molecules) is considered as a sum of independent binary collisions between the components of the both systems. In such a case, which in general is valid at large relative velocities of the systems, the cross section has the form :

$$\sigma = \sum_{i=1}^{n_A} \sum_{j=1}^{n_B} \iint f_A(\mathbf{v}_i^A) \, f_B(\mathbf{v}_j^B) \, \sigma^{\text{b.e.}}(\mathbf{v}_i^A, \mathbf{v}_j^B) \, \mathrm{d}\mathbf{v}_i^A \, \mathrm{d}\mathbf{v}_j^B \,, \quad (4)$$

where $f_A(\mathbf{v}_i^A)$ and $f_B(\mathbf{v}_j^B)$, being called the velocity distribution functions, describe in a probabilistic way the motion of individual particles in isolated systems, A and B, and $\sigma^{\text{b.e.}}(\mathbf{v}_i^A, \mathbf{v}_j^B)$ is the binary encounter cross section.

The other completely different approach, valid in general at weak interaction between systems, at large distances between systems, deals with the interaction

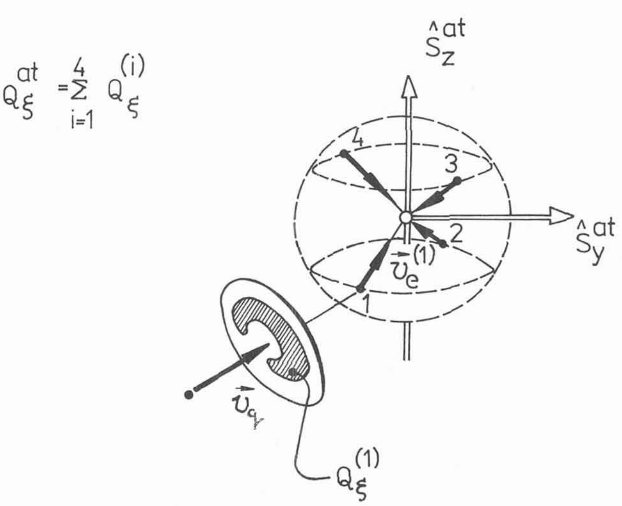

Fig. 2. — In the binary encounter approximation (b.e.a.) atomic cross sections is the sum of cross sections for collisions with atomic components (usually with atomic electrons).

of the whole systems through unperturbed collective fields [11]. Formally, this is again the two body problem, however now with very complicated interaction. To reduce mathematical difficulties and to enable physical interpretation, the atomic potential is usually expanded in series and a few of the first terms of the expansion are used in calculations. Experience show that in many cases it is sufficient to operate with the two first terms of the expansion only — the one which describes the static part of the field and the second which describes time variations of the field. Interaction between atoms can therefore be reduced to the atomic potential function of the following form :

$$\varphi^{\text{at}}(\mathbf{r}, t) \simeq \frac{C_n^\omega(\hat{r})}{r^{n+1}} \sin(\omega t) + \frac{C_m(\hat{r})}{r^{m+1}} \,, \quad (5)$$

where coefficients C_n^ω and C_m represent the main electric multipoles and their Fourier components. If all coefficients describing the atomic field, that is n, m, C_n^ω, C_m and ω, are known trajectories of colliding atoms can be determined, and cross section describing some sort of phenomena, elastic collisions for instance, can be calculated.

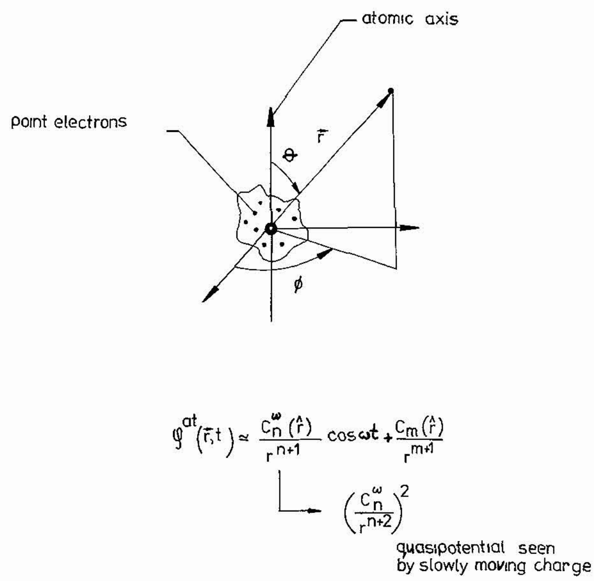

Fig. 3. — Atomic potential at large distances from the atom can be reduced to the two terms of the series expansion — the static and dynamic (oscillatory) multipole.

3. **Initial conditions for the atomic collision problem.** — To carry out concrete collisional calculations some at least informations about the colliding atoms (molecules) must be known. To derive the ionization cross section for instance, one must know how the electrons in the atom (molecule) are grouped, what are the binding energies of electrons and roughly what their motion is. Let us denote the number of electrons in the s shell by N_e^s, the ionization potential by U_i^s

and the atomic velocity distribution function, which describes the motion of electrons in the respective shell of the atom, by $p^s(v_e/\bar{v}_e^s)$. Then in the binary encounter approximation the ionization cross section formula, has the form :

$$\sigma_i = \sum_s N_e^s \int_0^\infty \sigma_i^{\text{b.e.}}(u_i^s, v_e) . p^s\left(\frac{v_e}{\bar{v}_e^s}\right) \mathrm{d}\left(\frac{v_e}{\bar{v}_e^s}\right), \quad (6)$$

where the sum is taken for all shells of the atom and $\sigma_i^{\text{b.e.}}$ is the binary encounter ionization cross section. Distribution of electrons and binding energies, until we are not concerned with complicated molecules, are known sufficiently well. It is not in the case of the velocity distribution. The knowledge of the velocity distribution function which is in fact equivalent to the knowledge of the all details of the electron motion in the atom, is at the moment very unsatisfactory. In some calculations, however, the details of the electron motion play a secondary role and the knowledge of the mean electron velocity $\bar{v}_e^s$ in the shell can be quite satisfactory. The electron ionization cross section for instance can be calculated with a relatively high degree of accuracy from the following simplified relation :

$$\sigma_i \simeq \sum_s N_e^s \, \sigma_i^{\text{b.e.}}(u_i^s, \bar{v}_e^s) . \quad (7)$$

This is a sufficiently good procedure in the case of ionization by fast heavy charged particles too, but it yields completely wrong results in the case of ionization by slow heavy particles [8, 12-14] (if velocities of the latter are distinctly smaller than $\bar{v}_e^s$). This follows from the fact that the greatest amount of energy which can be transfered to the light electron from the heavy projectile depends upon the velocity of the previous

$$\Delta E_{\max} \simeq 2\, m_e\, v_q(v_q + v_e) . \quad (8)$$

Ionization can exist until $\Delta E_{\max} < U_i$, that is until the projectile velocity is high enough — higher than the threshold velocity v_q^{thr}, which at $v_e \gg v_q$ is

$$v_q^{\text{thr}} \simeq U_i/2\, m_e\, v_e . \quad (9)$$

It follows from the above, that nontrivial threshold (at $E_q > U_i$) disappears with the electron velocity approaching infinity. Since the threshold is not experimentally observed the following conclusion can be drawn : electron velocities in the atom are unlimited. The only possibility of satisfying the above conclusion is synchronic zero angular momentum motion of all atomic shell electrons [15-17]. This is the motion which in the early twentiets was considered by Bohr and Sommerfeld and was rejected on the basis of arguments which in view of the later discovered properties of the electron appeared to be invalid [16].

In the case of a free-fall atomic model, with zero

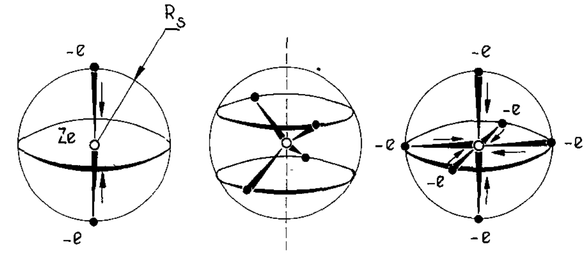

Fig. 4. — Free-fall atomic model — the first step towards the precise description of the atom.

angular momentum exactly radial electron orbits, the electron velocity distribution function has the form :

$$p\left(\frac{v_e}{\bar{v}_\theta^s}\right) = \frac{4}{\pi} \frac{1}{[1 + (v_e/\bar{v}_e^s)^2]^2} . \quad (10)$$

With the free-fall velocity distribution as given above many calculations were carried out and good agreement with experimental data was obtained [13, 14, 18].

Within the unperturbed collective fields approximation effective calculations are possible if at least first multipoles of the atomic field expansion in series are known. Unfortunately the knowledge of the latter, because of inquisitorial attitude of the quantum-mechanics ideology towards the classical concepts of atomic physics [16-20] is almost none. At the moment only very rough atomic model do exist (free-fall atomic model) and the rich experimental material of atomic collision physics and spectroscopy, which implicitly contains valuable informations about the atomic field, needs reinterpretation in the spirit of the

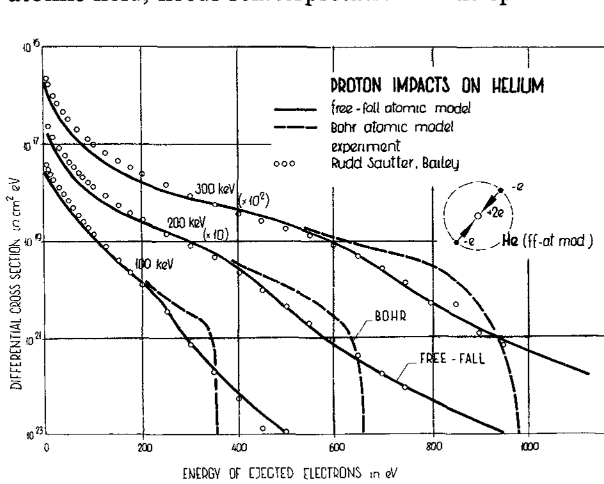

Fig. 5. — Ejection of electrons from helium atom by protons — one of many experiments investigated on the grounds of classical collision theory. Free-fall atomic model yields results which are in excellent agreement with the experimental data.

deterministic concepts outlined above (in quantum-mechanical approach atomic interaction appears as a result of polarization of initially exactly spherical distribution of a static electron cloud while in the Newton-Coulomb approximation the interaction is determined by the time dependent and aspherical from the very beginning potential of the collection of point charges being in dynamic equilibrium).

In result of reinterpretation of the low energy electron-atom and atom-atom scattering data [11] the two leading terms of the atomic field of noble atoms were deciphered. Those, excluding two-electron Helium atom, are : dynamic quadrupole and static octupole. In spherical coordinates the atomic potential of the noble atom has, therefore, the form :

$$\varphi(\mathbf{r}, t) \simeq A \frac{3\cos^2\theta - 1}{r^3} \sin \omega t + B \frac{\sin^3\theta \cos^3\phi}{r^4}, \qquad (11)$$

and the only difference between different noble atoms is in the value of coefficients A and B, and ω.

In the same way it has been found that dynamic octupole is the first term of the series expansion of the field of the hydrocarbon molecules C_nH_{n+2} and dynamic dipole is characteristic for the chemical π-bond [11].

Investigation of atomic energy level shifts [21], which are directly related to the deviation of the atomic core potential from the Coulomb potential, leads to the similar conclusions. Analysis of energy level shifts of alkalic metals, which have the noble-atom like atomic core, shows again that the octupole is a leading term of a static part of the atomic field of the noble atoms.

4. **Present possibilities of the classical collision theory.** — Effective application of the classical collision theory to analysis of elementary processes in ionized gases encounters two series of difficulties : mathematical, as we are concerned with the many body problem, and physical, as the knowledge of atomic systems specifying initial conditions of the collision problem is at the moment only fragmentary.

Nevertheless, at the present knowledge of atomic systems, and with the two approximate methods of analysis described above that is with the b.e.a. and with the u.c.f.a. some processes can be with accuracy satisfactory for plasma investigations effectively calculated. Among others are :

a) ionization (including inner shell ionization and multiply ionization),

b) excitation (including some $nl - n'\,l'$ transitions),

c) slowing down,

d) scattering of electrons from atoms and molecules,

e) atom-atom interactions.

The first three are those which can be effectively described with the b.e.a. and the other two with the u.c.f.a.

In the binary encounter approach, energy exchange cross section $\sigma_{\Delta E}$, which describes transfers of energy in a collision between two charged particles, forms the basis for almost all basic inelastic collision calculations. In result of appropriate integrations over ΔE one obtains :

a) ionization cross section

$$Q_i = \int_{u_i}^{\Delta E^-_{\max}} \sigma_{\Delta E}\, \mathrm{d}(\Delta E), \qquad (12)$$

b) excitation cross section

$$Q^n_{\mathrm{exc}} = \int_{u_n}^{u_{n+1}} \sigma_{\Delta E}\, \mathrm{d}(\Delta E), \qquad (13)$$

c) stopping power

$$S = \int_{\Delta E^-_{\max}}^{\Delta E^+_{\max}} \Delta E . \sigma_{\Delta E}\, \mathrm{d}(\Delta E), \qquad (14)$$

where the symbols U_i, U_n, $\Delta E^-_{\max}$ and $\Delta E^+_{\max}$ stand respectively for : ionization potential, excitation potential, and for the maximum gain and loss of energy in the individual binary collision.

Since b.e. cross sections depends upon velocities of colliding particles averaging over v_e and v_q must be carried out to obtain experimentally observed cross sections. Usually averaging over relative orientation of velocity vectors is the first step of calculations

$$\sigma(v_e, v_q) = \frac{1}{2} \int_{-1}^{+1} \sigma(v_e, v_q\,;\, \hat{v}_e . \hat{v}_q) . f(\hat{v}_e . \hat{v}_q)\, \mathrm{d}(\hat{v}_e . \hat{v}_q), \qquad (15)$$

while averaging over the atomic electron velocity is the next step of calculations

$$\sigma^{\mathrm{at}}(v_q) = \int \sigma(v_e, v_q) . f^{\mathrm{at}}(v_e)\, \mathrm{d}(v_e). \qquad (16)$$

This is the final formula of atomic collision physics. In plasma physics and in the physics of ionized gases averaging over v_q that is over velocity of plasma particles must be yet carried out :

$$\sigma^{\mathrm{pl}} = \int \sigma^{\mathrm{at}}(v_q)\, f^{\mathrm{pl}}(v_q)\, \mathrm{d}v_q. \qquad (17)$$

The two important distribution functions describing some idealistic situations in a plasma are :

a) Maxwell distribution function (describing the velocity distribution in a thermal equilibrium plasma).

b) Druyveistein distribution function (describing the velocity distribution of electrons in the gas at presence of electric field).

The other velocity distribution function derived recently during the analysis of magnetically insulated discharges, which play the fundamental role in ion beam fusion investigations, is the electron velocity distribution function for collisionless plasma at presence of crossed electric and magnetic fields. At negligibly small electron temperature the distribution has the form :

$$f_{(u)}^{\mathbf{E}\times\mathbf{H}} = \frac{1}{8\,\pi}\,\frac{1}{u^2}\,\frac{1}{\sqrt{1-u^2}}\,, \tag{18}$$

where u is the dimensionless electron velocity

$$u = \frac{v_e}{\sqrt{2}\,\dfrac{E}{H}}\,. \tag{19}$$

With the present computer technique all the cross sections listed above can be relatively easily calculated (see for instance Freeman and Jones [22]).

Analysis of processes within u.c.f.a. is a little bit more difficult, as one must usually start with numerical calculation of the individual particle orbit. Possibilities of deriving the cross sections in analytical form are almost none. In u.c.f.a. the latter can obtained in very specific situations only. Collisions at large impact parameters in one of them, as the relation between the scattering angle θ, which is very small then, and the impact parameter D can be obtained in analytical form. If moreover the relation $\theta = f(D)$ can be explicitly solved with respect to D the scattering cross section in explicite form can be determined. It is for instance possible when the atomic field description can be reduced to the one term of the series expansion. The scattering cross section has then the form :

a) if the leading term of atomic field expansion is a static multipole [23]

$$Q(\theta) \simeq \pi\left(\frac{C}{E.\theta}\right)^{2/(n+1)}, \tag{20}$$

b) if the leading term of atomic field expansion is a dynamic multipole [11]

$$Q(\theta) \simeq \begin{cases} \pi\left(\dfrac{C}{E.\theta}\right)^{2/(n+1)} & \text{for large velocities}\,, \\ \pi\left(\dfrac{v}{\omega}\right)^2 \ln^2\left(\dfrac{2}{\theta}\right) & \text{for small velocities}\,, \end{cases} \tag{21}$$

where E is the energy of scattered particle.

Excluding the above and few other specific cases, numerical analysis is the only possibility of effective calculations of concrete plasma collision problems in unperturbed collective field approximation.

5. **Coulomb logarithm and the screening radius.** — The energy loss function — S plays a fundamental role in analysis of transport properties of a plasma. It determines for instance extremely important in plasma research — the relaxation rates ; the precise knowledge of S is necessary in analysis of penetration the charged particles in different targets, particularly for calculation of deposits of energy in solid or gaseous pellets in ion beam fusion. Unfortunately the logarithmic term appearing in the binary encounter formula:

$$S \propto \ln\frac{m_e\,v_q^2\,D_{\max}}{Z_q.e^2}\,, \tag{22}$$

contains not well specified the impact parameter $D_{\max}$. Usually, in plasma calculations $D_{\max}$ is assumed to be equal to the Debye radius ; in atomic stopping power calculations one assumes, following Bethe, that $e^2/D_{\max}$ is equal to the mean ionization potential of the atom. The argument of the logarithm in the first case is usually a large number and the whole term, called the Coulomb logarithm, is in plasma calculations considered a constant quantity with the value somewhere between 10 and 20.

Intuitive, not exactly equivalent in the both cases, physical reasoning was the only justification for estimation of $D_{\max}$ [24]. The problem has however a more rigorous solution. The latter can be achieved by applying the appropriate method of mathematical analysis. This is the method of perturbation calculus developed by Gauss for analysis of evolution of planet any orbits. Simple analysis shows that the energy which can be transfered to the electron bound in the Coulomb field of nucleus from the charged particle moving at a distance D from the atom, at distances much larger than the distance between the nucleus and the electron, is

$$\Delta E \simeq 2\,\frac{Z_q^2.e^4}{D^2\,m_e\,v_q^2}\,e^{-\omega D/v_q}\,, \tag{23}$$

where ω is the angular frequency of the orbital motion of the electron, v_q is the velocity of the projectile and $Z_q.e$ is its charge. Until D is smaller than v_q/ω the interaction between the bound electron and projectile can be considered as the isolated binary collision. When the impact parameter becomes larger than v_q/ω, the interaction between the electron and the nucleus becomes dominant and a rapid decrease in energy transfer is observed. It is evident from the above that :

$$D_{\max} = v_q/\omega\,. \tag{24}$$

The result will be exactly the same if one assumes that the electron is not exactly free but is bound around some fixed point of space with a small but the finite force proportional to the displacement

$$\delta\mathbf{f} \simeq -\,k\,\Delta\mathbf{r}\,.$$

The result again has the form of eq. (23), where now

$$\omega = \sqrt{k/m_e}\,. \tag{25}$$

In the case of plasma electrons, which are bound with heavy ions through collective fields, the binary encounter limit is determined by the plasma frequency

$$\omega_{pl} = (4\,\pi n_e . e^2/m_e)^{1/2}\,. \tag{26}$$

In the particular case of the heavy particle moving in a plasma with a thermal velocity, eq. (24) and (26) yield the following formula :

$$D_{max}/\omega = \omega_{pl}\,,\; v_q = \overline{v}_q^{\text{thermal}} = (kT/4\,\pi n_e . e^2)^{1/2}\,, \tag{27}$$

which represents nothing else than Debye radius.

In general however D_{max} is different from the Debye radius and the formula (24) should be used. The correct expression for the Coulomb logarithm, therefore, is :

$$\ln \Lambda = \ln\left(\frac{m_e\, v_q^2}{Z_q . e^2}\,\frac{v_q}{\omega}\right), \tag{28}$$

where ω implicitly represents the interaction of electrons with heavy components of the matter (with positively charged nuclei).

6. **Other possibilities of the theory.** — Although b.e.a. and u.c.f.a. play the decisive role in analysis of atomic collisions, there are some processes which need for interpretation other or more precise mathematical treatment, or which within the Coulomb interaction law and newtonian dynamics can not be interpreted at all.

The capture of electrons by protons, for instance, represents the first case. It is a typical three body problem, which only numerically can be accurately solved. One can try to find of course the appropriate approximate methods — the concept of the switched binary encountery collision is one known possibility [4, 25] and two-fixed center problem is another [26].

The excitation and ionization through cumulation small amounts of energy is a process which in some cases may be extremely important. The process can be very effectively investigated with the mentioned above the perturbation method of Gauss [27]. Analysis of ionization in many electron atom collisions requires inclusion of statistics to binary encounter calculations [28, 29].

Some important features of the small angle scattering can be found on the grounds of the second order perturbation calculus [30]. It has been found for instance that quasipotential of the dynamic multipole, including the second order term, has the form

$$\varphi \simeq \frac{e^{-\omega r/v}}{r^{n+1}} + \varepsilon\left(\frac{1}{r^{n+1}}\right)^2,$$

where ε is much smaller than unity (in result quasipotential of the noble atom as seen by slowly moving charge has the form shown in figure 6).

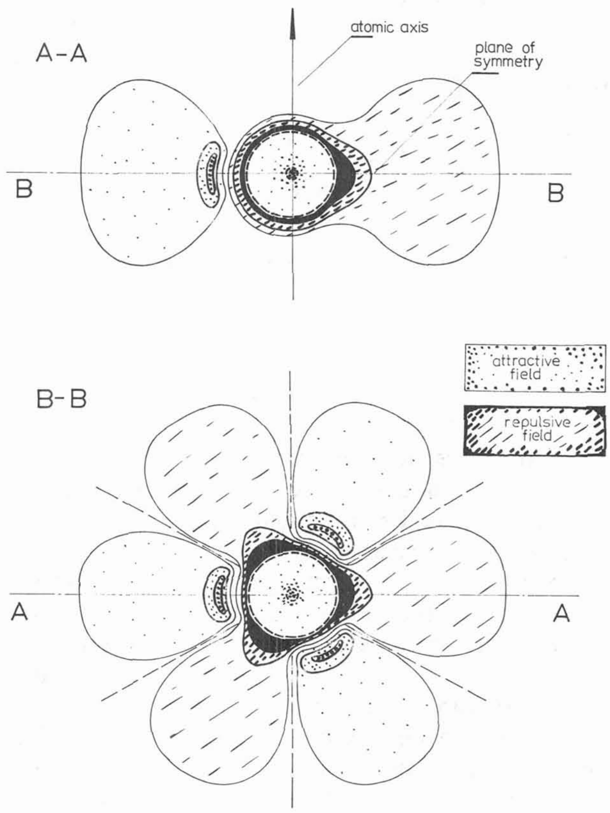

Fig. 6. — Quasipotential of the noble atom, as seen by slowly moving electron.

The problems which remain outside the scope of the Coulomb-Newton approximation are of course radiation phenomena — which as it has been shown previously are related with the gyromagnetic properties of the electron [31-33]. Gyromagnetic properties of the electron play an important role in orientation of atoms in external fields, what in some particular collision problems may be important. The other process which cannot be investigated with spin properties of the electron being neglected are polarisation effects.

At the moment, however, the main limitations in application of the classical collision theory to practical problems arise from the lack of information about the electron orbits in atomic systems. Further possibilities of effective description of processes in ionized gases of practical interest depend, therefore, mostly on further progress in deciphering of the electronic structure of atomic systems. Atomic collision physics may help much in solving this problem as investigation of atomic systems can be carried out with properly designed atomic collision experiments.

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