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INFLUENCE OF CRYSTAL LATTICE
ON MOTION OF ENERGETIC
CHARGED PARTICLES

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Synopsis

The paper describes a theoretical approach to the problems of directional effects for energetic charged particles moving through solids. Introductory comments on some aspects of directional effects are given in § 1. The fundamental approximations of the description are stated in § 2, and the associated simple concept of a string of atoms is introduced. A transverse continuum potential is a natural consequence of the basic approximations. The limit of applicability of continuum potentials is given by a critical angle. At high particle energies the critical angle is of an especially simple type. The critical angle separates particles behaving essentially as in a random substance from particles which do not come close to e.g. strings, with corresponding strong reduction of most physical processes. A number of examples are discussed, and critical angles belonging to atomic planes, strings, and pairs are compared. Characteristic features of a quantal treatment are briefly sketched.

§ 3 treats basic statistical estimates in calculations of directional effects. As a function of transverse energy, E_{\perp} , the slowing-down is calculated for electronic and nuclear collisions. Multiple scattering, i.e. lack of conservation of transverse energy, is studied in § 4. The normal multiple scattering, due to nuclear collisions, is strongly reduced for low values of E_{\perp} .

The rate of physical processes depends on the external angle between a beam and a crystal. In § 5 it is found that in simple cases the average of such rates over direction gives the same result as in a random system. Similar rules hold for spatial averages.

In § 6 experiments on directional effects are discussed from a theoretical point of view. The main effects to be taken into account are summarized. The order of magnitude of dip minima is estimated. The possibilities are discussed of using as an experimental tool the shadow belonging to e.g. strings. A few comments are made on recent experiments connected with string effects.

A more detailed investigation of classical deflections by lattice atoms, and the limits of validity of continuum potentials, is given in Appendix A, where also critical angles of particle emission from perfect strings are estimated. In Appendix B quantal corrections to the classical description are studied, and it is found that—in contrast to the familiar case of single collisions—the corrections are small at high velocities.

§ 1. Introduction

Measurements of range distributions and energy loss in single crystals have revealed directional effects, both for slow, heavy ions¹⁾ and, more recently, for protons²⁾. The first indications of directional effects for slow charged particles seem to be in observations on sputtering³⁾. Further indications were found in digital computer studies⁴⁾ of simplified models of penetration through lattices at extremely low particle energies.

The purpose of the present paper is to show that a comprehensive theoretical analysis may be made of directional effects in penetration of charged particles through crystal lattices. This analysis leads to conditions for the occurrence of a peculiar effect, described as atomic string effect. The corresponding string approximation is a well-defined approximation procedure by means of which primary and secondary directional effects can be treated. It then turns out that directional phenomena provide an interesting tool for solid state investigations, mainly because lattice points can be distinguished by means of a shadow effect. The theoretical results were summarized briefly in a recent note⁵⁾, and experiments were started along these lines⁷⁾.

At this point may be mentioned the well-known fact that, as a consequence of lattice periodicity, interference patterns of waves can be observed for both electromagnetic radiations and massive particles of not too short wave length. However, directional effects of that kind are not the subject of the present discussion, where mainly shadow phenomena are treated, with classical mechanics as a starting-point. Usually, the wave lengths of incoming particles are required to be exceedingly small and incoherence prevails, so that interference patterns are absent.

The basic case of the present approximation method is the case of high particle momenta. The classical orbital description of directional effects, as used in the following, is simple in this limit. In this connection it is also important that the classical approximation in directional phenomena turns out to be the better the higher the particle momentum, in contrast to most collision problems, where quantum mechanics takes over at high energies.

In the following chapters it is merely intended to present the general theoretical framework, with emphasis on a few basic phenomena and supplemented by a number of examples which can elucidate crucial problems. Several aspects, like quantal effects and thermal vibrations, are treated only in a cursory manner and need further study. Other problems, like the details of slowing-down, are not treated fully, because they are of secondary importance to the crucial questions discussed here.

The present chapter contains comments on some aspects of directional effects. A few facts are mentioned concerning slowing-down of charged particles.

Random systems

Although the spatial structure of a medium must have some influence on slowing-down and scattering of charged particles, the effect is normally disregarded. Several approximations are contained in a disregard of structure. They may be characterized by three mutually connected assumptions: homogeneity, isotropy, and randomness of the medium. The first two assumptions are often contained in the last one. An anisotropy due to lattice structure can thus result from some kind of correlation between collisions.

Suppose, that a penetrating particle has a certain differential cross section for scattering by single atoms, that its collisions with atoms of the medium are separable and independent, and finally, that the atoms are randomly distributed in space, with random orientation. Obviously, the slowing-down process is then independent of direction; the probability distribution in energy loss and scattering angle depends only on the mass per cm^2 penetrated, and is to be computed in a familiar way from single collisions. This is essentially a gas picture, and may be called a random system—implying homogeneity, isotropy, and random collisions. However, it is important to realize that the approximation of a random system is not confined to randomly distributed atoms or molecules, but may also be applied to media with lattice structure. As an example, one would a priori expect that a polycrystalline substance in many respects can be regarded as a random system.

Governed and ungoverned motion

A single crystal is a typical example of a medium in which directional effects in stopping might appear, due to both inhomogeneity, anisotropy and lack of randomness. We may classify directional effects for charged particles

moving through single crystals, or other media, by two labels: 1) un-governed motion, and 2) governed motion. By un-governed motion is meant the approximation where the path of the particle may be assumed to be essentially unaffected by the structure of the substance. Governed motion means that the path deviates definitely from that in a random system, because the path is determined by the structure of the medium. Ungoverned motion will be found to show merely fluctuations in physical effects due to correlations, whereas governed motion leads to more fundamental changes in physical processes.

In both categories of directional effects we may further distinguish between those cases where a) both direction and position of path are involved, and those where b) only direction is involved.

Direction and position

If a particle can be assumed to move classically along a straight line through a thin single crystal, the direction of the line of motion is important, as well as its position in the lattice (dependence on position indicates inhomogeneity, on direction: anisotropy). Thus, assume that the path is parallel to a major axis in the lattice. If then it is in between the atoms, there is a reduction of all those physical effects which require a close collision between particle and atom. If the particle is very close to atomic positions there is an increase in these effects.

Now, on the one hand, one can hardly hit e.g. only the space between atoms in a lattice, since a beam of projectiles will be spread over a large area, and thus one fraction of the beam may pass between atoms, while another fraction passes close to atoms. On the other hand, the impinging beam can be rather well collimated in direction, and thus a fraction of projectiles moving in straight lines might conceivably keep away from atoms for considerable distances of penetration.

As an example, consider the energy losses suffered by a beam of particles moving through a thin crystal film, where the energy loss remains small compared to the particle energy. The energy loss by a particle to an atom may be assumed to be a function of the impact parameter only. However, if the particles have un-governed motion, the average energy loss (but not the fluctuations) remains the same as in a random system. This result is evident, since the particle beam consists of parallel randomly distributed paths. An average of energy losses over randomly distributed parallel paths must give the same result as an average over randomly distributed atoms.

In the case of governed motion, the paths do not remain independent of the lattice, and the average energy loss is expected to deviate from that of a random system. In the following, we are interested in possible occurrence of governed motion in a lattice, where effects depend on both direction and position of particle path, and where e.g. averages over external position of the path are not in conformity with results for random systems.

Direction only

For comparison, we briefly consider effects concerned with direction only, i.e. not associated with position in space of the particle path. Such purely directional effects may be divided in two.

The first case can be indicated by an example. Suppose that the medium is a homogeneous plasma in a constant external magnetic field parallel to the z -axis. The energy dissipation by a particle is then independent of its localization in space, but depends on the angle between the direction of motion and the z -axis. This directional effect is a property of the medium, and subsists even though the particle moves approximately along a straight line.

The second case occurs e.g. for wave interference patterns due to lattice periodicity. Such effects require an extended wave, in sharp contrast to a classical localization of the particle within the lattice. As mentioned previously, we shall not here treat wave interference.

Channelling

The concept of channelling was introduced in recent papers on penetration in crystals, at first for slow ions^{4) 1)} and later for swift protons. By channelling is meant that a particle path near the centre of channels along a major axis in a crystal may have a certain stability. Particles moving along channels are subject to periodic forces, mainly focusing and occasionally defocusing. If the forces are of harmonic type and the focusing force is preponderant, this leads to a familiar solution of the equations of motion. The transverse motion in a channel is roughly a long-wave oscillation, combined with a short-wave vibration with the lattice period. The long-wave motion has a constant amplitude and wave-length v/ω , where ω is the period of average transverse harmonic oscillation and v the particle velocity. If the amplitude is large, the oscillation no longer remains harmonic. Any kind of oscillation within a channel we describe as proper channelling. A theoretical treatment of channelling is given by LEHMANN and LEIBFRIED⁸⁾

in a special case. Studies of individual paths at low energies by means of digital computers were performed by ROBINSON and OEN⁴⁾, and by others.

It is worth while to indicate in a qualitative way the possible occurrence of channelling and its relation to other phenomena. Suppose that a particle moves along the centre line of a channel, with oscillations about the centre line. If the energy of oscillation exceeds the barrier to a neighbouring channel, the particle escapes readily from the channel. We can roughly estimate the barrier for such escape either from the harmonic force in the centre of the channel, or from direct estimates at the channel border line. We introduce a barrier energy for channels, E_c , presumably of order of 5 eV for protons, and depending on Z_1 and on the medium. Let ψ be the angle between particle motion and channel direction when the particle is at the channel axis. If the energy in the transverse motion, $E \sin^2 \psi$, is larger than E_c , the ion can escape from the channel; we need not discuss details as to the probability of escape. Thus, we find a critical angle

$$\alpha_c = \left(\frac{E_c}{E} \right)^{1/2}, \quad (1.1)$$

where E is the energy of the particle. Only if the incident ion both has an angle less than α_c with the channel axis and also starts close to the channel axis, can its escape from the channel be disregarded and proper channelling take place. This corresponds to a solid angle for proper channelling,

$$\Omega_c \sim \pi \frac{E_c}{E}. \quad (1.2)$$

Within this solid angle, channelling can occur with a finite probability. In a wide channel, where the atoms in the walls are relatively closely packed, the energy E_c —and thus the solid angle Ω_c —is expected to be larger than in a narrow channel.

One consequence of (1.1) and (1.2) is that the critical angle depends strongly on the energy of the particle, while its charge and mass do not appear directly in the formula. Still, the barrier E_c depends somewhat on the atomic numbers Z_1 and Z_2 , and changes with lattice direction.

Already the above cursory considerations indicate that at high particle energies the probability of channelling is negligible. At low energies the probability becomes larger, although some effects have a disturbing influence (cf. e.g. (A.13)). However, the probability of remaining in one channel is

not of much physical importance, except for a special group of phenomena. In the following chapters we arrive at a more complete picture of the phenomena at high and low particle energies.

Electronic and nuclear stopping

There are two sources of energy loss by a charged particle¹²⁾. Electronic stopping is due to electronic collisions, where the particle excites or ejects atomic electrons, with loss of energy. The corresponding momentum transfer is small because electrons are light particles. Nuclear stopping arises from nearly elastic collisions with atoms, with transfer of both energy and momentum. Deflections of a particle are thus due to nuclear collisions, where large forces and heavy masses are involved. This simple fact is of significance in problems of directional effects.

One may distinguish between several regions of velocity in normal uncorrelated slowing-down of a charged particle. First, at high particle velocities, electronic stopping is completely dominating, and nuclear stopping is $\sim 10^3$ times smaller. This limiting case applies for protons, or heavier ions, when $v > v_1 = Z_1^{2/3} v_0$, Z_1 being the atomic number of the particle, v its velocity, and $v_0 = e^2/\hbar$. A quantal perturbation treatment of the excitation of the atomic system may then be applied (Bethe-Bloch treatment), the stopping being proportional to Z_1^2 and decreasing approximately as v to a power between -1 and -2 . Second, at velocities $v < v_1$, electronic stopping can still remain dominating and is nearly proportional to velocity⁶⁾ 13).

Third, the slowing-down of heavy ions of low velocities is dominated by nuclear stopping. In random systems, nuclear stopping can dominate over the electron stopping when $\varepsilon < 10$, where ε is a dimensionless measure of energy, of Thomas-Fermi type⁶⁾,

$$\varepsilon = \frac{a \cdot E}{Z_1 Z_2 e^2} \cdot \frac{M_2}{M_1 + M_2}. \quad (1.3)$$

In (1.3), the atomic number of the medium is Z_2 , the atomic screening radius is $a = a_0 \cdot 0.8853 \cdot (Z_1^{2/3} + Z_2^{2/3})^{-1/2}$, and $E = M_1 v^2/2$ is the energy of the particle. The parameter ε is convenient in the description of nuclear collisions.

The stopping of charged particles illustrates the necessity of distinguishing between electronic and nuclear collisions, and between several velocity regions. In the present context the actual stopping is not of primary importance, as discussed in § 2, but it remains a significant secondary phenomenon.

§ 2. Foundations of Theory

In order to find the proper approximation procedure for the treatment of directional effects, we must distinguish between primary and secondary phenomena. The energy loss of a particle (e.g. slowing-down by electronic collisions) is a secondary phenomenon, since it is determined by the path, but does not by itself govern the path. The possible governing of the path must be due to deflections of the particle in collisions with atoms, and thus a deflection is a primary phenomenon. Because of this simple fact, we can immediately introduce four basic assumptions⁵⁾, leading to a consistent approximation procedure for the treatment of possible governed motion of particles.

First, the angles of scattering of the particle may be assumed to be small. Not only does this usually hold for fast heavy particles, but scattering by large angles would imply that the original direction is completely lost, as well as correlations associated with the direction. The scattering of the particle is due to nuclear collisions, where it interacts with the charge distribution of an atom as a whole, the collision being nearly elastic. If the angles of scattering in the laboratory system, φ , and in the centre-of-gravity system, Θ , are small, we find for an elastic collision,

$$\operatorname{tg}\varphi = \frac{M_2 \sin\Theta}{M_1 + M_2 \cos\Theta} \rightarrow \varphi \cong \frac{M_2}{M_1 + M_2} \Theta, \quad \text{for } \varphi < 1, \quad \Theta < 1, \quad (2.1)$$

where M_1 is the particle mass and M_2 the mass of the atom, initially at rest. If we are interested in the motion of the particle only, we may find the correct scattering angle, φ , from the potential between particle and atom, calculating as if the atoms were infinitely heavy. In fact, the classical formula for scattering at small angles is

$$M_1 \varphi = M_0 \Theta = -\frac{1}{v^2} \int_{-\infty}^{+\infty} dz \frac{\partial}{\partial p} V(\sqrt{z^2 + p^2}), \quad (2.1')$$

where p is the impact parameter and $V(R)$ the potential between ion and atom at distance R . For the present purpose, the accuracy of the Thomas-Fermi potential between particle and atom is ample in most cases, and it leads to a simple comprehensive description. If the potential far away from an atom is needed, other estimates of potentials may be useful.

Second, since a collision demands that the particle comes close to the atom, strong correlations between collisions occur if the particle moves at a small angle with a row of atoms; if it passes close to one atom in the row, it must also pass close to the neighbouring atoms in the same row. This leads us to the concept of a string of atoms, characterized merely by the constant distance of separation, d , of atoms placed on a straight line. We describe this as the perfect string. In first approximation, collisions occur with one string at a time, string collisions being independent and uncorrelated. The physical importance of the string is emphasized by the fact that practically all physical processes caused by the particle, or influencing its path, demand that it comes close to the string. One exception is resonance excitation of atomic electrons, which may take place many lattice distances away from the particle, if it has a high velocity. The simplicity of the string approximation is partly due to the circumstance that the lattice structure does not enter, the only lattice parameter being the distance d between atoms in the string. Strings belonging to low index directions have a small value of d , and are the most pronounced ones. Correlations weaker than those of strings are expected for crystal planes, atomic pairs etc.

Third, classical orbital pictures may be used to a large extent. They may be applied in locating the particle in the lattice, because the wave length λ , is small. It is less obvious that classical orbital pictures may be used in describing collisions with e.g. strings of atoms. In fact, since individual collisions with atoms need quantal corrections either when the quantity $\kappa = 2Z_1Z_2e^2/\hbar v$ is not large compared to unity, or when the impact parameter is large, the classical approximation might seem to be doubtful in several cases. However, contrary to such expectations the classical description of many successive collisions with atoms in a string does not become invalid at high velocities. The quantal corrections are discussed below, cf. Appendix B.

Fourth, the idealized case of a perfect lattice, and a perfect string, may be used as a first approximation. The most important deviations are vibrations of strings, i.e. thermal and zero point vibrations. Again, some of the effects of vibrations are reduced by successive collisions with many atoms in a string.

On the basis of the above four assumptions it is possible to construct, step by step, a theory of directional effects for energetic charged particles. The discussion of correlations and small angle deflections has led to the basic concept of a string of atoms. This concept is not to be considered as a fixed model, but rather as a starting-point for an approximation procedure

applicable to directional effects. In this sense there is an analogy to the ideal gas as a starting-point for descriptions of real gases, or an ideal lattice as a starting-point for solid state theory.

Transverse continuum potential of a string

In order to study the effect of correlated small angle deflections on the motion of a particle, we may at first introduce the continuum string approximation. The basis of the continuum approximation is to assume that many consecutive atoms contribute to the deflection of the orbit. Having found the particle orbits in the continuum approximation, we may next ascertain whether these orbits are actually determined by many collisions, i.e. we can find a condition for validity of the continuum picture. A discussion of the connection between continuum string and perfect string is given in Appendix A, where the combined effect of successive classical collisions is considered in some detail.

In the continuum approximation we introduce the average potential at a distance r from the string, i.e.

$$U(r) = \int_{-\infty}^{+\infty} \frac{dz}{d} V(\sqrt{z^2 + r^2}), \quad (2.2)$$

where $V(R)$ is the ion-atom potential and d the distance between atoms in the string. Although $U(r)$ is determined as an average potential belonging to a string, it is of interest to notice that $d \cdot U(r)$ determines the scattering already in a single collision with an atom, according to (2.1').

If R is not very much larger than a , the potential $V(R)$ is essentially of Thomas-Fermi type, and we may put

$$V(R) = \frac{Z_1 Z_2 e^2}{R} \varphi_0\left(\frac{R}{a}\right). \quad (2.3)$$

Here, a is the screening length of the ion-atom interaction, equal to* $a = a_0 \cdot 0.8853 \cdot (Z_1^{2/3} + Z_2^{2/3})^{-1/2}$, and $\varphi_0(R/a)$ is the Fermi function belonging to one isolated atom^{6) 9)}. It is seen from (2.2) that, as a general rule, the variation of U with $1/r$ is by one power less than the variation of V with $1/r$. When (2.3) holds, we can write U as

* In the following it is often implicitly understood that $Z_1 \ll Z_2$, so that a is put equal to $a_0 \cdot 0.8853 \cdot Z_2^{-1/3}$.

$$U(r) = \frac{Z_1 Z_2 e^2}{d} \cdot \xi(r/a), \quad (2.4)$$

which formula is valid if the Thomas-Fermi type potential (2.3) applies.

A comparatively accurate estimate of $\xi(r/a)$, at moderate values of r/a , is given in ref. 10. For the present purpose we shall use somewhat simpler estimates. In order to get qualitative insight in the behaviour of ξ , i.e. of U , we note that $\varphi_0 \approx 1$ for $R/a \ll 1$, and according to (2.2) and (2.4) the function $\xi(r/a)$ must then increase logarithmically for small r , or

$$\xi\left(\frac{r}{a}\right) \approx 2 \log \frac{Ca}{r} \quad , \quad \text{for } r < Ca, \quad (2.5)$$

where $2 \log C$ is a constant of integration, determined by the screening. An approximation somewhat better than (2.5), and applicable for all values of r , is given by the expression, in the following described as the standard potential,

$$\xi\left(\frac{r}{a}\right) = \log \left[\left(\frac{C \cdot a}{r} \right)^2 + 1 \right]. \quad (2.6)$$

According to (2.6), $\xi \sim (Ca/r)^2$ for $r > Ca$. Even though (2.6) decreases rapidly for large r , it becomes less accurate when $r \gg a$. As a standard value for C we shall use $C = \sqrt{3}$, which gives a fairly good over-all fit. The best fit at small r/a would be obtained for a lower value of C , while large r/a would require a slightly higher value. Besides such estimates of $U(r)$ we shall sometimes consider the important atomic region where $R \sim a$ and $r \sim a$, so that V behaves as $\sim R^{-2}$, and $\xi(r/a)$ becomes $\xi \sim \pi a/2r$. The accuracy of the above approximations is indicated in reference 10.

The formula (2.6) corresponds to simple expressions for the density of electrons, $\varrho(R)$, and for the atomic potential $V(R)$ in (2.5), i.e.

$$\varrho(R) = \frac{3}{4\pi} Z_2 \frac{(Ca)^2}{(R^2 + (Ca)^2)^{5/2}} \quad , \quad (2.6')$$

$$V(R) = Z_1 Z_2 e^2 \left\{ \frac{1}{R} - \frac{1}{(R^2 + C^2 a^2)^{1/2}} \right\}. \quad (2.6'')$$

The limitation of the standard atomic potential in (2.6) is clearly seen if we attempt to compute the average of the atomic radius squared, $\overline{R^2}$. This

quantity diverges logarithmically, according to (2.6'). However, this is usually not of importance in the present calculations.

Condition for continuum approximation and critical angles*

A qualitative condition for the continuum approximation is obtained if we demand that the scattering in the vicinity of the minimum distance of approach is due to many atoms. Thus, the collision time, Δt , multiplied by the velocity component parallel to the string $v \cos \psi \approx v$, must be large compared to d . The collision time is of order of $r_{\min}(l)/(v \sin \psi)$, where l is the impact parameter with the string, and $r_{\min}(l)$ the corresponding minimum distance of approach. The condition is thus

$$\Delta t \cdot v \cos \psi \simeq \frac{r_{\min}(l)}{\psi} > d. \quad (2.7)$$

Let us apply the condition (2.7) in its most restrictive form, so that we demand its fulfilment for $l = 0$, i.e. for $r_{\min}(0)$. The latter quantity is a function of ψ . For brevity we simply write r_{\min} instead of $r_{\min}(l = 0, \psi)$. The minimum distance of approach is determined by

$$U(r_{\min}) = \frac{1}{2} M_1 v^2 \cdot \sin^2 \psi. \quad (2.8)$$

It is seen that r_{\min} increases rapidly as ψ decreases. According to (2.7), the critical angle is obtained by inserting $r_{\min} = d \cdot \psi$ in (2.8).

If the energy, $E = M_1 v^2/2$, is increased at fixed ψ , r_{\min} in (2.8) tends to zero. We may therefore expect that at high energies (2.5) applies, so that the condition (2.7) together with (2.8) leads to

$$\frac{Ca}{\psi d} \cdot \exp \left\{ -\frac{\psi^2 d}{2b} \right\} > 1,$$

where $b = Z_1 Z_2 e^2/E$ is the collision diameter belonging to laboratory system coordinates.

For ψ increasing from zero, the inequality is violated first by the rapid decrease of the exponential, provided $Ca/\psi d$ can remain large. Condition (2.7) therefore remains fulfilled if

$$\psi < \psi_1 = \sqrt{\frac{2b}{d}} = \sqrt{\frac{E_1}{E}}, \quad E_1 = \frac{2Z_1 Z_2 e^2}{d}, \quad (2.9)$$

* For a detailed treatment cf. Appendix A; in particular (A. 8), (A. 20) and (A. 21).

provided $Ca/\psi_1 d$ is larger than unity, i.e. approximately

$$\psi_1 \lesssim \frac{a}{d}, \quad \text{or} \quad E > E' = 2Z_1 Z_2 e^2 \frac{d}{a^2}, \quad (2.9')$$

where $a/d \sim 20^{-1}$, so that the energy E' is several hundred times larger than E_1 . According to (1.3), the condition (2.9') may also be stated as $\varepsilon > \varepsilon' = 2(d/a) \cdot M_2/(M_1 + M_2)$, and if $M_1 \lesssim M_2$ this corresponds to $\varepsilon \gtrsim 2d \cdot Z_2^{1/3} a_0^{-2}$.

If ψ fulfils the condition (2.9), the continuum potential (2.4) may be used and, accordingly, the particle cannot come closer than $\sim a$ to the centre of the string. Since E_1 is normally much larger than E_c in (1.1), the angle ψ_1 is large compared to the critical angle α_c for channelling. Therefore, in a well-defined high energy region given by (2.9'), where electronic stopping dominates, we may use the transverse potential (2.4), with a critical maximum angle $\propto \psi_1$, i.e. an effective maximum height of the transverse potential $\propto 2Z_1 Z_2 e^2/d$. In several respects, this maximum potential is remarkably simple. It is independent of the total energy of the particle and of the atomic screening radius a . It is a function of $Z_2 e/d$, the charge per unit length of the string.

At low energies, where (2.9') is no longer valid, we obtain an approximate expression for the critical angle by introducing (2.6) in (2.8) and (2.7). This leads to the condition

$$\psi < \psi_2 = \left(\frac{Ca}{d\sqrt{2}} \psi_1 \right)^{1/2}, \quad (2.10)$$

and since $C/\sqrt{2} \approx \sqrt{3}/\sqrt{2} \sim 1$, the critical angle ψ_2 applies when

$$\psi_1 > \frac{a}{d}, \quad \text{or} \quad E < E', \quad (2.10')$$

cf. (2.9'). An interesting consequence of (2.10) is that the potential energy barrier, obtained by squaring the right-hand side of (2.10) and multiplying by E , decreases proportionally to $E^{1/2}$, instead of remaining constant as in the high energy region. In contrast to ψ_1 in (2.9), the critical angle ψ_2 in (2.10) depends on the atomic radius a and on the behaviour of the screened atomic potential. For this reason, (2.10) is only a rough estimate and can hardly be expected to hold accurately at very low energies. In the following discussion we treat mainly the case of high energies, where (2.9) and (2.9')

apply. The other limit, (2.10), will only be discussed briefly, but in a general sense the following description applies also when (2.10) holds.

Already the result (2.9) gives a qualitative idea of the behaviour of a beam of particles moving through a lattice. If the initial angle ψ is less than $\sim \psi_1$, the continuum picture of the string applies, and there are separate repulsive collisions with strings, the particle leaving the strings at the same angle ψ as it had prior to the collision. Such particles hardly come close to atoms, and their angle ψ is not changed as it would be by normal multiple scattering. This may be called the aligned beam of particles, the condition being that $\psi < C'\psi_1$, where C' turns out to be of order of 1-2. For the aligned beam, the approximation of uncontrolled motion, mentioned in § 1, can not be valid.

From the formula (2.5) for the continuum potential it might seem as if there were an infinitely high barrier at $r = 0$. However, firstly we have seen from (2.9) that the continuum picture is not quite applicable when $\psi \gtrsim \psi_1$ (cf. Appendix A for a more detailed computation of critical angles). Secondly, if we use a continuum picture already the thermal vibration of atoms would lead to a smearing of the potential near $r = 0$, with a maximum $\sim Z_1 Z_2 e^2 d^{-1} \log(C^2 a^2 / \varrho^2)$, where ϱ is the amplitude of vibration, and the resulting maximum potential remains of the order of E_1 . From both points of views, if $\psi > C'\psi_1$ the particle moves rather freely through the lattice, and may easily be scattered by atoms in the usual way. In most respects, the penetration phenomena are then as in a random system. We therefore denote this part of the beam as the random beam.

Classical Rutherford shadow behind one atom

A simple and illustrative phenomenon is the shadow behind a repulsive scattering centre in an external, parallel beam of particles. The scattering is assumed to be classical (cf. (B.4) and (B.5)), and we suppose that there is a screen perpendicular to the beam, at a distance d behind the scattering centre. This idealized experiment may be said to represent a pair of atoms, the scattering centre being one atom, the second atom being placed in the screen, so that we ask for the probability of hitting the second atom.

An example of nearly isolated atomic pairs is found e.g. for nearest neighbours in the diamond lattice, i.e. in the $\langle 111 \rangle$ -direction. Such pairs may also be regarded as incomplete strings, with successively two occupied and to unoccupied sites. The pair effect can occur not merely in a monatomic substance like Si, but also in e.g. ZnS, where all S atoms are shielded by Zn atoms in one direction, and conversely in the opposite direction.

For simplicity, we consider merely Rutherford scattering, corresponding to impact parameters $p \lesssim a$. Let the scattering centre be placed on the z -axis, the beam being parallel to this axis. A particle with impact parameter p hits the screen at a distance r from the z -axis, and for small angles of deflection r is given by

$$r = p + \frac{b}{p}d, \quad (2.11)$$

where $b = Z_1Z_2e^2/E$. The distance r has a minimum, $r_{\min} = 2\sqrt{bd}$, for $p = \sqrt{bd}$. The shadow region therefore has a parabolic shape, as a function of the distance d , since its edge is at $r = r_{\min} \propto d^{1/2}$.

In order to hit the centre of the screen, we must tilt the beam by an angle $\psi_{\min} = 2\sqrt{b/d} = \psi_1/\sqrt{2}$, where ψ_1 is given by (2.9). The intensity distribution on the screen is easily obtained from (2.11). Let $f(r)$ be the intensity on the screen, the external beam containing one particle per unit area. Then, for large r , $f(r)$ tends to unity, whereas $f(r) = 0$ for $r < r_{\min}$. The particles aiming at $r < r_{\min}$ are pushed just outside r_{\min} , where $f(r)$ has a peak. In fact,

$$f(r) = \begin{cases} 0, & r < r_{\min} \\ \frac{1}{2} \left[\left(1 - \frac{r_{\min}^2}{r^2} \right)^{1/2} + \left(1 - \frac{r_{\min}^2}{r^2} \right)^{-1/2} \right], & r > r_{\min}. \end{cases} \quad (2.12)$$

The sharp edge at $r = r_{\min}$ is blurred when quantal corrections are taken into account, the blurring remaining small only when $\kappa = 2Z_1Z_2v_0/v$ is large compared to unity (cf. (2.29)).

The number of particles missing on the screen inside r_{\min} is πr_{\min}^2 . The number missing inside r is $\pi r^2 - \int_{r_{\min}}^r 2\pi r dr f(r) = \pi r^2 (1 - (1 - r_{\min}^2/r^2)^{1/2})$. For large r this implies that only half the missing number is compensated in Rutherford scattering with $p \ll d$. It is easy to show that, for screened atomic fields, the full compensation occurs for r larger than a . In fact, when (2.6') holds, a 75 per cent compensation is obtained for $r = Ca$. Thus, for fast particles obeying eq. (2.9') the compensation is divided in two equal parts, one occurring at $r \gtrsim 2(bd)^{1/2}$, or $\psi \gtrsim \psi_1/\sqrt{2}$, and the other at $r \sim Ca$, or $\psi \sim Ca/d$.

The critical angle ψ_{\min} for a pair of atoms is apparently quite similar to that of a perfect string. Still, there are differences of major importance.

If we tilt by an angle of e.g. $\psi_{\min}/2$, the nearest approach to the centre of the screen will be $r_{\min}/2 = \sqrt{bd}$, which distance is much smaller than the corresponding distance of approach to a perfect string, $\sim a$, if (2.9') is valid. In fact, both for strings and atomic pairs we must assume validity of (2.9'), in order that Rutherford scattering remains responsible for the phenomenon. The atomic pair is therefore much less effective than the string in pushing particles away from the atom. Another difference between atomic pairs and strings is that the atomic pair is less classical because there is only one repulsive collision instead of many. However, the most important difference between atomic pairs and strings is the small multiple scattering in the latter case, as will be discussed below.

Atomic planes

Another case of interest is that of a plane of atoms. Consider a particle moving not in any major string direction, but still nearly parallel to a plane in a lattice. There must then be some correlation between collisions with atoms, although in a weaker and less well-defined manner than for a string. Accordingly, one may expect effects of atomic planes in penetration. Like in the case of atomic pairs it is of interest to find the comparative merits of planes and strings.

A plane can give rise to governed motion of a particle, if the orbit of the particle, as derived from the continuum potential, involves many collisions with atoms. We therefore evaluate first of all the potential of a continuum plane, as obtained by smearing the atoms evenly in the plane*. As a function of the numerical value, y , of the distance from the plane, the continuum potential is

$$Y(y) = N \cdot d_p \int_0^{\infty} 2\pi r dr \cdot V(\sqrt{y^2 + r^2}), \quad (2.13)$$

where $N \cdot d_p$ represents the average number of atoms per unit area of the plane, d_p being the distance between planes. The ion-atom potential $V(R)$ is given by (2.3). The potential $Y(y)$ is similar to the string potential (2.2), but lower by a factor $\sim 2a/d$, when $r \lesssim 2a$. Further, in the plane—i.e. for $y = 0$ —the potential (2.13) has a finite value,

$$Y(0) = N \cdot d_p \cdot \int_0^{\infty} 2\pi R dR V(R) = \pi Z_1 Z_2 e^2 \cdot N d_p \cdot \bar{R}, \quad (2.14)$$

* The perfect plane has no preferred direction. The atoms may be assumed to be distributed as a two-dimensional liquid or, in simple estimates, random gas.

where \bar{R} is the average radius of the 'atom', $\bar{R} = Z_2^{-1} \int_0^{\infty} 4\pi\rho(R) \cdot R^3 dR$. The LENZ-JENSEN model⁹⁾ leads to $\bar{R} = 2.68 a$, whereas (2.6') implies $\bar{R} = 2Ca$.

By means of the standard atomic potential (2.6') a simple estimate is obtained for the potential $Y(y)$

$$Y(y) = 2\pi Z_1 Z_2 e^2 \cdot N d_p \cdot [(y^2 + C^2 a^2)^{1/2} - y], \quad (2.15)$$

which expression may be compared with the corresponding one for a string, (2.6).

The criterion for use of continuum potential for a plane is more involved than for a string. Let the particle, when far away from the plane, have an angle θ with it, i.e. transverse energy $E_{\perp} = E \cdot \theta^2$. Even though many atoms contribute to the deflection of a particle, there remains an uncertainty in the nearest approach y_{\min} to the plane. In contrast to the case of a string, the particle will usually not be deflected by atoms directly below its orbit, but it may happen that there is an atom directly below the orbit at minimum approach. Let us therefore demand that in this eventuality the deflection in the single collision is smaller than φ . According to (2.15), i.e. for the standard atomic potential, y_{\min} is given by

$$\theta^2 = 2\pi b \cdot N \cdot d_p \cdot [(y_{\min}^2 + C^2 a^2)^{1/2} - y_{\min}], \quad (2.16)$$

and we demand

$$\theta > \varphi = -\frac{d \cdot U'(y_{\min})}{2E} = b \cdot \frac{1}{y_{\min}} \frac{1}{1 + \frac{y_{\min}^2}{C^2 a^2}}, \quad (2.17)$$

where the expression on the right-hand side is derived from the standard atomic potential (2.6'). When combining (2.16) and (2.17) we find that they contain two dimensionless parameters, $\zeta = y_{\min}/Ca$ and $\alpha = E_p/E$, where

$$E_p = \frac{Z_1 Z_2 e^2}{2\pi C^3 a^3 N \cdot d_p} \sim Z_1 Z_2^2 \cdot 30 \text{ eV}. \quad (2.18)$$

The condition (2.17) is then equivalent to

$$\zeta^2(1 + \zeta^2)^2 [(\zeta^2 + 1)^{1/2} - \zeta] > \alpha. \quad (2.19)$$

If we demand that $y_{\min} \approx a$, this leads to $E > 3E_p$. In point of fact, the inequality (2.19) shows, on the one hand, that the continuum potential hardly ever holds at distances small compared to a , even though the energy E is very large. On the other hand, even for quite low energies the potential applies down to distances comparable with the atomic radius, $\bar{R} \sim 2Ca$. In view of the comparatively slow variation of $Y(y)$ with y , we may then normally assume that the potential barrier of a plane is not higher than

$$Y_{\text{eff}} = Y(0)/2, \quad (2.20)$$

and for quite low values of E/E_p the barrier becomes somewhat lower. So far, we have discussed merely one of the conditions for a continuum description of planes. We supplement this insufficient discussion by the description of a plane as a string of strings.

Plane described as string of strings

The limits of applicability of a continuum description are less obvious for planes than for strings. Some aspects of the properties of planes are illustrated by the following idealized picture. A plane of atoms can be treated as a string of strings, if the angles with a major string are not very large compared to ψ_1 . This case is of particular interest also for studies of the way in which string effects and plane effects join.

Suppose that the angle ψ with a set of parallel major strings is of order of the characteristic angle ψ_1 , so that for a wide region of impact parameters, l , with strings, the strings can be considered as continuum strings. The deflection can then be described in terms of the two-dimensional motion in the plane perpendicular to the strings, i.e. the transverse motion. Strings are arranged in a regular lattice, so that a plane consists of a row of strings, i.e. it can be conceived as a string of continuum strings. The transverse motion has a velocity $v_{\perp} = v \cdot \psi$, and the deflection by a string is determined by $U(r)$. If the angle of deflection φ_{\perp} in the transverse motion is small, it is obtained easily from the integrated force, and the result can be expressed in terms of the previously calculated plane potential Y in (2.13),

$$\varphi_{\perp} = -\frac{d_s \cdot Y'(l)}{2E \cdot \psi^2}, \quad (2.21)$$

where d_s is the distance between strings. It is seen from (2.13) that the product $d_s \cdot Y$ depends on lattice constants only through $d_s \cdot N \cdot d_p = d^{-1}$, where d is the atomic spacing in the strings.

We may at first discuss the shadow behind one string, in analogy to the way in which we treated the Rutherford shadow behind an atom. This enables us to study both the case of a pair of strings and the validity of the continuum plane approximation. Consider a particle with transverse motion in the positive x -direction, and impact parameter l with a string placed in the origin, $(x,y) = (0,0)$. According to (2.21), the particle hits the line $x = d_s$ at a distance y from the x -axis, where

$$y = l + \frac{d_s^2 Y'(l)}{2E \cdot \psi^2} . \quad (2.22)$$

We may write $y = \Phi \cdot d_s$, and find from (2.22) the minimum angle Φ_{\min} at which the centre of a string may be hit, due to the shadow from the previous string,

$$\Phi_{\min} = \frac{3}{2} \left(\frac{\pi \psi_1^2 C^2 a^2}{2 \psi^2 d_s^2} \right)^{1/3}, \quad \text{if} \quad \psi^2 \ll \psi_1^2 \frac{\pi \cdot d_s}{2Ca} . \quad (2.23)$$

If the inequality in (2.23) is not fulfilled, estimates of Φ_{\min} are not quite well-defined, since for small impact parameters l the continuum string is no longer applicable. If the inequality is fulfilled, the angle $\psi \Phi_{\min}$ remains smaller than that belonging to the continuum plane potential. In fact, the effective potential energy corresponding to Φ_{\min} is

$$Y_\psi = E \cdot \psi^2 \Phi_{\min}^2 = Y(0) \cdot \frac{9}{4} \frac{1}{(4\pi)^{1/3}} \cdot \left(\frac{\psi^2 Ca}{\psi_1^2 d_s} \right)^{1/3} . \quad (2.24)$$

Thus, the effect of a plane disappears gradually in the neighbourhood of a string direction. This means that a string can stand out distinctly within a plane. However, for strings of high index number, the barrier belonging to (2.9) or (2.10) may be less than the barrier of the plane, and such strings can be engulfed by the planar effect.

Comparison of transverse potentials

In three cases, i.e. for channels, strings and planes, we have estimated continuum potentials, and we have also treated the case of atomic pairs. At high particle energies, cf. (2.9'), the potential barriers for major strings (and atomic pairs) are of order of $4Z_1 Z_2 e^2/d \sim Z_1 Z_2 \cdot 20 \text{ eV}$, since $d \sim 5a_0$. The barriers of major planes are, cf. (2.20), $5Z_1 Z_2 e^2 N d_p a \sim 5 \cdot Z_1 Z_2^{2/3} \text{ eV}$, and thus lower than those of strings by a factor of $\sim 4Z_2^{1/3}$, such that critical angles are less by $\sim 2Z_2^{1/6}$. The barrier for proper channelling, perhaps $\sim 5 \text{ eV}$ for protons, is considerably lower than the two others. When comparing effects of strings and planes, however, one must first of all bear in mind that the string potential decreases more rapidly with distance than does the plane potential; the two potentials become equal at distances of order of $d/2$. The rapid decrease of the string potential makes penetration to the centre of string atoms more sensitive to e.g. temperature vibrations of atoms,

as will be discussed below. Moreover, there is a difference between strings and planes, because in the former case the particle motion is two-dimensional, while in the latter it is one-dimensional. However, strings and planes have in common the division of a particle beam into an aligned part which does not penetrate the potential barriers, and a random part which does. The aligned beam remains at distances larger than $\sim a$ in both cases. In the two latter respects, atomic pairs differ from strings and planes.

Quantal shadow behind an atom

As a counterpart to the classical shadow behind an atom, we may finally consider the quantum mechanical shadow in the limit where quantal perturbation theory applies for single collisions. This will also indicate a characteristic feature of string effects in a wave picture. The essential point in the following calculation is that we are not concerned with the standard case of scattering theory, where the scattered wave is recorded at infinity.

As before, we consider a scattering centre located at the origin, with potential $V(\vec{R})$, where $\vec{R} = (x, y, z)$. At a distance d behind the centre is placed a screen, i.e. with coordinates $\vec{R}' = (x', y', z' = d)$. The incoming particle has a wave function $\exp(ikz)$, where $k = M_1 v / \hbar$. Scattering angles are assumed to be small. The range, a , of the potential is small compared to the atomic spacing d . In first order perturbation theory, the wave function $\psi(\vec{R}')$ becomes

$$\psi(\vec{R}') = e^{ikd} - \frac{M_1}{2\pi\hbar^2} \int \frac{e^{ik|\vec{R}-\vec{R}'|}}{|\vec{R}-\vec{R}'|} V(\vec{R}) e^{ikz} d^3R. \quad (2.25)$$

Since all coordinates in the x and y directions are small compared to d , we find by series development of $|\vec{R}-\vec{R}'|$, and performing the integration over z ,

$$\psi(\vec{R}') = e^{ikd} \left[1 - \frac{M_1}{2\pi\hbar^2} \int dx \int dy U(r) e^{\frac{ik}{2d} \{ (x-x')^2 + (y-y')^2 \}} \right], \quad (2.26)$$

where $U(r)$ is given by (2.2) and (2.4).

At this stage it is essential to notice that the exponential in the integrand is a rapidly oscillating function. In fact, since U contains the screening length a , the exponential varies rapidly if

$$\frac{a^2}{\lambda \cdot d} \gg 1. \quad (2.27)$$

For $Z_2 \gg Z_1$ and with $d \approx 5a_0$, the inequality (2.27) is equivalent to

$$\frac{M_1}{m} \cdot \frac{v}{v_0} \cdot \frac{1}{5Z_2^{2/3}} \gg 1, \quad (2.27')$$

and therefore the condition (2.27) is easily fulfilled for heavy particles. Another way of expressing (2.27') is to say that the momentum of the particle, M_1v , should be very large compared to the average momentum, $mv_0Z_2^{2/3}$, of an electron in the Thomas-Fermi atom. We conclude that even in the quantal perturbation treatment there is a considerable localization of path in analogy to the classical treatment. This is because the distance d between atoms is not large, in the sense stated by (2.27).

The results obtained in (2.26) and (2.27) show that, in a general quantal treatment, the contributions to the wave function at a certain point in space are due to scattering by atomic fields within a narrow cone opposite to the direction of motion. The disregard of all atomic fields except those within the cone (or e.g. the string), is equivalent to the basic assumptions on page 9ff.

We introduce (2.4) in (2.26),

$$|\psi(\vec{R}')|^2 = \left| 1 - \frac{\kappa}{4\pi} \iint \frac{dx dy}{\lambda d} \xi\left(\frac{r}{a}\right) e^{\frac{i}{2\lambda d} [(x-x')^2 + (y-y')^2]} \right|^2, \quad (2.28)$$

where $r^2 = x^2 + y^2$. Suppose that $x' = y' = 0$, and apply the estimate (2.6) for $\xi(r/a)$. Then, for low values of κ and when (2.27) holds,

$$|\psi(0, d)|^2 \cong \left| 1 - \frac{\kappa}{2} \left(\frac{\pi}{2} + i \log \left(\frac{a^2 C^2 \gamma}{2\lambda d} \right) \right) \right|^2 \sim 1 - \frac{\kappa\pi}{2}, \quad (2.29)$$

where γ is Euler's constant. The right-hand side is the limit for small κ of a familiar result belonging to a pure Coulomb field, $|\psi(0, d)|^2 = \pi\kappa[\exp(\pi\kappa) - 1]^{-1}$. For attractive fields we may here regard κ as a negative quantity, and obtain an increase in intensity behind the scattering centre.

§ 3. Statistical Treatment and Energy Loss

The previous chapter was concerned with basic problems and with the accessibility of different regions in a crystal lattice. In order to study in more detail the total behaviour of a beam of particles in a crystal lattice, we may, as a first approximation, apply the simple continuum picture of strings (and planes).

The continuum picture implies conservation of the velocity component parallel to the string. The motion may therefore be studied completely in terms of its projection on a plane perpendicular to the string. In this transverse motion, the velocity far from a string is $v_{\perp} = v \sin \psi \simeq v \psi$, and the corresponding transverse energy is $E_{\perp} = E \cdot \sin^2 \psi \simeq E \cdot \psi^2$. The potential is $U(r)$, and we shall use several of the approximate formulae for $U(r)$ introduced in § 2.

Available phase space in transverse motion

The use of statistical mechanical estimates is a powerful alternative to detailed studies of separate successive collisions with strings. We shall at first consider statistical estimates of particularly simple type. We use the continuum picture, and we need consider only the transverse motion; all angles ψ can be assumed to be small. For fixed values of velocity v and transverse energy E_{\perp} , we then ask for the two-dimensional probability distribution in a total potential $U_{\text{tot}} = \sum U(\vec{r} - \vec{r}_i)$, where U is given by (2.4), and $\vec{r}_i = (x_i, y_i)$ is the position of the i 'th string of atoms. Evidently, we

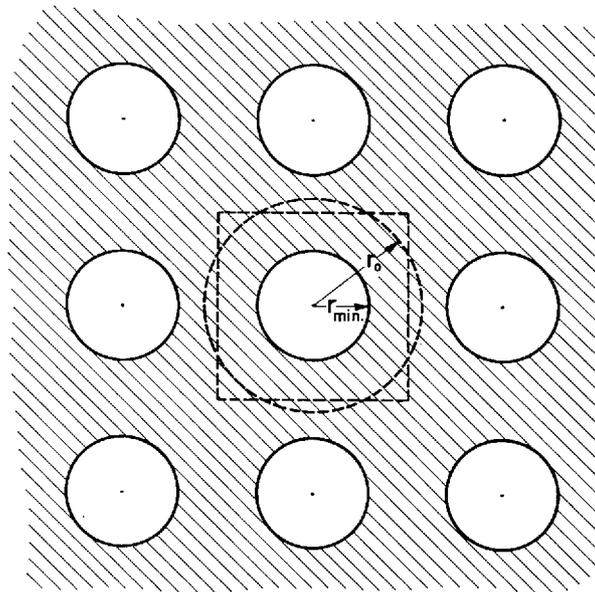


Fig. 1. Transverse plane of strings for simple cubic lattice. The square indicates unit cell, and the dashed circle with radius r_0 is approximate unit cell. Shaded area outside circles with radius r_{min} illustrates accessible portion of the plane for a given transverse energy. There is uniform probability distribution in shaded area according to two-dimensional continuum picture.

may usually confine the treatment to one unit cell in the two-dimensional \vec{r} -plane, containing one string. For most purposes, we can assume that the unit cell is a circle around the string, with radius r_0 , such that its area is $\pi r_0^2 = (N \cdot d)^{-1}$. We often disregard the potential due to neighbouring strings, so that the potential becomes simply $U_{\text{tot}} \approx U(r)$; this approximation applies if the transverse energy is not exceedingly low.

The beam of particles has some initial probability distribution, e.g. corresponding to a given direction in p_{\perp} -space. As a function of time t , or depth of penetration $z = vt$, the distribution will be $P(\vec{p}_{\perp}, \vec{r}, t)$. There will be a trend towards statistical equilibrium in the transverse phase space. Let us consider the equilibrium distribution within a transverse energy shell. We introduce the available momentum space as a function of \vec{r} , when the transverse energy is between E_{\perp} and $E_{\perp} + dE_{\perp}$. Since the volume in two-dimensional momentum space is proportional to dE_{\perp} , the equilibrium probability distribution becomes

$$P_0(E_{\perp}, \vec{r}) = \begin{cases} \frac{1}{A} & , \quad E_{\perp} > U_{\text{tot}}(\vec{r}), \\ 0, & E_{\perp} < U_{\text{tot}}(\vec{r}), \end{cases} \quad (3.1)$$

where the constant A is the accessible area in a unit cell with total area $A_0 = N^{-1}d^{-1}$. When the accessible portion of the unit cell is large, or $A \approx A_0$, we can simply disregard the overlapping of string potentials. This leads to $P_0 = 1/A \cong 1/A_0$, and $U_{\text{tot}}(\vec{r}) = U(r)$, where r is the distance from a string.

One-dimensional distribution

It is interesting to notice the extreme simplicity of the probability distribution in two-dimensional space, i.e. (3.1), as compared to both one- and three-dimensional spaces. Thus, the one-dimensional equilibrium on an energy shell, corresponding to continuum planes, becomes

$$P_0(E_{\perp}, y) = \begin{cases} \frac{C}{d_p} \left(\frac{E_{\perp}}{E_{\perp} - Y(y)} \right)^{1/2}, & E_{\perp} > Y(y), \\ 0, & E_{\perp} < Y(y), \end{cases} \quad (3.2)$$

where d_p is the distance between planes and C a normalization constant. In the one-dimensional motion the particles stay with maximum probability at the edges of forbidden regions, where the velocity is lowest. The formula (3.2) has several consequences different from those of (3.1). Thus, when E_{\perp} is large, higher than Y_{max} , all values of y are allowed, but the particle still feels the potential—in contrast to (3.1)—and stays with increased probability near the planes, where Y is highest.

Trend towards equilibrium on transverse energy shell

Having studied the equilibrium distribution on an energy shell in the transverse motion, we may next estimate how quickly the equilibrium distribution is attained. A measure of this is the change of average transverse momentum, $\langle \vec{p}_\perp \rangle$. Suppose that strings can be considered a good approximation. It is easily shown that

$$\langle \vec{p}_\perp \rangle = \langle \vec{p}_\perp \rangle_0 \cdot \exp(-z/\lambda_\perp), \quad (3.3)$$

where $\langle \rangle_0$ denotes initial averages for $z = 0$, and where the mean free path length λ_\perp of the particle is

$$\frac{1}{\lambda_\perp} = N \cdot d \cdot \sin \psi \int_{-\infty}^{+\infty} dl \cdot (1 - \cos \varphi(l)), \quad (3.4)$$

$\varphi(l)$ being the scattering angle of the transverse motion as a function of impact parameter with the string. It is to be noted that $\lambda_\perp \cdot \sin \psi$ is the so-called transport mean free path of the transverse motion, i.e. on the average the particle moves $\lambda_\perp \cdot \sin \psi$ in the transverse plane, in the direction of $\langle \vec{p}_\perp \rangle_0$.

If we assume that the minimum distance of approach exceeds $\sim a$, and the approximation $\xi = \pi a/(2r)$ is used for the string potential in (2.4), we get by a simple computation a direct estimate of λ_\perp ,

$$\frac{1}{\lambda_\perp} = \frac{\pi^2}{4} \cdot N \cdot d \cdot a \frac{\psi_1^2}{\psi}, \quad \text{for} \quad \xi \left(\frac{r}{a} \right) = \frac{\pi a}{2r}. \quad (3.5)$$

Therefore, when $\psi < \psi_1$ the mean free path λ_\perp is less than $1/(Nda\psi_1)$, the latter quantity being of order of 1000 atomic layers or less. After an energy loss of perhaps 1-10 keV, a proton attains equalization of distribution within the transverse energy shell.

The results (3.4) and (3.5) are based on random collisions for the transverse motion in the two-dimensional lattice of strings. However, as discussed in § 2, p. 19, this lattice contains strings of strings, or planes. When the direction of \vec{p}_\perp is not far from a plane direction, there is again a reduction of scattering, but now in the two-dimensional motion. In this limit, continuum planes are applicable and the primary equalization of the distribution is in the one-dimensional motion, leading to the equilibrium described by (3.2). The mean free path for the one-dimensional equalization must be of order

of $\lambda_p \sim d_p/\varphi$, where φ is the angle between \vec{v} and the plane. At this stage we need not treat further such questions of more detailed kind.

The quick scattering in azimuthal angle indicates that an assumption of statistical equilibrium on a transverse energy shell is often a fair approximation. Moreover, suppose that experimental conditions are such that initially an average is actually performed around a string direction, i.e. with respect to azimuthal angle. We then start from equalization on the transverse energy shell, which distribution has stable symmetry in the continuum picture.

Basic statistical averages over transverse motion

These results justify, so far, the use of (3.1). As a consequence of (3.1), we can for any function f , depending on \vec{p}_\perp and \vec{r} , obtain first its average on an energy shell

$$f(E_\perp) = \frac{1}{A} \int dx \int dy f(\vec{p}_\perp, \vec{r}), \quad (3.6)$$

or, equivalently, for not too low E_\perp ,

$$f(E_\perp) = \frac{1}{\pi(r_0^2 - r_{\min}^2)} \int_{r_{\min}}^{r_0} 2\pi r dr f(p_\perp, r), \quad (3.6')$$

where $f(p_\perp, r)$ is the average of $f(\vec{p}_\perp, \vec{r})$ over angles, and r_{\min} is determined by E_\perp through the relation $U(r_{\min}) = E_\perp$. The formula (3.6') is utilized repeatedly in the following. If $r_{\min}^2 \ll r_0^2$, the normalization factor is $(\pi r_0^2)^{-1} = N \cdot d$, and the upper limit in the integration may often be replaced by ∞ .

When the transverse energy is so low that the motion is confined to small unconnected areas (proper channelling), the integration in (3.6) can be approximately within an ellipse or circle around minimum of potential, and with area A .

Second, we can determine the final average f of $f(E_\perp)$ over the probability distribution in ψ , i.e.

$$\langle f \rangle = \int g(E_\perp) f(E_\perp) dE_\perp, \quad (3.7)$$

where $g(E_\perp)$ is the probability density per unit transverse energy.

The function $g(E_\perp)$ will change with penetration depth, because of multiple scattering, i.e. lack of conservation of transverse energy. Multiple scattering is treated in § 4. Before doing that, we find further properties be-

longing to particles with a given transverse energy. In fact, we have so far assumed that the total energy of a particle is conserved. We must therefore estimate the nuclear and electronic stopping for a particle of given transverse energy.

Statistical estimate of nuclear stopping

When the particle passes one atom at a distance r , and has a small angle of deflection φ , one obtains directly in terms of $U(r)$ defined in (2.2), cf. also (2.1'),

$$\varphi = -\frac{d \cdot U'(r)}{2E}, \quad (3.8)$$

and therefore the energy transfer in this elastic collision is

$$T_n = \frac{d^2}{2M_2v^2} [U'(r)]^2. \quad (3.9)$$

For aligned particles with a given value of E_{\perp} , we may average (3.9) over the available part of the unit cell according to (3.6), and obtain

$$T_n(E_{\perp}) = \frac{d^2}{2M_2v^2} \frac{1}{A} \int dx \int dy \sum_j U'^2(|\vec{r} - \vec{r}_j|), \quad (3.10)$$

where \vec{r}_j are the transverse coordinates of strings. Since we normally do not consider extremely low transverse energies, we may introduce (3.6') in (3.10), assuming $r_{\min}^2 \ll r_0^2$,

$$T_n(E_{\perp}) = \frac{\pi N \cdot d^3}{M_2v^2} \int_{r_{\min}}^{\infty} r dr U'^2(r), \quad (3.10')$$

where the usual upper limit of the integration, r_0 , is more correctly replaced by ∞ . The average energy loss in (3.10) and (3.10') is equal to $T_n(E_{\perp}) = N \cdot d \cdot S_n(E_{\perp})$, where $S_n(E_{\perp})$ is the stopping cross section for a given value of E_{\perp} . The integration in (3.10') may be performed explicitly and the result expressed in terms of E_{\perp} , if the standard atomic potential (2.6) is used.

The main contribution to the integral in (3.10') is in the vicinity of the lower limit, r_{\min} . If $U(r)$ varies as $r^{-\nu}$ when $r \approx r_{\min}$, we get directly from (3.10') the nuclear stopping as a function of transverse energy

$$S_n(E_\perp) = \frac{\pi \cdot \nu}{4} d^2 \frac{E_\perp^2}{E} \cdot \frac{M_1}{M_2}, \quad (3.11)$$

because $U(r_{\min}) = E_\perp$. Since ν is nearly equal to 1 for $a < r_{\min} < 2a$, increasing slowly to values ~ 2 for $r_{\min} > 2a$, the value of ν in (3.11) is not very sensitive to the magnitude of E_\perp^2 , and (3.11) gives a useful first estimate of the nuclear stopping. At the same time, the distribution in magnitude of the individual energy losses is also implicitly given by (3.10'). The stopping cross section (3.11) may be compared with the normal nuclear stopping in a random gas, cf. (4.2). When comparing with (4.2), (3.11) is found to imply that $L_n(E_\perp) = (\nu/2) \cdot (E_\perp/E\psi_1^2)^2$, which is much smaller than for normal nuclear stopping at high energies, where $L_n = \log(1.29\varepsilon) \sim 5-10$; it should be noted that (3.11) is applicable only for $E_\perp \lesssim E\psi_1^2$. In any case, for swift particles the nuclear stopping cross section S_n is quite small compared to electronic stopping S_e .

Nuclear energy loss in single collision with string

The above application of phase space in transverse motion resulted in statistical estimates, (3.10) and (3.11), of average nuclear stopping. However, it is also of interest to find the energy loss in an individual encounter between ion and string, characterized by the energy E of the particle, and its initial angle ψ and impact parameter l with the string.

The energy loss to one atom, at a distance r , is given by (3.9). In a string collision r is a certain function of time, $r = r(t)$. Integrating (3.9) over the orbit, we thus obtain the energy loss to the string, $\tau_n(l, \psi)$,

$$\tau_n(l, \psi) = \frac{d}{2M_2\nu} \int_{-\infty}^{+\infty} U'^2(r(t)) dt. \quad (3.12)$$

The integration in (3.12), containing the radial motion $r(t)$ as a function of time, is usually not simple, but may be readily performed if the potential $U(r)$ is proportional to r^{-1} or to r^{-2} . It can then also be verified that an integration of (3.12) over all impact parameters results in the stopping cross section (3.10'). In the present context we omit more detailed evaluations of type of (3.12), one reason being that except at exceedingly low energies the nuclear energy loss is negligible compared to electronic energy loss.

Electronic stopping

Even though we made only cursory estimates of nuclear stopping, that case can be treated in a comprehensive manner, and the accuracy may be easily improved. The electronic stopping is less simple because we must

distinguish between a number of different cases. Still, one qualitative expectation can be stated generally; at a fixed particle energy E , but decreasing E_1 , the electronic stopping is expected to decrease more slowly than does nuclear stopping. The ratio between electronic stopping and nuclear stopping should therefore be higher in the aligned beam than in the random beam.

We study primarily the important case of electronic stopping at those high particle velocities—and low charge numbers Z_1 —where the Bethe-Bloch formula applies. This formula may be written as

$$\frac{dE}{dR} = S_e \cdot N \cdot Z_2 = \frac{4\pi Z_1^2 e^4}{mv^2} Z_2 \cdot N \cdot L_e, \quad (3.13)$$

where N is the number of atoms per unit volume, and S_e the stopping cross section per electron. The factor L_e is approximately given by

$$L_e \cong \log \frac{2mv^2}{I}, \quad (3.14)$$

provided the velocity is so high that $x = v^2/(v_0^2 Z_2) \gg 1$, and^{13) 14)} $v/v_0 > Z_1^{2/3}$. The quantity I is the average excitation potential, $I \approx I_0 \cdot Z_2$, and $I_0 \approx 10$ eV.

When (3.14) applies, one may divide collisions with electrons in two groups, the distant resonance collisions and the close collisions with large momentum transfers to electrons (cf. BOHR¹²⁾). Since the phenomena are largely of quantum mechanical type, one may not apply classical orbital pictures in every detail for collisions between an electron and the particle. The precise distinction between close and distant collisions is in terms of, respectively, large and small momentum transfers. However, one may distinguish between the particle being outside the electronic orbit, where only resonance collisions occur, and inside the orbit, where close collisions occur with a probability distribution given essentially by the Rutherford scattering law. In a qualitative way, it is well-known from the derivation of the Bethe formula^{12) 15)}, that for very fast particles the stopping is asymptotically contributed equally by close and distant collisions. This turns out to hold also in a precise manner (equipartition rule¹⁶⁾), at not too low particle velocities. A detailed discussion of the dependence of energy loss on the space track of a particle of arbitrary velocity requires a generalization of the usual description and will be published separately.

From these considerations it seems proper, for large x , to replace (3.13) by

$$\frac{dE}{dR}(\vec{R}) = S_e \cdot [(1 - \alpha)NZ_2 + \alpha \cdot \varrho(\vec{R})], \quad (3.15)$$

where $\varrho(\vec{R})$ is the density of electrons at the point in space through which the particle moves, and where $\alpha \gtrsim 1/2$, α being the closer to 1/2 the higher the value of $x = v^2/(v_0^2 Z_2)$. This result means directly that the stopping cross section for a swift particle penetrating a thin foil can at most be reduced by a factor $\approx 1/2$. As we shall see, it can also increase by a factor slightly above unity, cf. § 5.

The increase per path length in square fluctuation of energy loss, $d(\Delta E)^2/dR$, in the case where (3.13) applies, is proportional to $Z_2 N$. The fluctuation contribution is due to close collisions only. In the present case, this contribution must be obtained by replacing the average electron density $Z_2 N$ by $\varrho(\vec{r})$. This straggling contribution, as a function of \vec{r} , becomes (cf. Bohr¹²⁾)

$$\left(\frac{d(\Delta E)^2}{dR}\right)_e = 4\pi Z_1^2 e^4 \cdot \varrho(\vec{R}). \quad (3.16)$$

A somewhat similar formula¹³⁾ holds at velocities $v < v_0 Z_2^{1/2}$. According to (3.16), the straggling depends more strongly on ϱ than does the stopping cross section (3.15).

We consider statistical equilibrium at a certain transverse energy E_\perp , and introduce an effective charge number $Z_2^*(E_\perp)$ such that with $U(r_{\min}) = E_\perp$ the number of electrons per atom outside the distance r_{\min} from the string is $Z_2^*(E_\perp)$. Averaging (3.15) by means of (3.6'), the electronic stopping cross section is found to be

$$S_e(E_\perp) = S_e \cdot \left[1 - \alpha + \alpha \frac{Z_2^*(E_\perp)}{Z_2}\right], \quad (3.17)$$

where S_e is given by (3.13). The ratio $Z_2^*(E_\perp)/Z_2$ is according to (3.22) and (3.6'),

$$\frac{Z_2^*(E_\perp)}{Z_2} = \frac{d \cdot r_{\min} \cdot U'(r_{\min})}{2Z_1 Z_2 e^2}. \quad (3.18)$$

Thus, $Z_2^*(E_\perp)/Z_2$ is approximately equal to $vE_\perp/(E\psi_1^2)$, if $U(r) \propto r^{-\nu}$ near r_{\min} , cf. also (3.11). When the atomic model (2.6) is introduced in (3.18), the following simple formula is obtained

$$S_e(E_\perp) = S_e \cdot \left[1 - \alpha \exp\left(-\frac{2E_\perp}{E \cdot \psi_1^2}\right) \right]. \quad (3.19)$$

The formula (3.19) shows that the dip in electronic stopping is somewhat narrower in angle ψ than are string effects where penetration to the centre of strings is necessary. The direct significance of the characteristic angle ψ_1 is also clearly indicated. It is noteworthy that the atomic screening radius a does not enter, in spite of (3.19) being based on (2.6), where the screening radius is an important parameter. The formula (3.19) contains the usual error belonging to continuum potentials, i.e. the stopping does not rise above the normal stopping S_e when $E_\perp \gtrsim E\psi_1^2$, and compensation of the dip (cf. § 5) is not obtained. The error is not serious, however, because the rise above normal stopping is rather small.

The average straggling energy loss is immediately found from (3.16) and (3.6'),

$$\left(\frac{d(\Delta E)^2}{dR}\right)_e = 4\pi Z_1^2 e^4 N \cdot Z_2^*(E_\perp), \quad (3.20)$$

where $Z_2^*(E_\perp)$ may be replaced by the estimates in (3.18) or (3.19).

Electronic energy loss in single collision with string

The electronic energy loss, $\tau_e(l, \psi)$, in a single collision with a string, at impact parameter l and initial angle ψ , can also be derived on the basis of (3.13) and (3.15). But we disregard the resonance stopping, i.e. the first term in (3.15), since it takes place independently of a string collision. The energy loss in a single collision with an atom at impact parameter r is then, from the second term in (3.15),

$$T_e(r) = \frac{S_e}{2} \cdot d \cdot \varrho_s(r) = \frac{S_e}{2} \int_{-\infty}^{+\infty} dz \cdot \varrho(\sqrt{z^2 + r^2}), \quad (3.21)$$

where $\varrho(R)$ is the electron density in an atom, at a distance R from the nucleus, and where the electron density $\varrho_s(r)$ of the continuum string is

$$\varrho_s(r) = \frac{1}{4\pi Z_1 e^2} \frac{1}{r} \frac{d}{dr} (rU'(r)). \quad (3.22)$$

As an example, we choose again the approximation $U = Z_1 Z_2 e^2 \pi a / (2dr)$, and obtain

$$e_s(r) \cong \frac{Z_2 a}{8d} \frac{1}{r^3}. \quad (3.23)$$

We next integrate (3.21) over the encounters with atoms along a string, using (3.23) and the hyperbolic orbit of an r^{-1} -potential. The electronic energy loss in one collision with a string becomes, at a transverse energy $E_{\perp} = E\psi^2$ and impact parameter l ,

$$\tau_e(l, \psi) = \frac{S_e \cdot Z_2 \cdot a}{8d} \cdot \frac{1}{lg\psi} \cdot \frac{1}{l^2} \left(1 - \frac{b_{\perp}}{2l} \operatorname{arctg} \frac{2l}{b_{\perp}} \right), \quad (3.24)$$

where b_{\perp} is defined by $U(b_{\perp}) = E_{\perp}$, i.e. $b_{\perp} = \pi a \psi^2 / (4\psi^2)$. If we integrate (3.24) over all l , we obtain the formula (3.18), with $\nu = 1$.

In order to estimate the straggling in energy loss, we can compare the maximum energy loss in a string collision, i.e. $\tau_e(0, \psi)$ in (3.24), with the usual maximum energy transfer to an electron, $2mv^2$. The ratio $\tau_e/2mv^2$ can be large compared to unity. If in (3.13) we introduce $L \cong 1.5 \cdot x^{1/2} = 1.5 \cdot (v^2/v_0^2 Z_2)^{1/2}$, which formula applies approximately when x is of order of 1^{13} , (3.24) leads to

$$\tau_e < \tau_e(0, \psi) \approx \frac{a_0}{a} \left(\frac{a_0}{d} \right)^{1/2} \cdot \left(\frac{M_1}{m} \right)^{1/2} Z_1^{3/2} \cdot 70 \text{ eV}, \quad (3.25)$$

which would be $\sim 3 \text{ keV}$ for protons. Since this is an upper limit to τ_e , the energy loss is normally divided into bits much smaller than (3.25), so that the straggling is small.

§ 4. Scattering of Aligned and Random Beams

We have seen that a beam of fast particles, having some probability distribution in direction, can be divided roughly in two parts. For angles less than ψ_1 (or ψ_2 , at low energies) we are concerned with the aligned part of the beam, while angles large compared to ψ_1 constitute the random part of the beam. The part between $\sim \psi_1$ and \sim twice ψ_1 is a transition region. In most respects, the two parts have a quite different behaviour. Thus, the aligned part was found to have a smaller stopping cross section $S(E_{\perp})$ than has the random part. Moreover, in first approximation the two parts of the beam appear not to communicate at all. Consider an ion in the random part of the beam. It can easily collide with atoms and be scattered to other directions within the random beam. If it were to be scattered into the aligned beam, a comparatively close collision is required—i.e. impact parameters much smaller than a . However, when the ion subsequently emerges from essentially the centre of the string, it cannot easily become aligned, since ions in the aligned beam do not come closer to the string than $\sim a$. Scattering

from random beam to aligned beam therefore seems prohibited. Conversely, an ion in the aligned beam will in the continuum approximation keep a constant ψ far away from strings, i.e. a constant transverse energy E_{\perp} , changing merely its azimuthal angle in a more or less random manner. This indicates the difficulty of being scattered into the random beam.

It is therefore important to discuss those phenomena which may be responsible for transitions between aligned and random beam and for angular diffusion within the beams, i.e. lack of conservation of transverse energy. In the discussion we may distinguish between three groups of phenomena responsible for transitions between aligned and random beams.

The first group concerns deviations from the picture of parallel continuum strings, with a potential $U(r)$ or $U_{\text{tot}}(\vec{r})$, cf. (3.1). Deviations can be due to thermal vibrations, including zero-point vibrations of atoms, which implies that the force on the particle fluctuates; the effect of fluctuation of atomic positions will be studied in some detail. Deviations must also occur when there are defects and impurities in the lattice. Defects and impurities lead to important scattering effects, but are of variable size and can be quite small in pure and perfect crystals. A special kind of deviation arises from the periodicity of a perfect string, which gives fluctuations of the path as compared to the motion in a continuum potential $U(r)$. The periodicity of perfect strings normally gives rise to only a small scattering effect (cf. Appendix A).

The second kind of scattering is due to deviations from classical motion in a conservative force field. It is necessary to estimate the magnitude of quantum mechanical corrections to classical mechanical motion (cf. Appendix B). Moreover, a single collision between an ion and an atom is quasi-elastic, so that the force field is not strictly conservative. In first approximation, the deviations from elastic collisions are included in electronic stopping and the damping effect, cf. below.

The above two groups of phenomena lead to an average increase of E_{\perp} . A third effect may be singled out, especially because it tends to reduce E_{\perp} . Suppose that electronic stopping is dominating, and that the motion is in a continuum potential. Now, if the slowing-down force is directed against the motion and the energy loss is δE , the corresponding average change in E_{\perp} turns out to be $\delta E_{\perp} \cong -\beta \cdot \delta E \cdot E_{\perp}/E$, where $\beta \sim 0.5 - 1$. Although small, this damping effect can in some cases compete even with multiple scattering. We may also compare the damping with the change of transverse potential barrier. At high energies E , the transverse barrier is constant, while at low energies it may decrease as $E^{1/2}$ during slowing-down, cf. (2.10'). The damping by itself thus exceeds the decrease of the barrier.

Multiple scattering

When discussing the changes in ψ , or E_1 , along the particle paths, it is useful to consider at first the normal case of multiple scattering in a random system. Let ψ_x and ψ_y be the angles with the z -axis of the projection of the direction of motion on the $x-z$ and $y-z$ planes, respectively, so that $\vec{\psi} = (\psi_x, \psi_y)$ and $\psi = (\psi_x^2 + \psi_y^2)^{1/2}$. The average square fluctuation in angle is then $\Omega^2 = \langle (\vec{\psi} - \langle \vec{\psi} \rangle)^2 \rangle$. We study the change of Ω^2 as a function of penetration depth. It is well known (cf. BOHR¹²) that the increase in average square fluctuation in angle, due to nuclear collisions, is approximately given by

$$(\delta\Omega^2)_n \simeq \frac{M_2}{M_1} \cdot \frac{(\delta E)_n}{E} = \frac{(\delta E)_e}{E} \cdot \frac{Z_2 m}{M_1} \cdot \frac{L_n}{L_e}, \quad (4.1)$$

where⁶)

$$\left(\frac{dE}{dR}\right)_n = \frac{4\pi Z_1^2 Z_2^2 e^4}{M_2 v^2} N \cdot L_n, \quad L_n \cong \log(1.29 \varepsilon), \quad (4.2)$$

the reduced energy ε being given by (1.3). The formulae (4.2) and (4.1) apply for ε large compared to unity. When $\varepsilon \gtrsim 10^3$, it is seen that $L_n \sim 5-10$, so that L_n is not sensitive to the value of ε .

There is a similar increase in average square fluctuation in angle, due to electronic collisions, and derived from Rutherford scattering in close collisions between particle and atomic electrons,

$$(\delta\Omega^2)_e = \frac{m}{2M_1 E} \cdot S_e \cdot \varrho(\vec{R}) \cdot \delta R. \quad (4.3)$$

In a random system, where the density of electrons $\varrho(\vec{R})$ is replaced by its average, NZ_2 , the electronic contribution is much smaller than the nuclear one, (4.1), by a factor $\sim 2Z_2 L_n / L_e$. The formula (4.3) is valid only if v is larger than the electronic orbital velocities, or rather $x = v^2 / v_0^2 Z_2 \gg 1$.

In the case of the random beam, where all nuclear collisions are permitted, we can apply formula (4.1), with neglect of the electronic contribution (4.3). We can also use (4.1)—both for the random and aligned beams—in the case of interstitials, impurities that break the symmetry, amorphous surface layers, etc. Then, N represents the density of scattering centres, Z_2 being their atomic number.

In the present context, it is appropriate to consider ψ_1 as a standard angle, also for a random system without string effects. We introduce the path length, l_{n, ψ_1} , for which the average square multiple scattering in nuclear

collisions (4.1), applicable for the random beam, becomes equal to ψ_1^2 . Evidently,

$$l_{n, \psi_1} = \frac{2}{\pi N d^2 \cdot L_n \psi_1^2} \quad , \quad (4.4)$$

and the corresponding total energy loss of a random beam, or in a random system, is according to (3.13)

$$\delta E_{\psi_1} = \frac{2 Z_1 e^2 L_e}{d L_n} \cdot \frac{M_1}{m} \quad , \quad (4.5)$$

i.e. of the order of $Z_1 \cdot A_1 \cdot 10$ keV in the case of swift particles, for which $L_e/L_n \sim 1/2$.

In connection with (4.4) and (4.5), one should also consider single scattering by angles larger than ψ_1 . The mean free path for such single scattering is larger than (4.4) by a factor $2L_n \sim 10$. We may therefore often disregard single scattering, but for special purposes it becomes important, cf. (6.15).

Starting from an initially well-defined direction, e.g. corresponding to polar angle $\Psi = 0$, the distribution becomes approximately Gaussian,

$$P(\Psi) 2\pi \Psi d\Psi \cong \exp\{-\Psi^2/\Omega^2\} 2\Psi d\Psi/\Omega^2, \quad (4.6)$$

where Ω^2 is obtained by integration of (4.1). The Gaussian is a consequence of many small scattering processes. For large Ψ the actual distribution has a tail decreasing more slowly than (4.6), and due to large angle single scattering. The approximation of WILLIAMS and BOHR^{12) 17)} may be applied. If (4.3) is not negligible, it must be added to (4.1), and (4.3) contributes to the Gaussian only—not to the tail.

Consider next particles in the aligned beam. We may at first estimate the contribution to multiple scattering from electronic collisions. In analogy to (4.4), we introduce the path length l_{e, ψ_1} , for which $(\delta\Omega^2)_e$ becomes equal to ψ_1^2 . Averaging (4.3) according to (3.6'), we obtain

$$l_{e, \psi_1} = \frac{4Z_2}{\pi N d^2 L_e \psi_1^2} \cdot \frac{Z_2}{Z_2^*(E_1)} \quad . \quad (4.7)$$

The factor $Z_2/Z_2^*(E_1)$ is given by (3.18) or (3.19), and tends to unity for the random beam, while for the aligned beam it becomes large when $\psi \rightarrow 0$. The path length l_{e, ψ_1} is larger than l_{n, ψ_1} in (4.4), by a factor of at least $2Z_2$.

The strong multiple scattering (4.1) for a random system disappears completely for the aligned beam colliding with continuum strings, i.e. when conservation of transverse energy applies. In § 3 it was found that part of the multiple scattering reappears as a quick trend towards uniform distribution on the transverse energy shell, cf. (3.4). Another part reappears due to deviations from perfect strings. Thus, suppose that in one transverse atomic plane there is a deviation $\delta\vec{K}(\vec{r})$ from the usual transverse force $\vec{K} = -\text{grad}U(\vec{r})$. This gives a change in the transverse momentum \vec{p}_\perp , i.e. approximately

$$\delta\vec{p}_\perp = \frac{d}{v} \delta\vec{K}(\vec{r}). \quad (4.8)$$

When the square of this scattering is summed over the atoms along a string (or over successive transverse atomic planes), we obtain the change in average transverse energy, due to string imperfections, i.e. on the path length δR ,

$$\delta\langle E_\perp \rangle = \sum \frac{(\delta\vec{p}_\perp)^2}{2M_1} = \frac{d}{4E} \cdot \langle \delta\vec{K}(\vec{r})^2 \rangle \delta R, \quad (4.9)$$

where $\langle \dots \rangle$ denotes an average over positions in transverse motion of the particle, i.e. (3.6) can be applied.

If the average square amplitude, ϱ^2 , of the thermal vibrations (cf. (6.5)) may be considered as small, the corresponding force fluctuation becomes

$$\langle \delta\vec{K}(\vec{r})^2 \rangle = \frac{1}{2} \varrho^2 \langle K^2(r)r^{-2} + K'^2(r) \rangle, \quad (4.10)$$

in the case of axial symmetry. The total diffusion can be expressed in terms of the result (4.1) for a random system,

$$\delta\langle E_\perp \rangle = (\delta\Omega^2)_n \cdot E \cdot \gamma, \quad (4.11)$$

where the reduction factor $\gamma = \gamma_n(E_\perp, \varrho) + \gamma_e(E_\perp)$ is a sum of contributions from nuclear and electronic collisions. According to (4.9) and (4.10), the magnitude of γ_n becomes approximately

$$\gamma_n(E_\perp, \varrho) \approx \frac{1}{L_n} \cdot \frac{\varrho^2}{C^2 a^2} e^{E\psi_1^2} \left(1 - e^{-\frac{2E_1}{E\psi_1^2}}\right)^3, \quad (4.12)$$

if the standard atomic model (2.6) applies.

For comparison, we rewrite the electronic scattering contribution (4.7), introducing the standard atomic model by means of (3.19),

$$\gamma_e(E_\perp) = \frac{1}{L_n} \cdot \frac{L_e}{2Z_2} \left(1 - e^{-\frac{2E_\perp}{E\psi_1^2}}\right). \quad (4.12')$$

Although (4.12) and (4.12') are merely cursory estimates, it is apparent that—in contrast to random systems—the electronic contribution γ_e may exceed γ_n , if $2E_\perp/E\psi_1^2$ is small, and Z_2 low. Note, however, that the damping effect, cf. p. 33, can dominate over (4.12') when $M_1\psi_1^2 > 2m$.

When the increase in average square angle is known, the corresponding diffusion equation becomes

$$\frac{\partial}{\partial z} g(\vec{p}_\perp, z) = \text{div}_{\vec{p}_\perp} D(\vec{p}_\perp) \text{grad}_{\vec{p}_\perp} g(\vec{p}_\perp, z), \quad (4.13)$$

where $g \cdot dp_{1,x} dp_{1,y}$ is the differential probability, measured e.g. at potential $U = 0$. Further, $z = vt$ is the distance of penetration. The diffusion constant, D , is determined by $\delta\langle E_\perp \rangle$, and for axial symmetry one finds

$$2D(p_\perp) + p_\perp D'(p_\perp) = M_1 \frac{\delta\langle E_\perp \rangle}{\delta R}, \quad (4.14)$$

where the right-hand side is given by (4.11).

When the diffusion constant is known, the increase in square fluctuation of e.g. p_\perp can be derived. In order to compare with the increase in E_\perp we consider the quantity $\langle (p_\perp - \langle p_\perp \rangle)^2 \rangle / (2M_1)$, and obtain from (4.13), for initially well-defined E_\perp ,

$$\frac{\delta\langle (p_\perp - \langle p_\perp \rangle)^2 \rangle}{2M_1 \cdot \delta R} = \frac{D(p_\perp)}{M_1}. \quad (4.15)$$

If γ in (4.11) increases rapidly with E_\perp , the value of (4.15) is much less than $\delta\langle E_\perp \rangle / \delta R$. The smearing of the distribution by diffusion may then be disregarded, and the transverse energy remains well-defined, increasing steadily according to (4.9) or (4.11).

It can be of interest to solve the equations on the assumption of well-defined transverse energy. If the electronic contribution (4.12') can be disregarded, we obtain from (4.11), (4.12) and (4.4) the following change in E_\perp on a finite path length δR ,

$$\delta R \cdot \frac{4\varrho^2}{C^2 a^2 L_n} \cdot \frac{1}{l_{n,\psi_1}} = -\delta(1 - e^{-\frac{2E_{\perp}}{E\psi_1^2}})^{-2} \approx -\delta \left(\frac{E\psi_1^2}{2E_{\perp}} \right)^2, \quad (4.16)$$

where l_{n,ψ_1} is given by (4.4), and δ denotes the increase of the quantity in question. One interesting feature in (4.16) is not limited to this equation, but holds also for the more general diffusion based on (4.12); the path lengths for scattering are increased by a factor $\sim L_n \alpha^2 / \varrho^2$, as compared to (4.4), valid for random media. This result is essentially based on the validity of (4.10).

Single scattering

The reduction factor γ_n in (4.12) can become quite small. If the diffusion is sufficiently small, however, the dominant effect can be single scattering. By single scattering a particle may in one collision enter the random beam, or its fringes. Single scattering requires that the particle comes close to a nucleus, and the probability for single scattering is therefore proportional to the fraction of the total number of nuclei which may be hit by a particle with transverse energy E_{\perp} . This fraction turns out to be $\Pi_{\text{in}}(E_{\perp}) \approx P(r_{\text{min}}(E_{\perp}))$, where $r_{\text{min}}(E_{\perp})$ is the minimum distance of approach to a string, and $P(r)$ the probability for a nucleus to be more than the distance r away from the string, cf. § 6. The effective cross section for single scattering is thus

$$d\sigma_{\text{eff}}(E_{\perp}) = d\sigma \cdot \Pi_{\text{in}}(E_{\perp}). \quad (4.17)$$

For a given penetration depth, (4.17) can be applied to angles of deflection larger than those belonging to the Gaussian peak of multiple scattering.

§ 5. Rules of Angular Averages and Compensation

Suppose that we are concerned with a definite physical effect, like the energy loss per cm., the number of K-shell excitations, or the number of (p, γ) reactions. For random systems the effect occurs at a definite rate, independently of direction. In a crystal, due to e.g. string effects, the rate may change drastically within small solid angles. In § 3 we estimated some changes of this kind in the approximation of transverse potentials. However, it can be difficult to carry out estimates to a high degree of accuracy at all angles. It is therefore appropriate to ask for rules which hold irrespective of the use of e.g. transverse continuum potentials. In particular, it is of interest to know in how far the average of an effect over all directions of incidence in a crystal is equal to that of a random system. If this is the case, we say that there is compensation of the directional effect in question.

At first we can disregard slowing-down of particles, i.e. we assume conservation of total energy. We are then concerned with particles moving in a fixed potential in three-dimensional space. We can here utilize two concepts from statistical mechanics, i.e. reversibility and microcanonical distribution. The idealized experiment of interest in the following is to consider an external beam of particles, represented by e.g. a point source at A , and to ask for the probability of hitting a certain point of space, B , in the neighbourhood of one atom. This probability is to be compared with the corresponding one when e.g. all atoms in the crystal, except the one in question, are removed or brought in disorder.

Rule of reversibility

The first useful result is that of reversibility. We need not enter on details, and shall disregard magnetic fields. Not only can the motion of a particle in its orbit from one point A outside the crystal to a point B inside the crystal be reversed according to mechanics, but also the transition probabilities for direct and reversed processes are equal, $P_{AB} = P_{BA}$, if the potentials at A and B are equal (cf. below). More definitely, suppose that at A is emitted ν particles per second per unit solid angle, in a direction towards B , and that the cross section at B is σ . The rate P_{AB} of direct processes is equal to the rate P_{BA} of reversed processes, for which emission at B is ν per unit solid angle and cross section at A is σ . This result may be regarded as a consequence of Liouville's theorem. By finding the angular distribution outside the crystal of particles emitted by atomic nuclei in strings in the crystal, we have then also obtained the probability of hitting nuclei by an external beam of particles. These results are not changed by multiple scattering, where the processes are reversible too.

Reversibility can be violated in some cases. In fact, if slowing-down on the path between A and B is so large as to influence the deflections on the way, it may not be possible to reverse the path, neither for potential motion nor for multiple scattering effects.

Rule of angular averages

In order to obtain the second rule, i.e. the rule of simple angular averages, we introduce the probability P of a particle of energy E being at a space point, \vec{R} , inside the crystal. The probability is measured relative to that without a crystal. Let the initial state be a particle beam of given uniform intensity, and a direction specified by angles θ , φ . The probability is

then a function of ϑ and φ , $P = P(\vartheta, \varphi, \vec{R})$. It should be noted that P also depends on other variables, especially on the energy E , as well as on the type of particle (Z_1, A_1), and on the medium (Z_2 , lattice structure). If we average $P(\vartheta, \varphi, \vec{R})$ over all directions, and denote the average as $P(\vec{R})$, we obtain

$$P(\vec{R}) = \frac{1}{4\pi} \int P(\vartheta, \varphi, \vec{R}) \sin \vartheta d\vartheta d\varphi. \quad (5.1)$$

An average over external angles is equivalent to imposing on the system an external statistical equilibrium. The average can therefore be estimated from statistical equilibria, e.g. a microcanonical ensemble for one particle. For this purpose we introduce the particle-lattice potential $V_i(\vec{R})$ at the space point \vec{R} . If R is close to one atom, $V_i(\vec{R})$ should only include the potential from the other atoms, because we compare e.g. with the corresponding probability of coming near the atom in empty space (or in a random substance). Without considering details, we can state that $V_i(R)$ must be quite small, perhaps of order of few eV for protons, like E_c in (1.1), and thus usually much lower than the transverse potential $U(r)$. Since the available volume in momentum space is proportional to $pdE = \sqrt{2M_1(E - V_i(\vec{R}))} dE$, the average value of the probability $P(\vartheta, \varphi, \vec{R})$ is approximately

$$P(\vec{R}) \cong \left(\frac{E - V_i(\vec{R})}{E} \right)^{1/2} \cong 1, \quad (5.2)$$

where the deviation of P from unity can be disregarded, being approximately equal to $V_i/2E$. Now, probabilities, intensities or fluxes may differ by $[E - V_i(\vec{R})]/E$ to a power between perhaps -1 and $+1$, but such factors are quite close to unity, so that even without detailed estimates we may state that averages of type of (5.1) are equal to unity.

This leads to the rule of angular averages for energy conservation: Any quantity Q , depending linearly on $P(\vartheta, \varphi, \vec{R})$, has the same angular average as in a random system. By a random system is meant a system with the same density, but without directional effects, for instance because of lack of structure. Examples of quantities obeying the simple rule are electronic stopping, e.g. (3.15), and nuclear stopping, (3.10), at a fixed energy E . We may formulate the rule of angular averages as follows. If Q is given by

$$\left. \begin{aligned}
 Q(\vartheta, \varphi) &= a + \int b(\vec{R})P(\vartheta, \varphi, \vec{R})d^3R, \\
 \text{the average of } Q \text{ becomes, according to (5.1) and (5.2),} \\
 \langle Q(\vartheta, \varphi) \rangle &= \frac{1}{4\pi} \int d\Omega \cdot Q(\vartheta, \varphi) = a + \int b(\vec{R})d^3R.
 \end{aligned} \right\} (5.3)$$

Both in (5.3) and in (5.1) it is often possible to limit the average to a solid angle Ω small compared to 4π . In fact, suppose that at the borderlines of a solid angle Ω the particles are not deflected into or away from this solid angle, by deflections due to strings or planes. The separate average over Ω must then also fulfill (5.3).

If we apply the result of reversibility, the rule of angular averages can also be used for particles coming from any space point \vec{R} in the lattice and arriving at a point outside the lattice. In this case the rule is quite evident, even without use of reversibility and (5.3). In fact, imagine that atomic nuclei in the lattice emit α -particles, which process occurs at a fixed rate per unit solid angle. The α -particles are deflected away from string directions, and exhibit a certain angular distribution when emerging from the crystal. But, evidently, on a large sphere surrounding the crystal, all particles will be collected, independently of their possible deflections within the crystal. Moreover, if we collect within a relatively small solid angle around a string direction, the angular width still being large compared to string deflection, the number collected is the same as if the string were not there. Thus, the angular distribution has a complete compensation of the dip, characteristic of quantities linear in $P(\vartheta, \varphi, \vec{R})$. A similar problem was discussed in § 2, in connection with the classical shadow behind an atom.

Limitations of rule of angular averages

When we are concerned with definite physical observations, like those mentioned in the beginning of this section, the simple rule does not always apply, because in actual fact energy conservation is violated in slowing-down and the measured quantities may be strongly dependent on energy. By and large, physical effects depending on slowing-down will not obey the rule of angular averages. It can be useful to consider a few examples.

First, a basic quantity is the range of a particle. The stopping cross section $S(E_1, E)$, at a definite energy E , is linear in P and follows the rule of averages. The range, however, is of type of $\int dR = \int dE / (N \cdot S(E_1, E))$. It is

therefore not linear in P , and does not follow the rule. In fact, deviations can be quite large. In two cases will deviations from the rule become small. If $S(E_1) \approx S$, the latter being the stopping cross section for random slowing-down, we have $S(E_1)^{-1} \cong S^{-1} \cdot (2 - S(E_1)/S)$, which is linear in P . Moreover, in a polycrystalline medium where the size δR of each crystal corresponds to $\delta E = \delta R \cdot (S(E_1)N) \ll E$, the range will be as in a random system.

Second, an instructive example is afforded by a (p, γ) reaction for protons passing through a crystal. The reaction occurs at a definite energy E_0 , and has a width Γ , very small compared to E_0 . Suppose that Γ nevertheless remains so large that an energy loss $\sim \Gamma$ is obtained only by penetration of many atomic layers. The number ν of reactions is then proportional to $\nu \propto P(\psi, \vec{R}_n)/S_e(\psi)$, where $P(\psi, \vec{R}_n)$ indicates the probability of hitting a nucleus. Since the ratio P/S_e is not linear in P , its average over all directions need not correspond to a random system, and (5.3) does not apply. However, the probability of hitting an atomic nucleus may be essentially zero, except when E_1 is large. Since $S_e(E_1)$ has a rather narrow dip, cf. (3.19), we may have $S_e(E_1) \approx S_e = \text{const.}$, in the region where P is different from zero, in which case the compensation belonging to (5.3) is approximately obtained.

As indicated by these examples, there is a large number of combinations of effects which may influence the angular averages, when slowing-down comes into play. Therefore, a thin single crystal foil, where the energy loss remains small, is one of the few examples where physical effects can obey (5.3) in a straightforward manner.

In measurements of angular dependence of effects in the neighbourhood of strings and planes, the compensation in (5.3) is usually of interest in a qualitative way only. In other cases, e.g. if nuclear cross sections are to be measured with high accuracy in solids, the applicability of (5.3) can be of direct importance.

Rule of spatial averages

The previous averages were concerned with angles, but also averages over space give rise to interesting rules. Suppose that an external beam has a fixed direction given by (θ, φ) , e.g. close to a string direction, and consider a nuclear process with a constant, energy independent cross section. The rate of the process depends on the position of the nucleus in the lattice. Now, if the probability density of the distribution of nuclei is constant in a

transverse plane, the process has for these nuclei the same rate as in a random substance, simply because every particle must pass through some point of the transverse plane. Thus, for a fixed value of z , less than the penetration depth of every particle,

$$\langle P(\vartheta, \varphi, \vec{R}) \rangle_{xy} = \frac{1}{A_0} \iint_{A_0} dx dy P(\vartheta, \varphi, \vec{R}) = 1, \quad (5.4)$$

where P is the previously mentioned probability, normalized to unity for a random system. Any linear function $Q = a + b \cdot P(\vartheta, \varphi, \vec{R})$ has the average $\langle Q \rangle_{xy} = a + b$. Therefore, if—for fixed external direction ϑ, φ —there is a dip in reaction rate when the atomic position is at a string, there must be a rise above normal yield at positions in between strings. However, the area outside strings is much larger than the effective area of a string; the increase in rate is then quite small, of order of $Nd \cdot \pi a^2$. A somewhat larger effect would occur for planes. Still, because of the smallness of these changes, reaction rates may then instead be dominated by secondary string phenomena, like electronic stopping, cf. § 6.

§ 6. Idealized Experiments and Comments on Measurements

When discussing experiments—both idealized and actual experiments—it is instructive to bear in mind that, at low angles of incidence, particles are prevented from coming closer than $\sim a$ to the centre of strings (or planes). This indicates, firstly, experimental tools that may be chosen. In fact, there is a possibility of utilizing any physical process requiring that the particle is less than the distance a from the atomic nucleus (nuclear reactions, Coulomb excitation, inner shell excitation, wide angle Rutherford scattering, emission of charged particles from radioactive nuclei). Secondly, measurements of this kind give direct information about paths of particles in the lattice and their scattering, and hence enables one to study the important primary phenomena, which govern the particle motion, cf. p. 9. Thirdly, by means of the shielding inside $\sim a$ one is able to pin atomic positions with an accuracy $< a$ in the vicinity of lattice sites, so that e.g. a method of observing defects and positions of impurity atoms is available.

It is easy to visualize many further applications, but it seems proper to demonstrate first the way in which theory and experiments can cope with the primary task sketched above. When that is done, a quantitative basis

is obtained for estimating in how far the more complicated applications may be realized. In the present context, however, we shall merely discuss briefly a few aspects of the primary task.

Three stages in particle motion

The fate of particles on their way from an external source to e.g. an atomic nucleus in a crystal may be divided into three successive stages. These three stages appear in the opposite order for the reversed process of a particle coming from a nucleus and arriving at a detector outside the crystal. A calculation of the probability of a direct process is often equivalent to an estimate of the reverse process, cf. § 5.

A particle beam has an initial angular spread before entering the crystal surface. Let the initial distribution be $P(E\psi_e^2)d(E\psi_e^2)$, where ψ_e is the external angle with strings. It can be convenient to include in this spread the multiple scattering due to impurity layers in front of the crystal surface. It should be remembered that the angular distribution from scattering by a thin layer consists of a narrow Gaussian peak and a tail due to single scattering.

Consider particles arriving at the crystal surface at a definite angle ψ_e with a string (or a plane). The first stage is then the transition from immediately outside to immediately inside the crystal surface. We may introduce a transmission factor,

$$T = T(E_{\perp}, E\psi_e^2),$$

such that $T \cdot dE_{\perp}$ is the differential probability of transverse energy between E_{\perp} and $E_{\perp} + dE_{\perp}$, when the external angle is ψ_e . In the continuum description we get, if $U_{\text{tot}}(\vec{r}) \approx U(r)$,

$$T(E_{\perp}, E\psi_e^2) = \int_0^{r_0} \frac{2rdr}{r_0^2} \delta(E_{\perp} - E\psi_e^2 - U(r)), \quad (6.1)$$

because, at the point \vec{r} , the transverse energy becomes $E\psi_e^2 + U(r)$. In this way, the initial distribution $g(E_{\perp}, z = 0)$ can be obtained,

$$g(E_{\perp}, 0) = \int P(E\psi_e^2)d(E\psi_e^2)T(E_{\perp}, E\psi_e^2), \quad (6.2)$$

where the particle energy is E .

In (6.1) is assumed axial symmetry; the general formula corresponding to (6.1) is a normalized integration over the unit cell. Therefore, in the corresponding estimate for planes, the right-hand side of (6.1) is replaced by

$$\int_0^{d_p/2} \frac{2dy}{d_p} \delta(E_{\perp} - E\psi_e^2 - Y(y)),$$

where d_p is the distance between planes, ψ_e the angle with the plane, and $Y(y)$ the continuum plane potential. In (6.1) the direction of the transverse motion is disregarded and we shall omit estimates of e.g. $g(\vec{p}_{\perp}, \vec{r}, z = 0)$.

The second stage consists in the passage through the crystal from the surface to depth z . During this stage there is multiple scattering, i.e. a redistribution of transverse energy in a manner somewhat similar to diffusion. The redistribution depends strongly on the value of $E_{\perp}/E\psi_1^2$, cf. § 4. At the same time, the particles are subject to slowing-down, so that the energy E decreases. The slowing-down also depends on $E_{\perp}/E\psi_1^2$, cf. § 3. Accordingly, a redistribution factor R is obtained, giving the probability of energy E' and transverse energy E'_{\perp} , at depth z , if their values are E and E_{\perp} at the surface, i.e.

$$R = R(E', E'_{\perp}, z; E, E_{\perp}, 0),$$

where $R(E', E'_{\perp}, 0; E, E_{\perp}, 0) = \delta(E' - E)\delta(E'_{\perp} - E_{\perp})$. Usually, one can either disregard energy loss as compared to diffusion, or disregard diffusion and include only energy loss. This leads to considerable simplification in R . In some cases we can assume that both E and E_{\perp} change smoothly, without fluctuations, as functions of depth, so that R is a δ -function in both E' and E'_{\perp} .

When R is known, we can estimate the probability $g(E', E'_{\perp}, z)dE'dE'_{\perp}$ of energy in the interval dE' and transverse energy in the interval dE'_{\perp} ,

$$g(E', E'_{\perp}, z) = \int dE_{\perp} g(E_{\perp}, 0) R(E', E'_{\perp}, z; E, E_{\perp}, 0). \quad (6.3)$$

The third stage is the occurrence of the actual physical process, a nuclear reaction for instance. In processes of this kind, the particle essentially must penetrate to the centre of atoms, and the probability $\Pi_{\text{in}}(E_{\perp})$ for this will be discussed in some detail. If $\Pi_{\text{in}}(E_{\perp})$ is known, and the cross section for the process in question is σ , the effective cross section σ_{eff} at depth z becomes

$$\sigma_{\text{eff}}(z) = \int dE' \int dE'_{\perp} g(E', E'_{\perp}, z) \Pi_{\text{in}}(E'_{\perp}) \sigma(E'). \quad (6.4)$$

Cross sections $\sigma(E')$ for nuclear reactions can be of resonance type in the energy E' .

We refrain from discussing further the general case of superposition of the three stages mentioned. Instead, a few basic examples will be treated after the estimates of $\Pi(E_{\perp})$.

Particle emission from string atoms and $\Pi(E_{\perp})$

Several characteristics of basic phenomena in the string effect are illustrated by the following idealized experiment. A fast, positively charged particle leaves a nucleus by a process independent of lattice properties, e.g. an α -decay. The nucleus has some probability distribution in space. The first question to be solved is the probability $\Pi_{\text{out}}(E_{\perp})dE_{\perp}$ of transverse energy between E_{\perp} and $E_{\perp} + dE_{\perp}$.

We note that $\Pi_{\text{in}}(E_{\perp}) = \xi \cdot \Pi_{\text{out}}(E_{\perp})$ is the probability of the opposite process as described by (6.4), where ξ is a constant accounting for available space—or phase space—in the two opposite processes. In fact, in the continuum description ξ^{-1} is the fraction of the area of the transverse plane accessible to the particle, i.e. $\xi^{-1} = 1 - r_{\text{min}}^2(E_{\perp})/r_0^2$, and thus ξ is normally close to unity. The subsequent fate of the particle, as determined by multiple scattering and emergence through surface, can be treated separately, the former being determined by (6.3) and the latter by reversal of (6.2).

Suppose that the atomic nucleus is in the neighbourhood of an atomic position in a perfect string, with probability distribution $dP(r)$, where r is the distance from the string axis. The distribution in z -direction may be disregarded. For simplicity, a Gaussian type distribution will be used as an example in the following, i.e.

$$dP = e^{-\frac{r^2}{\varrho^2}} 2r dr \cdot \alpha / \varrho^2, \quad (6.5)$$

where r is the distance from the perfect string, and α is a normalization constant, $\alpha = \{1 - \exp(-r_0^2/\varrho^2)\}^{-1}$, i.e. $\alpha \approx 1$ if ϱ^2 is small compared to $r_0^2 = 1/(\pi N \cdot d)$. The distribution (6.5) might roughly represent zero-point and thermal vibrations of an atom with respect to its neighbours. If ϱ is large, (6.5) corresponds to a uniform distribution within the unit cell. It can therefore represent cases other than vibrations. The calculations of several effects, cf. (4.10) and (6.13), involve merely the average square vibration of an atom, ϱ^2 , and not the probability distribution as such. At low temperatures, ϱ^2 is determined by zero-point vibrations of lattice atoms, while at high temperatures it increases proportionally to temperature.

We ask for the initial distribution in transverse energy $\Pi_{\text{out}}(E_{\perp})$, of particles emitted into the lattice from an atom close to a lattice site. Consider

the approximation in Appendix A, where a transverse potential $U(r)$ may be used, and E_{\perp} is to be registered at the planes half-way between atoms. A particle initially at a distance r from the string, moving at an angle φ with the string and azimuthal angle ϑ , will be a distance r^* away from the string when it arrives at the half-way plane, where $r^{*2} = r^2 + (\varphi d/2)^2 + r\varphi d \cdot \cos\vartheta$. Therefore,

$$\Pi_{\text{out}}(E_{\perp}) = \int_{r=0}^{r_0} dP(r) \int d(E\varphi^2) \int_0^{2\pi} \frac{d\vartheta}{2\pi} \cdot \delta(E_{\perp} - U(r^*) - E\varphi^2), \quad (6.6)$$

and for planes an analogous formula holds.

If $\varphi d/2$ is small compared to the range ϱ of the distribution, we may put $r^* = r$, and (6.6) becomes

$$\Pi_{\text{out}}(E_{\perp}) = \int_{U(r) < E_{\perp}}^{r_0} dP(r). \quad (6.7)$$

Although (6.7) implies a dip quite similar to that in (6.6) for low values of E_{\perp} , the magnitude of (6.7) apparently cannot exceed unity, in contrast to (6.6). The shoulder of the distribution at $E_{\perp} \sim E\psi_1^2$ is therefore absent in the approximation (6.7).

By means of (6.7), (6.5) and the standard potential (2.6) a definite expression for Π_{out} is obtained

$$\Pi_{\text{out}}(E_{\perp}) = \exp\left\{-\frac{C^2 a^2}{\varrho^2} (e^{E\psi_1^2} - 1)^{-1}\right\} - \exp\left\{-\frac{r_0^2}{\varrho^2}\right\}, \quad (6.8)$$

where it is assumed that $\varrho \ll r_0$, i.e. $\alpha \approx 1$. When $E_{\perp} \rightarrow U(r_0)$, the expression in (6.8) tends to zero. However, the value of $\Pi_{\text{out}}(E_{\perp} \approx 0)$ is sensitive to the atomic potential, and to the behaviour of the probability distribution (6.5). The number of particles emerging from the crystal surface, at angles close to zero with the string, may therefore be strongly influenced by multiple scattering, etc.

In view of the variability of the maximum dip, it can be of interest to look for quantities less sensitive to multiple scattering. From (6.7) and (6.8) approximate estimates of the width of the dip in $\Pi(E_{\perp})$ may be easily obtained, but a precise definition of the width is less simple. However, the integrated dip is more well-defined. Since the dip from unity is $1 - \Pi_{\text{out}}(E_{\perp})$, we may integrate over positive values of this quantity. When (6.7) is introduced, we obtain an integrated dip

$$\Omega(\varrho) = \int (1 - H_{\text{out}}(E_{\perp})) 2\pi \sin \psi d\psi = \frac{\pi}{E} \int_0^{\pi} (1 - H_{\text{out}}(E_{\perp})) dE_{\perp} = \left. \begin{aligned} &= \frac{\pi\alpha}{E} \int_0^{r_0^2} \frac{d(r^2)}{\varrho^2} e^{-\frac{r^2}{\varrho^2}} U(r). \end{aligned} \right\} \quad (6.9)$$

When ϱ is large compared to a , but small compared to r_0 , we find by partial integration,

$$\Omega(r_0 \gg \varrho \gg a) = \frac{1}{\varrho^2 d \cdot E} \int 4\pi R^2 dR V(R) = \frac{Z_1 Z_2 e^2}{\varrho^2 d \cdot E} \pi \frac{2}{3} \overline{R^2}, \quad (6.10)$$

where $\overline{R^2} = Z_2^{-1} \int_0^{\infty} 4\pi R^4 dR \varrho(R)$ is the average square radius of the atom per electron.

In the LENZ-JENSEN description⁹⁾ the average square radius becomes $\overline{R^2} \simeq 15a^2$, which result agrees well with measurements as well as with the HARTREE treatment. For ϱ large compared to a , we may thus put

$$\Omega(\varrho) \simeq \pi \cdot \frac{\psi_1^2}{2} \cdot 10a^2/\varrho^2. \quad (6.11)$$

In the opposite limit of ϱ small compared to a we find readily, from (2.5),

$$\Omega(\varrho < a) = \pi \cdot \frac{\psi_1^2}{2} \log \left(\frac{C^2 a^2}{\varrho^2} \gamma \right), \quad (6.11')$$

where $\gamma = 1.78$ is Euler's constant. A qualitative estimate, applicable for all values of ϱ , is therefore

$$\Omega \simeq \pi \cdot \frac{\psi_1^2}{2} \log \frac{\gamma C^2 a^2 + \varrho^2}{\varrho^2}. \quad (6.12)$$

The formula (6.12), giving the dip as a function of transverse energy for $\varrho \ll r_0$, should in this case also give approximately the dip outside the crystal, if multiple scattering can be neglected. However, when ϱ in (6.9) becomes large compared to r_0 , there is a uniform probability distribution $dP(r)$ in the unit cell, $r < r_0$. The effects of exit from the surface are then most important, and according to the discussion in § 5, there is no dip outside the crystal. It so happens that (6.12) has the value zero in this limit, and in this sense represents better the external than the internal angular distribution. There is, however, a serious drawback in the formulae (6.7) – (6.12). A continuum potential has been used, and thus compensating shoulders are disregarded. It would be more correct to use (6.6) and apply the formulae in Appendix A, according to which the potential energy is to be measured at the planes half-way between atoms.

The equation (6.12) can be used in two ways. From knowledge of ϱ , the value Ω can be found approximately; from measurements of Ω , the value of ϱ^2 can be estimated qualitatively. Apart from such estimates, it is seen that Ω is proportional to $\psi_1^2 = 2Z_1Z_2e^2/d \cdot E$.

Lowest minimum yield

The minimum yield of e.g. nuclear reactions at a given depth corresponds to external angle $\psi_e = 0$. The lowest value χ of the minimum occurs at low depth, where the multiple scattering is small. If we disregard the multiple scattering, we find from (6.1) and (6.4) that there always remains a yield from thermal vibrations. If the continuum description applies, we obtain from (6.7) and (6.1) the first contribution χ_1 to the total χ ,

$$\chi_1 = N \cdot d \cdot \pi \varrho^2, \quad (6.13)$$

where ϱ^2 is the average square amplitude of atomic vibrations with respect to the string. It is noteworthy that (6.13) does not depend on the probability distribution, i.e. (6.5) need not apply. The magnitude of χ_1 is often $\chi_1 \lesssim 10^{-2}$, when $d \sim 3\text{\AA}$.

For several reasons, the effective lowest minimum can be higher than the above value. Particles in the exterior beam, which hit within $\sim a$ from the centre of a string, obtain transverse energy $\sim E \cdot \psi_1^2$, and they may after very little multiple scattering be able to hit the centre of atoms; the path length in question is $\simeq l_{n,\psi_1}$ in (4.4). This leads to the next, and less well-defined contribution to χ ,

$$\chi_2 \cong N \cdot d \cdot \pi a^2. \quad (6.14)$$

In the case of major strings, i.e. for $d \sim 3 \cdot 10^{-8}$ cm, the magnitude of χ_2 varies between ~ 0.03 in the lighter substances and ~ 0.005 in heavy substances. For planes, we roughly find $\chi_2 \sim 2a/d_p$.

The result (6.14) corresponds to the high energy case (2.9'). At low energies, or large values of d , there is a well-defined increase in the fractional area χ_2 corresponding to transverse energy above the barrier. According to (2.10) or (A.21) one obtains $\chi_2 \cong \pi N \cdot d^2 a \psi_1$, when ψ_1 is large compared to a/d .

It may be noted that the atoms at the surface can react directly with the particle. The effective number of layers, of thickness d , giving full contribution is ξ , where $\xi > 1$. Measurements confined to the first 10-50 layers cannot therefore yield very strong dips, and a certain amount of multiple scattering must always be included in the measurements.

Although a classical orbit remains outside the centre of atoms in a perfect string, there is a quantal penetration. However, particles with the

same value of Z_1/E have the same characteristic angle ψ_1 , but their wave length decreases proportionally to $(M_1E)^{-1/2} \propto (M_1Z_1)^{-1/2}$. The quantal penetration probability is in this sense an independent quantity which can be made quite small.

The presence of amorphous impurity layers on the surface of the crystal need not cause large multiple scattering. Still, effects of single scattering cannot be disregarded in the present context. Let the number per cm^2 of the i 'th atomic species be ν_i , while its collision diameter with the particle is b_i . The fraction of particles deflected by an angle larger than Θ , in single scattering, is then

$$\sum_i \nu_i \cdot \pi b_i^2 \cdot \Theta^{-2},$$

where it is assumed that Θ is so large that Rutherford scattering applies. If the particles originally have zero angle with a string direction, we have directly obtained a tail of the distribution in transverse energy, and the contribution χ_3 to χ is obtained,

$$\chi_3 = \sum_i \nu_i \pi b_i^2 \cdot E \int_0^\infty \frac{dE_\perp}{E_\perp^2} \Pi(E_\perp). \quad (6.15)$$

The integral in (6.15) may be evaluated by means of (6.6) or (6.7). At high particle energies and for $\varrho < a$ we may assume, crudely, that $\Pi \sim 0$ for $E_\perp < E\psi_1^2$, and $\Pi \sim 1$ for $E_\perp > E\psi_1^2$, leading to $\chi_3 \sim \psi_1^{-2} \sum \nu_i \pi b_i^2$. This result is interesting in several respects. The value of χ_3 can exceed χ_1 or χ_2 , if there is a substantial surface layer of not too low atomic number. It is also seen that at high particle energies both χ_1 , χ_2 and χ_3 may be proportional to the spacing d between atoms in the string. It is therefore expected that the minimum yield, when small, increases with d in a simple manner.

In any case, if measured dips are in the neighbourhood of the minima quoted above, it seems possible to study in detail the effects of multiple scattering, etc., as discussed in the beginning of this chapter.

Comments on experiments

Although detailed comparisons with experiments would be out of place, it may be proper to comment briefly on some measurements directly connected with the theory. We do this in the spirit of the introductory remarks in this chapter (p. 43), selecting primary directional effects.

In the exploratory measurements on (p, γ) reactions in Al and Si at

~ 400 keV, BØGH, DAVIES and NIELSEN⁷⁾ observed the expected reduction in yield in string directions. The yield is proportional to $H(E_{\perp})/S_e(E_{\perp})$, the probability distribution in E_{\perp} depending on external angle. The observed reduction by a factor ~ 5 was large enough to be promising⁵⁾, partly because the disturbing influence of electronic stopping could then be disregarded, and partly because it seemed comparatively easy to develop further this tool of solid state observations. The measurements are apparently, as to purpose and result, different from those of THOMPSON¹⁹⁾.

In continued measurements, also effects of planes were clearly seen, and higher proton energies were used²⁰⁾. In connection with (p,γ) reactions, with rate $\propto S_e^{-1}(E_{\perp})$, it may be mentioned that they might also be used for identifying interstitials, where peaks in yield, instead of dips, should appear for atoms outside strings when $\psi_e < \psi_1$ (cf. p. 43 and (3.19)).

The measurements by DOMENJ and BJÖRKEQVIST¹⁸⁾ are of particularly simple and informative kind. The angular distributions of α -particles, emitted by heavy ions stopped in W , showed dips by a factor ~ 4 and angular widths in agreement with (2.9). It could be concluded that most, if not all, ions ended up in lattice positions. In more detailed measurements, including changes of temperature, it should be possible to verify positions of ions in the lattice and even to check vibrations (cf. also (6.9)).

Observations utilizing wide angle Rutherford scattering would seem to provide a promising and versatile tool, because of the large cross sections, and the free choice of Z_1 , Z_2 and $E^5)$. The measurements by BØGH and UGGERHØJ²²⁾ of Rutherford scattering for 400 keV protons in Ta and with energy analysis of the emerging protons, provide the most definite and detailed information obtained so far. Strings of both low and high index numbers are clearly seen. The angular widths as functions of d and E are in accord with (2.9) and (2.10), and dips approach the lower limits (cf. p. 49 and ref. 5). An effect of planes is seen as a background of the dominating string dips. It may be added, as an example, that Rutherford scattering can be used for determining positions of impurity atoms, in lattice sites or in interstitial positions.

As to other processes requiring that the particle comes close to the nucleus, preliminary measurements of inner atomic shell excitation by ~ 100 keV protons have been performed by BRANDT et al.²¹⁾, but in the interpretation the repulsion by atomic strings was not taken into account.

As regards secondary directional effects (cf. p. 9), the most prominent one is slowing-down. For fast protons, the most accurate observations were performed by ERGINSOY, WEGNER and GIBSON¹¹⁾. These measurements

clearly reveal effects of planes and strings. The energy loss is found to be reduced by a factor of at most ~ 2 , in rough agreement with (3.15). The wide distribution in energy loss is not to be accounted for as usual straggling, which becomes quite small according to (3.20), but in terms of the statistics of the two first stages in particle motion mentioned on p. 44 ff.

Numerous careful experimental studies on penetration by heavy ions in the keV region have been performed, especially by DAVIES and co-workers (e.g. refs. 1 and 23), and by LUTZ and SIZMANN²⁴).

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Appendix A

Classical Scattering by Perfect String and Continuum Potential

The accuracy of the continuum string approximation may be assessed approximately within classical mechanics. Besides classical mechanics, the calculations in this appendix are based on the perfect string, i.e. atoms placed on a straight line with constant spacing d , and are easily generalized to a perfect lattice.

The first circumstance to be noted is the strict conservation of angular momentum with respect to the string. We shall at first discuss only the case of zero angular momentum. This is the least favourable case for conservation of transverse energy, because the particle penetrates the closest to the string.

Let atoms be placed on the z -axis, at $z = 0, \pm d, \pm 2d, \dots$. It is convenient to introduce the planes half-way between atoms, $z = \pm d/2, \pm 3d/2, \dots$, and measure transverse coordinates (x, y) at these planes. The distance

from the string is $r = (x^2 + y^2)^{1/2}$, and the motion is assumed to be in a plane containing the string (cf. above). We want to find the accuracy with which transverse energy is conserved between the two planes, the a -plane where $z_a = -d/2$, and the b -plane where $z_b = +d/2$. In the a -plane the distance from z -axis is r_a and the angle with the z -axis is ψ_a , and in the b -plane distance and angle are r_b and ψ_b . At $z = 0$, where the deflection

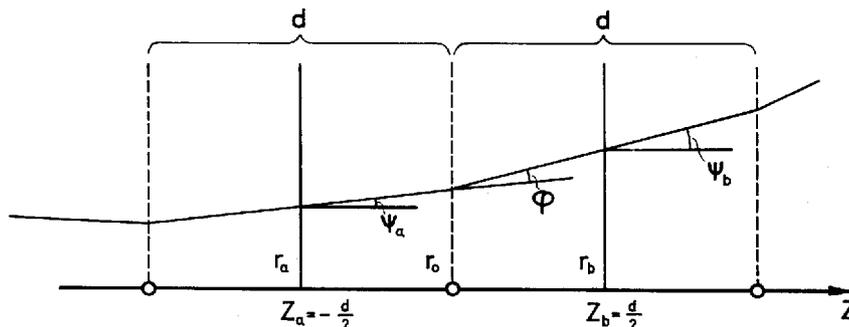


Fig. 2. Classical deflections of particle by perfect string, with coordinates recorded at half-way planes, cf. text.

occurs, the distance from the axis is r_0 . Then, $r_b = r_0 + \psi_b \cdot d/2$, and $r_a = r_0 - \psi_a \cdot d/2$. The deflection at r_0 becomes, cf. (2.1'),

$$\varphi = \psi_b - \psi_a = -\frac{d \cdot U'(r_0)}{2E}; \quad (\text{A.1})$$

r_0 and $r_b - r_a$ are given by

$$r_0 = \frac{r_a + r_b}{2} - \varphi \frac{d}{4}; \quad r_b - r_a = \frac{d}{2}(\psi_a + \psi_b). \quad (\text{A.2})$$

We here disregard terms of relative magnitude $(\psi_a + \psi_b)^2/2$ in r_0 , and of relative magnitude $\varphi r_0/d$ in $r_b - r_a$.

From these relations we may find the degree of conservation of transverse energy, retaining only powers of ψ less than ψ^4 ; the latter limitation is implicitly contained in the small angle approximation for ψ . We tentatively introduce transverse energies $E_{\perp}(r_a)$ and $E_{\perp}(r_b)$,

$$E_{\perp}(r_a) = E \cdot \psi_a^2 + W(r_a), \quad E_{\perp}(r_b) = E \cdot \psi_b^2 + W(r_b), \quad (\text{A.3})$$

and ask whether a transverse energy of this kind can be approximately conserved, i.e.

$$E_{\perp}(r_a) = E_{\perp}(r_b). \quad (\text{A.4})$$

If (A.4) holds, it is easy to calculate the angle of emergence ψ from the string, since $E \cdot \psi^2 = E_{\perp}$. An over-all validity of the continuum approximation would mean that the conservation in (A.3) holds not merely at the half-way planes, but is also accurate at other values of z .

Consider the difference between $E_{\perp}(r_a)$ and $E_{\perp}(r_b)$ in (A.3), and eliminate ψ_a and ψ_b by means of (A.1),

$$E_{\perp}(r_b) - E_{\perp}(r_a) = W(r_b) - W(r_a) - (r_b - r_a) \cdot U'(r_0). \quad (\text{A.5})$$

Since (A.2) is an implicit equation for r_0 , i.e.

$$r_0 = \frac{r_a + r_b}{2} + \frac{d^2}{8E} U'(r_0), \quad (\text{A.6})$$

r_0 and $U'(r_0)$ are only functions of the sum $r_a + r_b$, in the present approximation. The mean distance $(r_a + r_b)/2$ is, for brevity, denoted as r , and we may ask for the connection between differential changes in r and r_0 . From (A.6) is obtained

$$dr = dr_0 \left[1 - \frac{d^2}{8E} U''(r_0) \right]. \quad (\text{A.7})$$

If r_0 initially is large, and then decreases, the two terms dr and dr_0 remain approximately equal, until the term in brackets in (A.7) becomes zero. Thereupon, r increases rapidly as r_0 tends to zero. It is therefore appropriate to require

$$E > \frac{d^2}{8} U''(r_{\min}), \quad (\text{A.8})$$

in order that the transverse motion can be described by a continuum potential; in (A.8) the minimum distance of approach to the string is $r_{\min} = r_{\min}(E_{\perp})$ for transverse energy E_{\perp} . The criterion (A.8) is closely equivalent to those in (2.9), (2.10), or (2.7).

In order to find W , we expand in (A.5),

$$W(r_b) - W(r_a) = (r_b - r_a) \cdot W'(r) + \frac{1}{24} (r_b - r_a)^3 \cdot W'''(r) + \dots \quad (\text{A.9})$$

Assuming $r - r_0$ to be small, we also find

$$U'(r_0) = U'(r) + U''(r) \cdot \frac{d^2}{8E} U'(r) + \dots \quad (\text{A.10})$$

As a result of this, we find that if the last term in (A.9) is disregarded, (A.5) becomes equal to zero when the potential $W(r)$ is given by

$$W(r) = U(r) + \frac{d^2}{16E} [U'(r)]^2 + \dots \quad (\text{A.11})$$

However, it is easily verified that the condition (A.8) demands that the second term in (A.11) remains small compared to the first one. We may therefore identify $W(r)$ with the continuum potential $U(r)$. Nevertheless, the second term in (A.11) may be given a simple physical interpretation, accounting approximately for single scattering, albeit in an incomplete manner, cf. below.

We omitted the last term in (A.9). Since we need only a crude estimate, we may by means of this term find an upper limit to the lack of conservation of transverse energy in a collision with a string. In fact, suppose that this term represents twice the uncertainty in energy conservation when going from z_a to z_b . Suppose even that the uncertainties add. The total uncertainty in transverse energy after a string collision must be less than this sum. We write the sum as an integral, where we can put $(r_b - r_a)^2 = d^2 \cdot \psi_r^2 = d^2(E_1 - U(r))/E$, as well as $W(r) = U(r)$,

$$\delta E_1 \rightarrow \left. \begin{aligned} \int_{r_{\min}}^{\infty} \frac{d^2}{24E} \{E_1 - U(r)\} U'''(r) dr &= \frac{d^2 U'(r_{\min})^2}{48E} = \\ &= \frac{d^2}{48E} E_1^3 \cdot \frac{\nu^2}{r_{\min}^2} \end{aligned} \right\} \quad (\text{A.12})$$

where ν is the effective power of $U(r)$, $\nu = -d \log U(r) / d \log r$. The right-hand side becomes comparable to E_1 only if $E_1 > E \psi_1^2$, as was to be expected. Moreover, the right-hand side decreases as E_1 to a power between 3 and 4, since $\nu \sim 1 - 2$. It is therefore seen that transverse energy conservation must be accurately fulfilled, if E_1 is not large. We conclude that the conservation of transverse energy, as expressed by (A.4), is a good approximation, and that deviations from it must be due to e. g. atomic vibrations.

In connection with (A.3), (A.4) and (A.11) may also be noted the special case of a harmonic oscillator potential. Then, the higher derivatives of U vanish, and an exact solution is obtained. In fact, suppose that $U_{\text{tot}}(\vec{r}) = Cr^2/2$. The general two-dimensional motion obeys the equations (A.5) and (A.6), which may be solved to give

$$E\psi_a^2 + \frac{1}{2}Cr_a^2 \frac{1}{1 - \frac{d^2C}{8E}} = E\psi_b^2 + \frac{1}{2}Cr_b^2 \frac{1}{1 - \frac{d^2C}{8E}} \quad (\text{A.13})$$

One must therefore require that $E > d^2C/8$, in order that the motion does not diverge. This criterion coincides with (A.8). If the potential is not confined to the transverse plane of atoms, the critical energy is slightly reduced.

In the above, transverse energy E_{\perp} was shown to be conserved. However, the particle energy E in the laboratory system was unchanged during the collision, i. e. the recoil energy of the atom was disregarded. We may briefly show that, even when the latter effect is included, E_{\perp} may normally be taken to be conserved in a collision. To this end, consider an elastic collision, so that particle energy after the collision is $E - T_n$, where T_n is given by (3.9). The change of energy implies in itself a reduction of transverse energy, $\delta E_{\perp,1} = -T_n \cdot \psi_a^2$. Moreover, when there is transfer of energy and of angular momentum, the outgoing particle path is shifted outwards by an amount δr , cf. reference 10,

$$\delta r \cong \frac{T_n}{E} \left\{ \frac{U(r)}{r \cdot U'(r)} + \frac{1}{2} \right\} r \quad ;$$

the corresponding change of E_{\perp} in the collision is $\delta E_{\perp,2} = \delta r \cdot U'(r)$. The total change is then $\delta E_{\perp,1} + \delta E_{\perp,2}$. Suppose next that $U \propto r^{-\nu}$, and find the statistical average of δE_{\perp} for strings, according to (3.6). A simple calculation then shows that, for $r_{\min} \ll r_0$,

$$\frac{\langle \delta E_{\perp} \rangle}{E_{\perp}} = -\frac{\nu - 1}{3} \frac{\langle T_n \rangle}{E} \quad (\text{A.14})$$

Therefore, E_{\perp} is conserved quite accurately if $0 < \nu < 2$, cf. standard potential (2.6). For this reason, and since electronic stopping normally dominates over nuclear stopping—especially when E_{\perp} is small—we may often disregard the change in E_{\perp} due to elastic nuclear collisions in a perfect lattice. The change in E_{\perp} during penetration is then usually due to electronic stopping, and to the other effects mentioned in § 4.

General equations of motion

As an alternative to the above estimates we treat a somewhat different approach, associated with variational principles in dynamics and useful for numerical estimates. For this purpose we record the distance r_j at $z = j \cdot d$, where j is an integer. Since the basic equation of deflection is

$$\frac{r_{j+1} - 2r_j + r_{j-1}}{d} = \varphi_j = -\frac{d \cdot U'(r_j)}{2E}, \quad (\text{A.15})$$

we may form the sum

$$\sum L_j = \sum_{j=n+1}^m \left\{ E \cdot \frac{(r_j - r_{j-1})^2}{d^2} - U(r_j) \right\}, \quad (\text{A.16})$$

and the orbit for given values of coordinates r_n and r_m is determined by variation of all r_j , $j = n+1, \dots, m-1$, with a stationary value of (A.16).

So far, the deflection was assumed to occur in the plane $z = z_j$, the force being an approximate δ -function. At large distances from strings this is not quite correct. It is easy to introduce the smoothly varying force in the present formulation. In fact, let $V_{\text{tot}}(\vec{r}, z)$ be the total potential in the lattice. Then, the orbit from (\vec{r}_1, z_1) to (\vec{r}_2, z_2) is determined by the variational principle

$$\delta \int_{z_1}^{z_2} L(\vec{w}(z), \vec{r}(z), z) dz = 0, \quad \vec{r}(z_1) = \vec{r}_1, \quad \vec{r}(z_2) = \vec{r}_2, \quad (\text{A.17})$$

where

$$L(\vec{w}(z), \vec{r}(z), z) = \frac{1}{2} M_1 \vec{w}^2(z) - V_{\text{tot}}(\vec{r}(z), z), \quad \vec{w}(z) = v \frac{d}{dz} \vec{r}(z),$$

and all angles are assumed to be small, i.e. $w \ll v$. The Lagrangian formulations (A.16) and (A.17) may be turned into Hamiltonian equations, but owing to the explicit dependence of L on z , i.e. on the time variable, one does not obtain the normal simple conservation of energy.

Emission of particle from atom in perfect string

On the basis of the approximate conservation of transverse energy E_{\perp} in (A.4), we can discuss the emission of a particle from the centre of an atom in a string. It is of interest to find both the minimum angle and the angular distribution. It should be remembered, though, that this will not represent too well the actual emission from an atom in a lattice, because we disregard the vibrations of atoms, and in some cases quantal corrections should be included. However, we do obtain an alternative estimate of the validity of the continuum string picture.

The particle is emitted from the point $r = 0$, $z = 0$, at an angle Φ . Its total energy, $E_{\perp} = E \cdot \psi^2$, is then given by (A.3) and (A.11), where the energy is recorded at $z = d/2$, i.e. $r_b = d\Phi/2$, $\psi_b = \Phi$, and where we assume $W(r) = U(r)$,

$$E\psi^2 = E \cdot \Phi^2 + U(\Phi d/2). \quad (\text{A.18})$$

Since emission probability is proportional to differential solid angle $\approx 2\pi\Phi d\Phi$, the probability distribution in angle ψ is also contained in (A.18). If the second term in (A.11) is included, we must add $W_2 = Ed^2 \cdot U'^2(\Phi d/2) \cdot (4E)^{-2}$ on the right-hand side of (A.18).

In order to obtain quantitative estimates, we introduce the standard potential (2.6), and (A.18) becomes

$$\psi^2 = \Phi^2 + \frac{\psi_1^2}{2} \log \left(\frac{4C^2 a^2}{d^2 \cdot \Phi^2} + 1 \right), \quad (\text{A.19})$$

the additional term being $W_2 = \psi_1^4 (2\Phi)^{-2} (1 + \Phi^2 d^2 / 4C^2 a^2)^{-2}$.

It is interesting to compare the terms in (A.18) and (A.19) with the corresponding ones in scattering by a single atom, cf. p. 15 ff. In scattering by a single atom, with the same notation as in (A.18), one obtains

$$\psi^2 = \left(\Phi - \frac{d}{2E} U'(\Phi d) \right)^2 = \Phi^2 - \frac{\Phi d}{E} \cdot U'(\Phi d) + \frac{d^2}{4E^2} U'^2(\Phi d),$$

where the first term equals that in (A.19), whereas the second term tends to ψ_1^2 for low values of Φ . The third term dominates when Φ is small, and is similar to W_2 for $\Phi \rightarrow 0$. However, if $\psi_1 > a/d$, the third term can become $\sim W_2/16$. This indicates the ambiguity belonging to W_2 . In the following we disregard W_2 , primarily because its inclusion would not affect much the estimates of critical angles.

Returning to (A.19), we can estimate the minimum, ψ_{\min} , of the angle of emission, ψ . The minimum is obtained for

$$\Phi^2 = -\frac{2C^2 a^2}{d^2} + \left[\left(\frac{2C^2 a^2}{d^2} \right)^2 + \psi_1^2 \frac{2C^2 a^2}{d^2} \right]^{1/2}.$$

It is convenient to distinguish between two limiting cases. Suppose that ψ_1 is small compared to a/d . Then

$$\psi_{\min} = \psi_1 \cdot \left[\log \frac{\alpha C a}{\psi_1 d} \right]^{1/2}, \quad \text{for } \psi_1 < \frac{a}{d}, \quad (\text{A.20})$$

where $\alpha = 2^{3/2} \exp(1/2)$. The coefficient of ψ_1 is of order of 1.5-2, and is nearly independent of E and ψ_1 , if ψ_1 is small.

At lower energies, where $\psi_1 > a/d$, we find from (A.19) the minimum angle

$$\psi_{\min} = 2 \left(\frac{\psi_1}{\sqrt{2}} \frac{C a}{d} \right)^{1/2} = 2\psi_2, \quad \text{for } \psi_1 > \frac{a}{d}. \quad (\text{A.21})$$

There is a smooth transition between the limiting cases (A.20) and (A.21). These two formulae are in good agreement with the qualitative considerations in § 2, cf. (2.9) and (2.10). It should be added that in the low energy region, where increasingly large impact parameters become important, the standard potential (2.6), as well as (A.21), should not be considered as accurate estimates.

In the formula (A.21), where angles are large, hardly more than the first atom contributes much to the deflection near the critical angle. It is noteworthy that in spite of the simplified transverse potential description used here, the critical angle (A.21) is 14 per cent above the corresponding precise result obtained for scattering by one atom only, at a distance d . This gives a justification of the use of transverse continuum potentials in one limit.

Appendix B

Quantal Corrections to Classical Description

The following discussion is divided in three sections, of which the two first are meant as a preamble to the third. The first section, Single Collisions, concerns a familiar case of scattering, where a classical description is the more accurate the lower the velocity. The second section, Continuum String, illustrates that if the continuum picture were completely valid, the transverse motion of particles would be essentially classical. The third section, Perfect String, aims at an estimate of the quantal correction to classical deflection by an actual string. It is shown that, in contrast to other collision problems, the classical description is the better the higher the velocity of the particle.

Single Collision

In a single collision the condition for a classical treatment is determined by essentially two lengths, the wave length λ of the relative motion and $L_f = [\vartheta'(p)]^{-1}$, i.e. the focal length of the classical scattering, $\vartheta(p)$ being the deflection for impact parameter p . The total uncertainty, $\delta\vartheta$, in scattering angle can be obtained in a way analogous to that used by BOHR¹²⁾. We assume that the angle $\vartheta(p)$ is small, and thus determined by (2.1'). With a wave packet of width δr there are two contributions to $\delta\vartheta$, one from diffraction and one from classical uncertainty in position, i.e.

$$(\delta\vartheta)^2 = \frac{\lambda^2}{4(\delta r)^2} + (\delta r)^2 \cdot (\vartheta'(p))^2. \quad (\text{B.1})$$

The minimum value of (B.1) is obtained for $(\delta r)^2 = \lambda/(2\vartheta'(p))$, and becomes

$$(\delta\vartheta)^2 = \lambda \cdot \vartheta'(p). \quad (\text{B.2})$$

In order to obtain a well-defined orbit, we may demand $(\delta\vartheta)^2 < \vartheta^2$, or

$$\lambda \frac{d}{dp} \left(\frac{1}{\vartheta(p)} \right) < 1, \quad (\text{B.3})$$

which formula in the case of Rutherford scattering, $\vartheta = b/p$, leads to the inequality of BOHR¹²⁾

$$\kappa = \frac{2Z_1 Z_2 e^2}{\hbar v} > 1. \quad (\text{B.4})$$

For the screened field of the standard atomic potential, (2.6''), the condition (B.3) and the scattering formula (2.1') give the somewhat stronger condition

$$\kappa > 1 + \frac{3p^2}{C^2 a^2} \sim 1 + \frac{p^2}{a^2}. \quad (\text{B.5})$$

The above formulae apply for the relative motion, where $\lambda = \hbar/M_0 v$, and $\vartheta(p)$ is the deflection in the centre of gravity system. However, it may be shown that the results also apply in the laboratory system, if (2.1) is fulfilled, i.e. with $\lambda = \hbar/M_1 v$ and $\vartheta(p)$ the deflection in the laboratory system. This leads to a slight change in (B.1) and (B.2), since M_0 is replaced by M_1 . However, (B.3), (B.4) and (B.5) remain unchanged, because the particle masses do not enter in these formulae, cf. (2.1').

It should be strongly emphasized that (B.3), and similar conditions for the use of classical mechanics, are conditional and not absolute statements of limitations of classical estimates. Thus, (B.3) comes into play only if one desires a well-defined angle of deflection at very large distances from the scattering centre, in one-body or two-body scattering.

Continuum string

Let us assume that the continuum approximation is valid. We may then ask for the quantal correction to classical transverse motion. This is a quite straightforward problem, since both classically and in quantum mechanics there is conservation of transverse energy. As a simple example, we consider a string potential $U(r) = Z_1 Z_2 e^2 \pi a / (2dr)$, and a particle with trans-

verse energy E_{\perp} . The BOHR condition (B.4) applied to the transverse motion with initial velocity $v_{\perp} = v\psi$, and initial energy $E_{\perp} = E\psi^2$, becomes

$$\kappa_{\perp} = \kappa \cdot \frac{\pi a}{2d} \cdot \frac{1}{\psi} > 1. \quad (\text{B.6})$$

Since $\psi < \psi_1$, we find that κ_{\perp} is always larger than (we put $a \sim \alpha_0 Z_2^{-1/3}$)

$$\kappa_{\perp} \gtrsim \frac{\pi}{2} \left(\frac{M_1}{m} \right)^{1/2} \left(Z_1 Z_2^{1/3} \cdot \frac{\alpha_0}{d} \right)^{1/2}. \quad (\text{B.7})$$

The right-hand side in (B.7) is independent of energy E , and is certainly large compared to unity if M_1 is large compared to the electron mass m . In the general case of string deflection the formulae (2.21), (2.15) and (B.3) show that a classical description is applicable if $\lambda_{\perp} \ll a$. The essential point is that quantal tunnelling to the centre of a continuum string does not occur. The treatment can be extended, e.g. to continuum planes, but for the present purpose this is hardly necessary.

The following curious transformation from perfect string to continuum string may be illustrative. We start from a perfect string of atoms with spacing d . We imagine that each atom is cut in two equal parts, by a cut perpendicular to the string, retaining the electron distances from the string. The halves are placed with constant spacing $d/2$. Next, we cut each half in two, the spacing becoming $d/4$. This process can be continued, the string approaching more and more a true continuum string. On the one hand, consider an isolated collision between the moving particle and the fraction of an atom remaining at the n 'th stage. The Born approximation will take over and be the more accurate, the higher the stage, and orbital pictures of the deflection fail completely (cf. the previous section). On the other hand, the continuum description of the particle motion gets more and more accurate as the cutting proceeds, and the estimates in the present section become relevant. In point of fact, the motion becomes rather classical. But in any case, the use of a continuum description is not determined by the isolated scattering by single entities; the decisive parameter is the length of the time interval d/v , between successive collisions, as will appear from the following section, and from (2.27).

Perfect string

When considering quantal corrections to the classical treatment of a set of successive collisions, we must compare the relative magnitude of a number of quantities. We can introduce five basic quantities of this kind, i.e.

$$\lambda, \quad L_f = [\vartheta'(r)]^{-1}, \quad a, \quad d, \quad L_{\text{coll}}, \quad (\text{B.8})$$

where the first three parameters belong to single collisions too, whereas d is the distance between successive collisions, and $L_{\text{coll}} = v \cdot \Delta t$, cf. (2.7), the effective collision length with one string, combined of many separate atomic collisions. It is apparent that $L_{\text{coll}} > d \gg a$, and in the type of collisions considered here we also have $\lambda \ll d$.

Besides the above lengths, we are concerned with others, partly constructed from those in (B.8). Thus, if a wave-packet is formed in the transverse motion, of width δr , the wave-packet does not spread essentially on a path length $L_w = (\delta r)^2/\lambda$. We want to choose the size $(\delta r)^2$ of wave-packets, i.e. L_w , in an optimal way. A crucial question is whether L_w is large or small compared to d , the distance between successive collisions. Let us tentatively suppose that d could be large compared to L_w ; we would then have a set of randomly adding fluctuations. In the i 'th collision the angular fluctuation is analogous to (B.1),

$$(\delta\vartheta)_i^2 = \frac{\lambda^2}{4(\delta r)_i^2} + (\delta r)_i^2 \vartheta'^2(r_i), \quad (\text{B.9})$$

i.e. at minimum

$$(\delta r)_i^2 = \lambda/2\vartheta'(r_i), \quad (\delta\vartheta)_i^2 = \lambda\vartheta'(r_i), \quad (\text{B.10})$$

and totally the angular fluctuation would become

$$(\delta\vartheta)^2 = \lambda \sum_i \vartheta'(r_i). \quad (\text{B.11})$$

However, in this derivation we assumed that $d > L_{w,i}$, where $L_{w,i} = 1/2\vartheta'(r_i)$ according to (B.10). Since $\vartheta'(r_i) \approx \vartheta(r_i)/r_i$, this implies that $d > r_i/\vartheta_i$, which is in direct contradiction to the basic condition (2.7), requiring that several collisions take part in the repulsion of a particle, i.e. $L_{\text{coll}} > d$. We must therefore assume that $L_w \gtrsim d$, and can conclude that (B.11) does not apply. The conclusion that the wave-packets in consecutive collisions are not independent is in agreement with the inequalities (2.27), (2.27').

Disregarding the assumptions leading to (B.11), we must then consider a wave-packet which approximately retains its width during the whole set of collisions. If the width is δr , the total contribution to angular dispersion from diffraction becomes $(\delta\vartheta)_{\text{diff.}}^2 = \lambda^2/4(\delta r)^2$, which may be compared with the corresponding term $\Sigma \lambda^2/4(\delta r)_i^2$ in (B.9), (B.10). As to the total uncertainty in deflection of the particle by the successive force fields, we assume that there is a lack of coherence between successive collisions. If they were completely coherent, the uncertainty in total deflection would

disappear when transverse energy is conserved. In order to get a slight overestimate of the uncertainty, we assume incoherence between successive terms, i.e. totally

$$(\delta\vartheta)^2 = \frac{\lambda^2}{4(\delta r)^2} + (\delta r)^2 \sum_i \vartheta'^2(r_i), \quad (\text{B.12})$$

leading to

$$(\delta\vartheta)^2 = \lambda \cdot [\sum_i \vartheta'^2(r_i)]^{1/2}, \quad (\text{B.13})$$

and

$$(\delta r)^2 = \frac{\lambda}{2} [\sum_i \vartheta'^2(r_i)]^{-1/2}. \quad (\text{B.14})$$

According to (B.13) and (B.14), both $(\delta\vartheta)^2$ and $(\delta r)^2$ become smaller than the corresponding expressions (B.11) and (B.10) belonging to completely independent wave packets. Since $\vartheta'^2(r_i)$ decreases strongly with increasing r_i , it can for large E_\perp be permissible to include in (B.14) only the effect of the closest collision.

If we evaluate the summation in (B.13) as an integral, i.e. in the continuum approximation, we find

$$(\delta\vartheta)^2 = \lambda \cdot \frac{d^{1/2}}{2E} \left\{ \int_{-\infty}^{+\infty} dz U''^2(r(z)) \right\}^{1/2}, \quad (\text{B.15})$$

where $r(z)$ is the distance from the string as a function of the coordinate z measured along the string. The integral in the brackets depends only on E_\perp and on the impact parameter l in the transverse motion, but not on d . Therefore, (B.15) tends to zero for $d \rightarrow 0$, as it should do for continuum strings, in contrast to (B.11).

If (B.15) is multiplied by E , it represents the change in transverse energy in one collision. Let us consider a particle at different energies E , but in each case with the same transverse energy E_\perp . According to (B.15) its increase in transverse energy, by fluctuations due to quantal corrections, will then be proportional to the wave length λ of its translatory motion. The quantal corrections to classical description therefore decrease with increasing velocity v .

A more detailed discussion of quantal effects will be published shortly, in collaboration with PH. LERVIG and V. NIELSEN.

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