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INTEGRAL EQUATIONS GOVERNING RADIATION EFFECTS

(NOTES ON ATOMIC COLLISIONS, III)

BY

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Synopsis

A theoretical study is made of damage effects by particle radiations in matter, and their dependence on energy, mass and charge number of an incoming particle, as well as on the composition of the medium. Typical examples of damage effects are the number of ion pairs formed in a gas, or the number of vacancies created in a crystal. We are particularly concerned with the consequences of the competition between energy transfer to atomic electrons and to translatory motion of an atom as a whole. For these purposes, common integral equations are formulated and studied. We treat primarily average effects resulting from an atomic particle with given energy, but also their average fluctuation and probability distribution.

As an important example we study the division of the total energy dissipation, E, into energy given to recoiling atoms, ν, and energy given to electrons, $E-\nu$. Several radiation effects are accounted for from knowledge about E and ν.

The primary quantities in a study of radiation effects are the cross sections for all relevant collision processes. We use comprehensive estimates of cross sections, derived elsewhere in a Thomas-Fermi treatment. Various simple approximations are introduced; analytical and numerical estimates are made of solutions to the integral equations. For many purposes nuclear collisions and electronic collisions may be treated as if they were unconnected events, although this is not quite correct, especially at low energies. Considerable simplification is obtained by a suitable scaling of energy. A key to a common experimental and theoretical study is provided by an incoming particle identical with the atoms of the substance. Only few experiments can at present be compared quantitatively with theory.

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§ 1. Introduction

When an atomic particle is slowed down in a substance, a wide variety of damage effects may be observed. Familiar phenomena of this kind are the number of ion pairs formed in a gas, the number of electron-hole pairs in a semiconductor, or the number of defects in a solid. Other damage effects have been studied less, or not at all, like the number of electrons ejected from atomic K-shells, or the number of dissociations of molecules. The observations of damage phenomena may be divided into two classes. The one is particle detection, where the effect of a single incoming particle is observed and possibly recorded in time, and the other is the total damage due to many particles, as in reactor materials.

All damage effects depend on a competition between the cross sections for a multitude of different processes. Theoretical studies have been made by many authors concerning some aspects of excitation and ejection of electrons. Other theoretical studies have been concerned with the average energy required to form defects in solids. Less attention has been paid to the question of the competition between, on the one hand, energy transfer to atomic electrons and, on the other hand, energy transfer to translatory motion of an atom as a whole. Our knowledge of collision processes for slow heavy particles has been scanty, and the mentioned competition does in fact occur primarily for slow heavy particles.

To a wide extent all above damage processes may be described by integral equations which are formally equivalent. The differences concern mostly the inhomogeneous parts or boundary conditions. But the competition between energy transfer to electrons and to atomic recoils can be described by equations which have even more in common. This is because there are extensive similarity properties, of Thomas-Fermi type, between the competing processes in this case. The homogeneous integral equations in different substances are actually quite closely connected. It can therefore be worthwhile to study them in some detail. When we have gained insight in the equations we can handle not only average damage effects, but also fluctuations and even the distribution in probability.

We shall be concerned mainly with one effect which corresponds to the simplest homogeneous equations. This effect is the division of the dissipated energy between electrons and recoiling atoms in the substance. More precisely, for an incoming particle of energy E we ask for that part η of the total energy loss, E, which is ultimately given to electrons, and that part ν, which is ultimately left in atomic motion. Since this division is a useful and simple concept, we comment on it in some detail as an example of the application of the general equations.

It might seem as if the division into η and ν were not quite well-defined, since we are not concerned with the final thermal equilibrium. However, on the one hand, the energy once given to electrons can be transferred back to atomic motion only extremely slowly and in exceedingly small bits.* On the other hand, sufficiently slow atoms no longer excite electrons and their energy may be frozen in or become thermalized. This may give a qualitative justification of the separation into ν and η.

For the present purpose the quantities η and ν may be specified as follows. We consider η as the sum total of the energy given to electrons, i. e. for ejected electrons it is the kinetic energy plus the original binding while for excited electrons it is the excitation energy. Correspondingly, ν is the total energy given to atoms, excluding internal excitation of atoms. Thus, η and ν are quite well-defined, and have the sum $\eta + \nu = E$.** It is clear that there must be a probability distribution $P(\nu, E)d\nu$ in the variable ν, such that

$$\int_0^\infty P(\nu, E)\,d\nu = 1, \quad \bar{\nu}(E) = \int_0^\infty \nu\, P(\nu, E)\,d\nu,$$

and similarly for the higher moments. For the present we may disregard fluctuations and consider only e.g. $\bar{\nu} = \bar{\nu}(E)$.

We shall attempt to show how $\bar{\eta}(E)$, $\bar{\nu}(E)$ and other cumulative effects may be derived for all kinds of particles in any medium. Since $\bar{\eta}$ and $\bar{\nu}$ are determined by the competition between energy transfer to electrons and to atomic recoils in all collisions during slowing-down, they are expected to depend on the medium, on the type of particle and on its energy. This enormous variability can be reduced somewhat by studying at first the more basic cases.

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* An exception occurs if an electron by exciting atomic electrons gives rise to large vibrations or even disruption of bindings in molecules (through a Franck-Condon effect or an Auger effect). The energy transferred in this way from a moving electron into atomic motion can be appreciable. This effect must be studied separately, and is remarkable in that it does not occur in monatomic gases. – The role of the Auger effect is studied by Durup and Platzman (1961).

** If more subtle distinctions are necessary, we may divide E into components other than η and ν. Examples are the energy escaping as X-rays or as near-thermal excitations.

Let us start by considering the case where the medium consists of only one atomic species, of atomic number Z_2 and mass number A_2. Now, any incoming particle, irrespective of its type, gives rise to recoiling atoms of the medium, and we will have to make use of their value of $\bar{\nu}$ and $\bar{\eta}$. It follows that the simplest basic case occurs when the atomic number, Z_1, and the mass number, A_1, of the incoming particle are equal to those of the medium, i. e. $Z_1 = Z_2$, $A_1 = A_2$.

Suppose that a particle belonging to the medium ($Z_1 = Z_2$) initially has an energy E; we want to find $\bar{\eta}(E)$. Collisions with atoms result in recoiling atoms or ions which may have any energy E' within the interval $0 < E' < E$, and therefore the corresponding values of $\bar{\eta}(E')$ enter in the evaluation of $\bar{\eta}(E)$, as must also the differential cross section for energy transfer to recoiling atoms. Clearly, the procedure must be to build up $\bar{\eta}$ starting from zero energy, and the relative magnitude of the partial stopping cross sections $S_e(E)$ and $S_n(E)$ must be of direct importance. We shall therefore review briefly the behaviour of the relevant cross sections.

When deliberating the approach to these problems, one should first of all bear in mind that extreme accuracy and separate computation of each individual case cannot be the primary aim. Also, a discussion of quite low energies of heavy particles, less than 100 eV say, is either unnecessary or may be made separately. It is therefore desirable to use statistical methods, of type of the Thomas-Fermi treatment, as far as possible. Since at moderate energies the interpenetration of two atomic electron clouds can be considerable, many atomic electrons with moderate bindings play a part, and statistical methods seem promising. In the case $Z_1 = Z_2$, $A_1 = A_2$ the function $\bar{\eta}$ can depend on three variables, $\bar{\eta} = \bar{\eta}(Z_2, A_2, E)$. It turns out that the Thomas-Fermi treatment together with a suitable approximation to scattering reduces the number of variables. In fact, beside the energy measured in a suitable Thomas-Fermi scale there is only one further parameter, which even has approximately the same value in most cases. Such reductions in the number of variables lead to highly desirable simplifications in the theoretical treatment.

We shall already here give a brief summary of relevant stopping cross sections and differential cross sections. The cross sections are derived elsewhere (LINDHARD and SCHARFF (1961), and Notes on Atomic Collisions I and IV (unpublished)). We do not claim that the accuracy is very high, and in individual cases other authors may have obtained better estimates. The primary purpose for the present is to have available comprehensive formulas, applicable in as many cases as possible. Maybe the greatest uncertainty is the proportionality factor, k, in the electronic stopping. A considerable number of observations on range and on scattering have been made;

they appear to be in fair agreement with the formulas quoted here (LINDHARD, SCHARFF and SCHIØTT (1962)).

Stopping cross sections.

The nuclear stopping cross section $S_n = \int T_n d\sigma_n$ depends on the particle energy E, and on the parameters Z_1, Z_2, A_1 and A_2. An important region of low velocities corresponds to v less than $\sim 0.015\, v_0 Z^{2/3}$, where $Z^{2/3} = Z_1^{2/3} + Z_2^{2/3}$ and $v_0 = e^2/\hbar$. In this region S_n remains nearly constant, and we shall sometimes approximate S_n by the constant standard stopping cross section S_n^0 (similar to that quoted by BOHR (1948)),

$$S_n^0 = (\pi^2/2.7183)\, e^2 a_0 Z_1 Z_2 M_1 \cdot Z^{-1/3} (M_1 + M_2)^{-1}. \tag{1.1}$$

In a more accurate description S_n increases slowly towards a maximum (cf. Fig. 1), and (1.1) may be used in the neighbourhood of the maximum. Beyond it, S_n decreases corresponding to an increasing negative power of E, but always slower than E^{-1}. In fact, S_n approaches the classical stopping formula in a screened Coulomb potential.

It turns out that the nuclear stopping is most simply described by a suitable scaling of energy and cross section. Introduce the dimensionless quantities

$$\varepsilon = E \frac{a M_2}{Z_1 Z_2 e^2 (M_1 + M_2)} \quad \text{and} \quad \varrho = RNM_2 \cdot 4\pi a^2 \frac{M_1}{(M_1 + M_2)^2}$$

as measures of energy and range, where $a = 0.8853\, a_0 \cdot Z^{-1/3}$, while R is the usual range and N the number of atoms per unit volume. The derivative $(d\varepsilon/d\varrho) = S \cdot (M_1 + M_2)/(4\pi e^2 a Z_1 Z_2 M_1)$ is a dimensionless measure of the stopping cross section, S. To a good approximation all nuclear stopping cross sections are then described by one curve. This is shown in Fig. 1, where the solid curve was computed from the comprehensive scattering cross section in Fig. 2. The approximation $S_n = S_n^0$ is represented by the horizontal dotted line $(d\varepsilon/d\varrho)_n = 0.327$.

The electronic stopping cross section is nearly proportional to v in a considerable velocity interval, i.e. for $v < v_1 \simeq v_0 \cdot Z_1^{2/3}$, and is of order of

$$S_e \simeq 8\pi e^2 a_0 \frac{Z_1^{7/6} Z_2}{Z} \cdot \frac{v}{v_0}, \quad v < v_1. \tag{1.2}$$

This leads to an electronic contribution to stopping in an ε-plot $(d\varepsilon/d\varrho) = k \cdot \varepsilon^{1/2}$, where the quantity k as given by (1.2) depends somewhat on Z_1, Z_2, M_1 and M_2, but is often within the interval $0.10 < k < 0.20$. This holds in particular in the case of $Z_1 = Z_2$, $A_1 = A_2$, where $k = 0.133\, Z_2^{2/3} A_2^{-1/2}$, so that k varies only little with Z_2. Merely in the special case of $Z_2 \gg Z_1$, with Z_1 comparable to 1, does k appreciably exceed 0.20. The dashed straight line in Fig. 1 shows the electronic stopping for a representative value of k ($k = 0.15$). It cuts the horizontal line $S_n = S_n^0$ at an energy E_c corresponding to $\varepsilon_c = 4.75$.

In the neighbourhood of $v = v_1$ the electronic stopping has a maximum, upon which it decreases and gradually approaches the Bethe stopping formula.

Let us take the ratio $\xi(E) = S_e/S_n$ as a measure of the division of energy dissipation into electronic and atomic motion. The above summary of

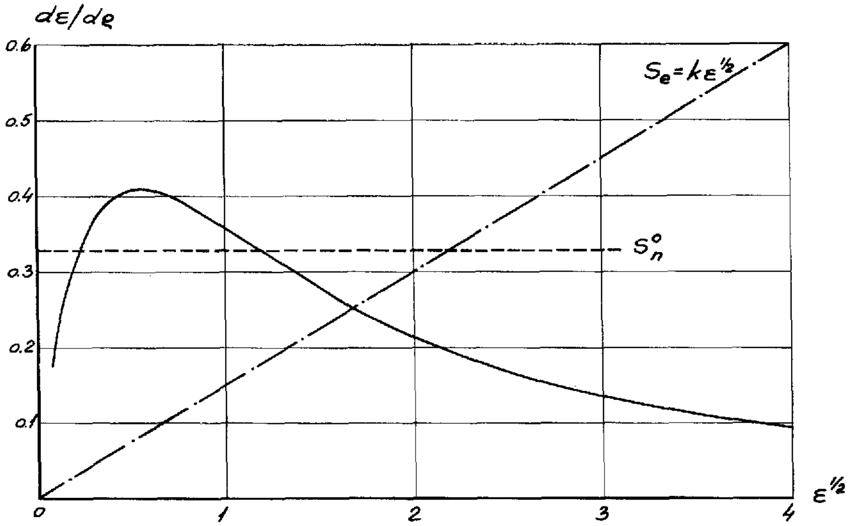

Fig. 1. Theoretical stopping cross sections in $\varrho-\varepsilon$ variables. The abscissa is $\varepsilon^{1/2}$, i.e. proportional to v. The solid curve is $(d\varepsilon/d\varrho)_n$ computed from the Thomas-Fermi cross section in Fig. 2. The horizontal dashed line indicates (1.1) and the dot-and-dash line is the electronic stopping cross section, $k\varepsilon^{1/2}$, for $k = 0.15$.

stopping cross sections then shows that there is a natural division into three regions of different behaviour. In the lowest energy region, region I, the nuclear stopping is dominating and relatively little energy goes into electronic motion. Region I is bounded upwards by an energy roughly equal to E_c. Above E_c the nuclear stopping falls off, while the electronic stopping goes on increasing as $E^{1/2}$. This is region II, with an upper bound given by v_1, i.e. ε_1 is of order of 10^3 or larger. In region II the ratio ξ increases rapidly, and the fraction of energy going into electronic motion must increase correspondingly. Finally, above ε_1 the electronic stopping starts decreasing, and the ratio ξ, though still increasing, approaches a maximum value of order of $2M_p/m \sim 4000$; this is region III. The division into three regions is convenient only when $Z_1 = Z_2$.

Differential cross sections.

Although the stopping cross sections are relevant and give a qualitative picture of the events, they contain only part of the necessary information. In fact, in the following the integral equations demand a detailed knowledge of the differential scattering cross section in nuclear collisions. As regards electronic collisions, we normally need no more than the stopping cross section itself.

We shall briefly recapitulate two different approximations to the differential cross section in nuclear collisions, assuming the scattering to be approximately elastic (LINDHARD and SCHARFF (1961), and Notes on Atomic Collisions, I). First, in an s'th power potential, $V(r) = Z_1 Z_2 e^2 a_s^{s-1} s^{-1} r^{-s}$, with $a_s \approx a = 0.8853\, a_0 \cdot Z^{-1/3}$, the differential scattering cross section is approximately equal to

$$d\sigma_n = \frac{C_n}{T_m^{1-1/s}} \cdot \frac{dT}{T^{1+1/s}}, \quad s > 1, \tag{1.3}$$

where the incoming particle with energy E transfers an energy T to an atom originally at rest. Here, $T \leq T_m = \gamma E = 4\, M_1 M_2 (M_1 + M_2)^{-2} E$, T_m being the maximum energy transfer in the collision. Furthermore, the constant C_n is connected to the stopping cross section S_n, and is approximately given by

$$C_n = \frac{\pi}{s}\left(b^2 a_s^{2s-2} \frac{3s-1}{8s^2}\right)^{1/s} \cdot T_m = \left(1 - \frac{1}{s}\right) S_n, \; b = \frac{2 Z_1 Z_2 e^2}{M_0 v^2},$$

M_0 being the reduced mass. In preliminary discussions these simple formulas are quite useful, especially for explorative purposes. The case of $s = 2$, where $S_n = S_n^0$ is independent of energy, appears to be a fair approximation at energies somewhat below E_c. At extremely low energies, $s = 3$ is preferable. At high energies s tends to 1.

A more accurate description is obtained from an interaction potential $V(r) = (Z_1 Z_2 e^2/r) \cdot \varphi_0(r/a)$, where $\varphi_0(x)$ is the Fermi function belonging to a single Thomas-Fermi atom. It turns out that the differential cross section is now to a good approximation, for all Z_1, Z_2, A_1, A_2 and all non-relativistic energies, equal to

$$d\sigma = \pi a^2 \frac{dt}{2t^{3/2}} f(t^{1/2}), \tag{1.4}$$

where $t = \varepsilon^2 \cdot (T/T_m) = \varepsilon^2 \cdot \sin^2 \frac{\vartheta}{2}$. The variable t is proportional to the energy transfer T, and to the energy E through ε^2/T_m. Thus, one universal function of a single variable, $f(t^{1/2})$, describes the scattering at all energies and scattering angles, and for all atom-ion pairs. The function f was computed numerically from the Fermi function, and is shown in Fig. 2. At high energies and not too small angles the expression (1.4) becomes equal to the Rutherford cross section, where $f(x) = (1/2x)$. The equations (1.3) and (1.4) are used in the following in order to get first estimates of radiation effects.

Some reservations should be made in connection with the cross section (1.4) and the accompanying curve on Fig. 2. First, at high energies $\varepsilon > \varepsilon_1$, the curve on Fig. 2 is not very accurate at small angles, because the screening of the potential is reduced, the ion being stripped of most of its electrons. However, since at these energies most of the scattering is Rutherford scattering anyway, no major error is committed.

Second, a more interesting correction is due to the circumstance that for large angle ion-atom scattering a considerable energy is spent in electron excitation or ejection. This was observed by FEDORENKO and also by EVERHART and co-workers (cf. FEDORENKO (1959)). The result is that such collisions are not elastic, and that there is a correlation between nuclear collisions and electron excitation. Although ap-

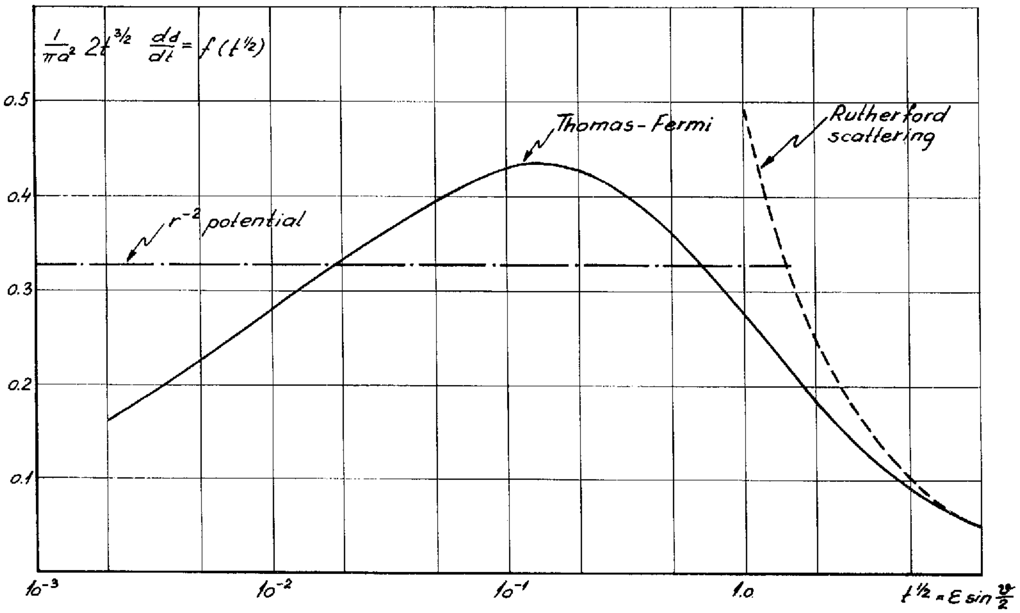

Fig. 2. Universal differential scattering cross section for elastic collisions, (1.4), based on a Thomas-Fermi type potential. At high values of $t^{1/2}$ it joins smoothly the Rutherford scattering. The cross section corresponding to power law scattering (1.3) with $s = 2$ is also shown.

proximate formulas may be quoted for the cross sections of such quasi-elastic collisions, the gain in generality hardly outweighs the complications due to the extra parameters in the treatment. Since the changes in our final results are presumably small (cf. p. 15), it seems preferable to verify at first the gross features of the simple formulas quoted above.

The general considerations in this introduction suggest a definite line of approach. It seems natural to develop first a formal theory of average damage effects, and to consider basic cases ($Z_1 = Z_2$) and possible simplifications, keeping in mind the main characteristics of the above cross sections. In this connection, the theory of fluctuations and of probability distributions should also be given. We therefore treat these general topics in § 2 and § 3. A direct application of the above cross sections to basic cases may then be made, first by analytical methods (§ 4) and next by numerical computations (§ 5). As an illustration of more complicated cases we consider a few examples, which also have bearing on experimental results (§ 6).

§ 2. The Basic Integral Equation

We shall now formulate and discuss the basic integral equation. The discussion, admittedly, is elaborate, but it seems profitable to make clear the contents of each assumption or approximation. We consider at first damage effects which are additive when due to independent events, so that e.g. saturation effects are excluded. The basic equation will be formulated in rather general terms, but immediate simplifications must be made when we treat solutions of actual cases. We study primarily the case where the particle belongs to the medium, and where the medium contains only one atomic species. When this case is solved, we may turn to equations for more complicated situations. For the present, we consider the simple case of average damage effects. Other averages, and the probability distribution in damage, will be discussed below.

We are concerned with a particle belonging to the medium, i.e. $Z_1 = Z_2$ (and $A_1 = A_2$). The particle has the energy E. We consider some unspecified physical quantity, φ, such as the number of ion pairs in a gas, the number of vacancies in a crystal, the energy given to electrons, etc. The quantity φ is arbitrarily taken to be zero before irradiation. The final average value of φ, after irradiation by a particle of energy E, we call $\overline{\varphi}(E)$. Although we use this simplified notation, the quantity $\overline{\varphi}$ depends not only on E, but also on Z_2 (and A_2), and to some extent on the physical state of the medium. Further, the physical quantity may be changed later by recombination processes, like in the case of ion pairs, but we shall disregard recombination effects and consider only the intermediate stage before recombination. In practice, recombination may be either avoided or accounted for separately. It is important that the physical quantity $\overline{\varphi}(E)$ in question is additive, i.e. for each separate slowing-down process all particles set in motion contribute additively to φ. This could hold for the three examples mentioned above.

The quantity $\overline{\varphi}(E)$ for the particle with energy E we may express in another way, if we suppose that the particle moves a path length dR in the medium with N atoms per unit volume. There is then a probability $NdRd\sigma_{n,e}$ for a collision specified by energy transfer T_n to the mass centre of the struck atom, together with energy transfer T_{ei} to electrons (electrons labelled by suffix i). The collision reduces the ion energy to the value $E - T_n - \sum_i T_{ei}$, i.e. the ion will now have a $\overline{\varphi}$-value equal to $\overline{\varphi}(E - T_n - \sum_i T_{ei})$. At the same time the struck atom gets the $\overline{\varphi}$-value $\overline{\varphi}(T_n - U)$, where U is the energy wasted in disrupting the atomic binding. Finally, the electrons produced are described by another φ-function, which we denote as φ_e, and their contribution to $\bar{\varphi}$ after the collision in question is then $\sum_i \bar{\varphi}_e (T_{ei} - U_i)$, where U_i are the corresponding ionization energies. The above probability times the total $\bar{\varphi}$-value after the collision gives the contribution of this collision to $\bar{\varphi}(E)$. Afterwards we integrate over all collisions. There is left a probability $1 - NdR \int d\sigma_{n,e}$ that no collisions occur; in this event the $\bar{\varphi}$-value remains $\bar{\varphi}(E)$.

Collecting the above contributions we may write the original $\bar{\varphi}(E)$ as

$$\bar{\varphi}(E) = NdR \int d\sigma_{n,e} \left\{ \bar{\varphi}(E - T_n - \sum_i T_{ei}) + \bar{\varphi}(T_n - U) + \sum_i \bar{\varphi}_e (T_{ei} - U_i) \right\} + \\ + \left(1 - NdR \int d\sigma_{n,e}\right) \bar{\varphi}(E),$$

which leads to the basic integral equation

$$\int d\sigma_{n,e} \left\{ \bar{\varphi}\left(E - T_n - \sum_i T_{ei}\right) - \bar{\varphi}(E) + \bar{\varphi}(T_n - U) + \sum_i \bar{\varphi}_e (T_{ei} - U_i) \right\} = 0 \qquad (2.1)$$

This equation may be said to state simply that the $\bar{\varphi}$-value of the particle before the collision is equal to the sum of the $\bar{\varphi}$-values of, respectively, the particle, the struck atom and the ejected electrons after the collision, averaged over the probability of occurrence of the individual processes.

It may be noted that there is no necessity for the total cross section $\int d\sigma_{n,e}$ to be finite, and thus we do not attempt to normalize the probability of the various events. The actual physical quantities entering are integrals of $d\sigma_{n,e}$ times quantities tending to zero as e.g. T_n, or faster. The cross sections quoted in § 1 do in fact diverge. Of course, if classical cross sections larger than the atomic size become important in the final results, it may not be possible to separate into collisions with single atoms.

In equation (2.1) we have tried to avoid unnecessary details of notation. Thus, in specifying $\bar{\varphi}$ for the incoming particle or for the struck atom we might include a dependence on the degree of ionization of the particle in question. We shall assume such specifications to be included if necessary, but the interpretation of $\bar{\varphi}(E)$, if there can be doubt about the state of ionization, would normally be that in $\bar{\varphi}$ the number of electrons carried by the ion is considered to be a function of the ion velocity, and equal to the average number of electrons on the ion at the velocity in question.

The solution $\bar{\varphi}(E)$ of the equation (2.1) can be found if $\bar{\varphi}_e$ is a known function. This is the case if $\bar{\varphi}$ represents e.g. the number of vacancies produced in a crystal, since electrons with moderate energies may not be able to produce vacancies because of their low momentum, and thus $\bar{\varphi}_e = 0$. However, in general there is an additional integral equation describing $\bar{\varphi}_e$. For an electron of energy E the differential cross section is denoted by $d\sigma'_{n,e}$ and the collision results in a recoil atom of energy T_n and an energy transfer T_{ei} to atomic electrons. In analogy to (2.1) we immediately find

$$\int d\sigma'_{n,e}\left\{\bar{\varphi}_e\left(E - T_n - \sum_i T_{ei}\right) - \bar{\varphi}_e(E) + \bar{\varphi}(T_n - U) + \sum_i \bar{\varphi}_e(T_{ei} - U_i)\right\} = 0. \quad (2.2)$$

Together with (2.1) the equation (2.2) leads to a solution for both $\bar{\varphi}$ and $\bar{\varphi}_e$. In equation (2.2) we may normally quite neglect the recoil of the nucleus; (2.2) then contains only $\bar{\varphi}_e$, and can be solved separately. An incoming electron usually gives only a small perturbation of the struck atom, and electron excitation may be separated into individual excitations. With a differential cross section $d\sigma'_e$ we thus find in all the simplified version of (2.2)

$$\sum_i \int d\sigma'_e \left\{\bar{\varphi}_e(E - T_{ei}) - \bar{\varphi}_e(E) + \bar{\varphi}_e(T_{ei} - U_i)\right\} = 0. \quad (2.2')$$

Equation (2.1), supplemented by (2.2) if necessary, describes the simplest situation. It may be useful to comment on the set of integral equations belonging to other and more complicated cases. We give only a summary treatment, since the generalizations to be made are fairly obvious.

Firstly, if $Z_1 \neq Z_2$ we denote by $\bar{\varphi}_1(E)$ the average physical effect produced by particle 1. The equation for $\bar{\varphi}_1(E)$ is obtained in the same way as (2.1)

$$\int d\sigma_{1n,e}\left\{\bar{\varphi}_1\left(E - T_n - \sum_i T_{ei}\right) - \bar{\varphi}_1(E) + \bar{\varphi}(T_n - U) + \sum_i \bar{\varphi}_e(T_{ei} - U_i)\right\} = 0, \quad (2.3)$$

where $d\sigma_{1n,e}$ is the differential cross section for collisions between particle 1 and the atom 2. Evidently, (2.3) requires that the solution of (2.1) is known. In this sense, equation (2.3) is secondary to (2.1); this applies also when we wish to compare experiments and basic collision theory. It is interesting to notice that (2.3), in contrast to (2.1), is not a typical integral equation; if $T_n + \sum_i T_{ei}$ is small, (2.3) becomes a differential equation.

Secondly, the substance may contain more than one atomic element. Then, primary cases are those where the incoming particle is one of the atoms in the substance, and the function $\bar{\varphi}^{(j)}(E)$ belongs to the case where the incoming particle is equal to the j'th atomic species of the substance. In place of (2.1) and (2.2) we now write generally

$$\sum_{j=1}^{m+1} \int dx\, S_{kj}(E, x)\, \bar{\varphi}^{(j)}(x) = 0, \qquad k = 1, 2, \ldots, m+1, \quad (2.4)$$

where m is the number of atomic elements in the substance, and $\bar{\varphi}^{(1)} \ldots \bar{\varphi}^{(m)}$ are the $\bar{\varphi}$-functions of these elements, while $\bar{\varphi}^{(m+1)}(E)$ represents $\bar{\varphi}_e(E)$. The integral operator S_{kj} is associated with collisions between the k'th element, of energy E, and the j'th element at rest. As an example, we quote the basic case (2.1) and (2.2), where $m+1 = 2$, and e.g. $S_{21} = \int d\sigma'_{n,e}\,\delta(x - T_n + U)$, according to (2.2).

Let us now return to the basic integral equation (2.1) and discuss the approximations which might be made in solving the equation. It is useful to classify these approximations; roughly, they may be divided into five types.

Discussion of approximations.

The first approximation, (A), was introduced above. It consists in assuming that the electrons do not produce recoil atoms with appreciable energies. This is usually quite correct and implies that $\overline{\varphi}_e$ may be obtained separately, i.e. (2.2) simplifies into (2.2′). (A) is therefore normally fulfilled. An interesting exception occurs if the disruption of atomic bindings has significant influence on the measured effects (cf. footnote on page 4). A more straightforward exception is the case of incoming electrons of energies so high ($\gtrsim 1\,MeV$) that in violent collisions bound atoms can be directly dislodged. In the following, approximation (A) is always used.

The second approximation, (B), consists in neglecting the atomic binding term U in (2.1) so that $\overline{\varphi}(T_n - U)$ is replaced by $\overline{\varphi}(T_n)$. Since the bindings are of order of some eV, we are normally quite justified in neglecting U, for heavy particles at energies where the electronic stopping has any influence at all on the events. Approximation (B) is used everywhere in the following, if not directly otherwise stated.

At this stage it may be of interest to mention cases where (B) is invalid. In fact, if the binding energies contribute to (2.1) in a significant way, the particle energy E is not exceedingly large compared to the binding term U. This implies, on the other hand, that the electronic stopping is small and may be neglected. The approximation may be called (B^{-1}), and we then obtain the simplified equation

$$\int d\sigma_n\left\{\overline{\varphi}(E - T_n) - \overline{\varphi}(E) + \overline{\varphi}(T_n - U)\right\} = 0, \tag{2.5}$$

where $d\sigma_n$ is the differential cross section for elastic ion-atom collisions. This equation is essentially that used by SNYDER and NEUFELD (1955), and by other authors. It should be noted that the binding term U is introduced in a rather symbolic way. A thorough study demands a detailed description of the mechanism by which an atom in a lattice may be removed from its environment. Thus, beside the energy wasted irreversibly, U, when an atom is quickly removed, there is e.g. the threshold energy for adiabatic removal of the atom. The generalization of (2.5) to a substance containing several different atoms in various binding states should be obvious from (2.4). Note also that the approximation (E), introduced below, may be useful in studies of (2.5).

The third approximation, (*C*), is to assume that the energy transfers T_{ei} to electrons are small in a relative measure, or $T_{ei} \ll E - T_n$. Like (*B*) this approximation should hold quite well if the particle energy is not too low. In fact, we have approximately at high velocities $T_{ei} \sim E$ times electron mass divided by ion mass. In all, (*C*) applied to (2.1) leads to

$$\left.\begin{aligned}\int d\sigma_{n,e}\Big\{\bar{\varphi}(E-T_n)-\bar{\varphi}(E)-\bar{\varphi}'(E-T_n)\sum_i T_{ei}+\\+\bar{\varphi}(T_n)+\sum_i\bar{\varphi}_e(T_{ei}-U_i)\Big\}=0,\end{aligned}\right\}\tag{2.6}$$

where approximation (*B*) is also included. Like the two previous approximations, approximation (*C*) is used generally in the following, exceptions being clearly stated.

The fourth approximation, (*D*), is separation of nuclear and electronic collisions. The idea is that only a negligible part of the electronic excitation occurs at the small impact parameters where nuclear collisions play a role. In point of fact, most of the electronic excitations are associated with large impact parameters. It is then natural to disregard the slight overlap of the two types of collision effects, and (2.6) becomes

$$\bar{\varphi}'(E)\cdot S_e(E)=\int d\sigma_n\Big\{\bar{\varphi}(E-T_n)-\bar{\varphi}(E)+\bar{\varphi}(T_n)\Big\}+\int d\sigma_e\sum_i\bar{\varphi}_e(T_{ei}-U_i),\tag{2.7}$$

where $d\sigma_n$ is the differential cross section for elastic nuclear collisions. $S_e(E)=\int d\sigma_e\sum_i T_{ei}$ is the electronic stopping cross section, $d\sigma_e$ being the differential cross section for energy transfers $T_{e1}, T_{e2}, \ldots, T_{ei}, \ldots$ to the individual electrons.

Approximation (*D*), as expressed by (2.7), is also used widely in the following. It contains a definite assumption, the justification of which is less apparent and less justified than the previous assumptions. In (2.7) we have disregarded the connection between electronic and nuclear collisions; they are even supposed to be separable. From a series development in (2.6) we find that the term neglected on the right hand side of (2.7) is approximately $\bar{\varphi}''(E)\int d\sigma_{n,e}T_n\sum_i T_{ei}$. It is of interest to investigate the justification of (2.7) using such correction terms.

In making approximation (*D*) we include approximation (*C*). This is reasonable since it implies only that $\bar{\varphi}(E)-\bar{\varphi}\left(E-\sum_i T_{ei}\right)=\bar{\varphi}'(E)\sum_i T_{ei}$. The correction for this approximation is therefore $\frac{1}{2}\overline{\varphi}''(E)\int d\sigma_{n,e}\left(\sum_i T_{ei}\right)^2$ on the left hand side of (2.7), but is presumably not large.

Finally, the fifth approximation, (E), is to assume that also T_n is small compared to the energy E. Since the maximum energy transfer is normally quite large, and even equal to E if $A_1 = A_2$, it might seem that this approximation is poor. However, because the cross sections are strongly forward peaked, the approximation remains fairly good, as we shall see in § 4. Approximation (E), together with the previous simplifications, leads to

$$\overline{\varphi}'(E)\{S_e(E)+S_n(E)\} = \int d\sigma_n \overline{\varphi}(T_n) + \int d\sigma_e \sum_i \overline{\varphi}_e(T_{ei}-U_i), \qquad (2.8)$$

where $S_n(E) = \int d\sigma_n T_n$, and where the quantity neglected, as compared to (2.7), is approximately $(1/2)\,\overline{\varphi}''(E)\cdot\int d\sigma_n T_n^2$ on the right hand side of (2.8). The approximation (E) may be regarded as an expedient to get an approximate solution of (D), i.e. (2.7).

An interesting consequence of approximation (E) may be noticed. Thus, if we disregard (D), and use only (E), i.e. T_n and $\sum_i T_{ei}$ are small, we obtain again equ. (2.8), but now $S_n = \int d\sigma_{n,e} T_n$, $S_e = \int d\sigma_{n,e} \sum_i T_{ei}$. Further, the cross sections on the right of (2.8) should be $d\sigma_{n,e}$. The separation in (2.8) is therefore obtained independently of the separability of nuclear and electronic collisions assumed in (D). Conversely, it can be difficult to relate the integral equations for $\overline{\varphi}$ to the degree of correlation between electronic and nuclear collisions, as referred to in § 1, p. 9. In Fig. 6, the good agreement between approximations (D) and (E) indicates that correlation corrections to $\overline{\nu}(E)$ can not be large.

We shall sometimes use an approximation, (E'), which is much closer to (D) than (E) itself

$$\left.\begin{aligned} -\frac{1}{2}\overline{\varphi}''(E)\Gamma_n(E) + \overline{\varphi}'(E)\{S_e(E)+S_n(E)\} &= \\ = \int d\sigma_n \overline{\varphi}(T_n) + \int d\sigma_e \sum_i \overline{\varphi}_e(T_{ei}-U_i)&, \end{aligned}\right\} \qquad (2.8')$$

where $\Gamma_n(E) = \int d\sigma_n T_n^2$.

When $\overline{\varphi}_e$ is determined by an equation like (2.2′) it only enters as a known source term in the basic integral equation (2.1). Clearly, the primary problem is then to find the complete solution of the homogeneous basic equation, i.e. omitting the $\overline{\varphi}_e$-term, in one of its formulations within the approximations (A) to (E).

It would be vain to ask for a detailed knowledge of $d\sigma_{n,e}$, let alone solve the equation (2.1) on this basis. However, from equations (2.7) and (2.8) it is seen that knowledge of the stopping cross sections S_e and S_n as functions of energy is essential to the solution of the basic integral equation. Apart from this, some knowledge of $d\sigma_n$ as a function of T_n is clearly required. This is seen in all versions of the basic integral equation, where the term $\int d\sigma_n \overline{\varphi}(T_n)$ always enters.

It need hardly be added that in the following we introduce approximations other than those listed above. Most of the approximations are connected with Thomas-Fermi-like properties or with the specific behaviour of the cross sections summarized in § 1. An example of general interest is the attempt to formulate asymptotic equations in the high energy limit, cf. (5.3) and (5.4).

§ 3. Fluctuations and Probability Distribution

Fluctuations.

So far, we have considered the average, $\overline{\varphi}(E)$, of an additive physical quantity, φ. However, it is of interest to discuss also other averages, for instance the average of the square of the physical quantity. In general, we might consider $<\varphi^m(E)>$, by which is meant the average over all events of the m'th power of φ, so that $<\varphi(E)> \equiv \overline{\varphi}(E)$. The equation governing $<\varphi^m(E)>$ is obtained in a similar way as (2.1), and we find in analogy to (2.1)

$$\left.\begin{aligned} \int d\sigma_{n,e}\Big\{ -<\varphi^m(E)> + <\Big[\varphi\Big(E - T_n - \sum_i T_{ei}\Big) + \varphi(T_n) + \\ + \sum_i \varphi_e(T_{ei} - U_i)\Big]^m>\Big\} = 0. \end{aligned}\right\} \quad (3.1)$$

In principle, (3.1) may be used to construct the average of any function $f(\varphi)$, e.g. by means of a power series development in φ. In practice, however, it is preferable to study instead the equation for the probability distribution in φ, $P(\varphi, E)$. A brief discussion of the probability distribution is given below.

How ever this may be, it is always of considerable interest to treat the case of $m = 2$ in (3.1). This case indicates how equations of type of (3.1) may be solved, and gives at the same time the average square fluctuation in φ. We therefore put $m = 2$ in (3.1) and average over independent quantities like e.g. the product $<\varphi(E - T_n - \sum_i T_{ei})\varphi(T_n)> = \overline{\varphi}(E - T_n - \sum_i T_{ei})\overline{\varphi}(T_n)$, where we average over the subsequent fate of two atoms of given energies, $E - T_n - \sum_i T_{ei}$ and T_n. We get thus

$$\left.\begin{aligned} &\int d\sigma_{n,e}\left\{\Omega_\varphi^2\left(E - T_n - \sum_i T_{ei}\right) - \Omega_\varphi^2(E) + \Omega_\varphi^2(T_n) + \sum_i \Omega_{\varphi e}^2(T_{ei} - U_i)\right\} = \\ &= -\int d\sigma_{n,e}\left\{\left[\overline{\varphi}\left(E - T_n - \sum_i T_{ei}\right) + \overline{\varphi}(T_n) + \sum_i \overline{\varphi}_e(T_{ei} - U_i)\right]^2 - \overline{\varphi}^2(E)\right\}, \end{aligned}\right\} \quad (3.2)$$

where we have introduced the average square straggling $\Omega_\varphi^2(E) = \langle\varphi^2(E)\rangle - \overline{\varphi}^2(E)$, and $\Omega_{\varphi e}^2(E) = \langle\varphi_e^2(E)\rangle - \overline{\varphi}_e^2(E)$.

The right hand side of (3.2) may be reformulated by means of (2.1), and we obtain

$$\left.\begin{aligned} &\int d\sigma_{n,e}\left\{\Omega_\varphi^2(E) - \Omega_\varphi^2(T_n) - \Omega_\varphi^2\left(E - T_n - \sum_i T_{ei}\right) - \sum_i \Omega_{\varphi e}^2(T_{ei} - U_i)\right\} = \\ &= \int d\sigma_{n,e}\left\{\overline{\varphi}\left(E - T_n - \sum_i T_{ei}\right) - \overline{\varphi}(E) + \overline{\varphi}(T_n) + \sum_i \overline{\varphi}_e(T_{ei} - U_i)\right\}^2. \end{aligned}\right\} \quad (3.3)$$

This is the integral equation which governs the straggling in φ, and it corresponds to the equation (2.1) describing $\overline{\varphi}$ itself. Also in a more formal respect (3.3) is similar to (2.1). In fact, if the right hand side of (3.3) could be neglected, the resulting equation for the quantity Ω_φ^2 would be exactly (2.1). Now, the right hand side of (3.3) is a positive source term completely determined by the known functions $\overline{\varphi}$ and $\overline{\varphi}_e$. It contains the square of a term whose average is zero, being the square of the change in $\overline{\varphi}$ in a collision, averaged over the different results of the first collision.

We shall not quote the separate equation for $\Omega_{\varphi e}^2(E)$, in analogy to (2.2) or (2.2'), since it would be of type of (3.3) and could be written down immediately. Moreover, simplifications in (3.3), corresponding to the approximations (A) to (E), are fairly straightforward. We consider explicitly only a few cases. Suppose that energy transfers to electrons are small, and that nuclear and electronic collisions are separable. This corresponds to approximation (D). In the cases where $\overline{\varphi}_e$ is zero we then get, in analogy to (2.7),

$$\left.\begin{aligned} S_e(E)\cdot\frac{d\Omega_\varphi^2(E)}{dE} &= \int d\sigma_n\left\{\Omega_\varphi^2(E - T_n) - \Omega_\varphi^2(E) + \Omega_\varphi^2(T_n)\right\} + \\ &+ \int d\sigma_n\left\{\overline{\varphi}(E - T_n) - \overline{\varphi}(E) + \overline{\varphi}(T_n)\right\}^2, \end{aligned}\right\} \quad (3.4)$$

where also the term $(\overline{\varphi}'(E))^2 \int d\sigma_e\left(\sum_i T_{ei}\right)^2$ is disregarded.

Assume here that T_n in (3.4) is small, i.e. approximation (E). From (3.4) we obtain, corresponding to the homogeneous part of (2.8),

$$\{S_n+S_e\}\frac{d\Omega_\varphi^2(E)}{dE}=\int d\sigma_n\,\Omega_\varphi^2(T_n)+\int d\sigma_n\{\overline{\varphi}(T_n)-T_n\overline{\varphi}'(E)\}^2. \qquad (3.5)$$

Although (3.5) appears to be simpler than (3.4), we shall find in § 5 that in a straightforward case equ. (3.4) has the advantage of simplicity.

Let us consider for a moment what kind of changes will result in (3.5), if approximation (D) is dropped and only (E) and (C) are kept. Then, T_n and $\sum_i T_{ei}$ are small, but a correlation between electronic and nuclear collisions remains. According to (3.3), all cross sections in (3.5) must be replaced by $d\sigma_{n,e}$, but moreover the term $(\overline{\varphi}(T_n)-T_n\overline{\varphi}'(E))^2$ on the right changes into $\left(\overline{\varphi}(T_n)-\overline{\varphi}'(E)\left[T_n+\sum_i T_{ei}\right]\right)^2$, and for this reason the effect of correlations can be distinguished. In this respect (3.5) differs from the corresponding equation (2.8), where we also discussed omission of approximation (D).

Corresponding to the equation (2.3) for $\overline{\varphi}_1(E)$, we shall also discuss the straggling in the case of $Z_1 \neq Z_2$. The average square straggling in φ_1 is denoted as $\Omega_{\varphi 1}^2(E)$. We consider again the case where φ_e does not contribute. Using approximation (D) an equation analogous to (3.4) is obtained

$$\left.\begin{aligned}S_{1e}\cdot\frac{d}{dE}\Omega_{\varphi 1}^2(E)=&\int d\sigma_{1n}\{\Omega_{\varphi 1}^2(E-T_n)-\Omega_{\varphi 1}^2(E)+\Omega_\varphi^2(T_n)\}+\\&+\int d\sigma_{1n}\{\overline{\varphi}_1(E-T_n)-\overline{\varphi}_1(E)+\overline{\varphi}(T_n)\}^2,\end{aligned}\right\} \qquad (3.6)$$

where $\overline{\varphi}(E)$ is given by (2.7), $\Omega_\varphi^2(E)$ by (3.4) and $\overline{\varphi}_1(E)$ by (2.3) in approximation (D), while $d\sigma_{1n}$ is the differential nuclear cross section for collisions between the particle 1 and an atom 2. Further, S_{1e} is the electronic stopping cross section per atom for the particle 1 passing atoms 2. It is seen that (3.6) contains (3.4) as a special case. In (3.6), terms of type of $\left(\sum_i T_{ei}\right)^2$ are omitted.

Finally, we apply the approximation (E) to (3.6), i.e.

$$(S_{1e}+S_{1n})\frac{d}{dE}\Omega_{\varphi 1}^2(E)=\int d\sigma_{1n}\,\Omega_\varphi^2(T_n)+\int d\sigma_{1n}\{\overline{\varphi}(T_n)-T_n\overline{\varphi}_1'(E)\}^2, \qquad (3.7)$$

where $\overline{\varphi}$, Ω_φ^2 and $\overline{\varphi}_1$ should be given in approximation (E) too. Note that (3.7) is a differential equation in the variable $\Omega_{\varphi 1}^2$, and may be integrated readily.

Probability distribution.

We have now studied average quantities, $\overline{\varphi}\,(E)$, described by rather simple equations, as well as fluctuations, $\Omega^2(E)$, which obey more elaborate equations. These are the first two steps in a series development, where successive moments $<\varphi^n>$ are calculated. The series development is convenient if the first moments give adequate information, since they may be calculated with comparative ease. Often, further information is needed. When the value of a series development becomes doubtful, a closed equation for the probability distribution itself is much to be preferred. Other approximation methods are then at our disposal.

It is thus of both theoretical and practical interest to study the probability distribution itself. We shall merely formulate the basic equations. Let us then ask for the equation analogous to (2.1), where one considers the effect of an incoming particle with energy E, and identical with the atoms in the medium. Introduce probability distributions $P\,(\varphi, E)$ and $P_e\,(\varphi, E)$ representing the probabilities that, respectively, the particle and an electron having energy E will produce the damage effect φ. Therefore, e.g. $\int_0^\infty \varphi P_e\,(\varphi, E)\,d\varphi = \overline{\varphi}_e\,(E)$ is the average effect produced by an electron of energy E. The equation governing $P\,(\varphi, E)$ is derived in the same way as (2.1), making the same assumptions. We find readily

$$\left.\begin{aligned}\int d\sigma_{n,e} P\,(\varphi, E) = \int d\sigma_{n,e} \int_0^\infty d\varphi' \int_0^\infty d\varphi'' \prod_j \int_0^\infty d\varphi_j P_e\,(\varphi_j, T_{ej} - U_j)\,\cdot \\ \cdot\, P\left(\varphi', E - T_n - \sum_i T_{ei}\right)\cdot P\,(\varphi'', T_n - U)\cdot\delta\left(\varphi - \varphi' - \varphi'' - \sum_i \varphi_i\right).\end{aligned}\right\} \qquad (3.8)$$

The equation states that the probability for the value φ prior to the collision is equal to the product of the individual probabilities belonging to ejected particles, when averaged over the frequency of occurrence of the different events. There is an integration over all possible φ-values of the ejected particles, with the condition that their sum is equal to the original φ-value, as expressed by the δ-function. Thus, (3.8) assumes independent behaviour of the separate events, i.e. product of P's, and additivity of damage effect, i.e. $\varphi = \varphi' + \varphi'' + \sum_i \varphi_i$.

Equ. (3.8) determines $P\,(\varphi, E)$ and P_e is considered as a known function. If (3.8) is multiplied by φ and integrated over φ from 0 to ∞, equ. (2.1) results.

There is a similar equation for $P_e\,(\varphi, E)$. We write it down assuming for simplicity that electrons produce no atomic recoils (approximation (A) and equ. (2.2'))

$$\left.\begin{aligned}\int d\sigma_e' P_e\,(\varphi, E) = \int d\sigma_e' \int_0^\infty d\varphi' \prod_j \int_0^\infty d\varphi_j P_e\,(\varphi_j, T_{ej} - U_j)\,\cdot \\ \cdot\, P_e\left(\varphi', E - \sum_i T_{ei}\right)\cdot\delta\left(\varphi - \varphi' - \sum_i \varphi_i\right),\end{aligned}\right\} \qquad (3.9)$$

where $d\sigma_e'$ is the differential cross section for transfer of energy T_{ei} to atomic electrons by an electron of energy E. There are further simplifications, if we take into account that an electron normally ejects at most one atomic electron in a collision.

In (3.8) let us assume that electrons do not contribute to the damage effect in question, i.e. $P_e(\varphi,E) = \delta(\varphi)$. In approximation ($D$) we then get, since $P(\varphi,0) = \delta(\varphi)$,

$$\left.\begin{aligned} S_e(E)\frac{\partial}{\partial E}P(\varphi,E) + \int d\sigma_n P(\varphi,E) &= \\ = \int d\sigma_n \int_0^\infty d\varphi' \int_0^\infty d\varphi'' P(\varphi', E-T_n)\, P(\varphi'', T_n)\, \delta(\varphi-\varphi'-\varphi''). \end{aligned}\right\} \quad (3.10)$$

The bond expressed by the δ-function can be inconvenient. It is natural to introduce Laplace transforms of the probability distribution,

$$\tilde{P}(\lambda,E) = \int_0^\infty d\varphi\, P(\varphi,E)\, e^{-\lambda\varphi}.$$

The Laplace transforms are particularly useful because of the additivity of φ. From (3.8) we obtain the alternative version

$$\left.\begin{aligned} \int d\sigma_{n,e}\tilde{P}(\lambda,E) = \int d\sigma_{n,e}\tilde{P}\Big(\lambda, E-T_n-\sum_i T_{ei}\Big)\tilde{P}(\lambda, T_n-U)\cdot \\ \cdot\prod_j \tilde{P}_e(\lambda, T_{ej}-U_j), \end{aligned}\right\} \quad (3.11)$$

and if $\overline{\varphi}_e$ is zero we have $\tilde{P}_e(\lambda,x) \equiv 1$.

§ 4. Analytical Approximations in Homogeneous Equation

The first step towards a solution of (2.1), or its simplified versions, is to discuss its homogeneous part, i.e. put $\varphi_e = 0$. Now, it so happens that the quantity $\overline{\nu}(E)$, introduced in § 1 and described as the average energy transfer to atomic motion, is normally a solution of the homogeneous part of equation (2.1), because the energy transfer from electrons to atoms is negligible to nearly all purposes. By solving the homogeneous equation, we have therefore found one important physical property in slowing-down processes. In the following, the normal boundary condition on $\overline{\nu}(E)$ is $\overline{\nu}(E)/E \to 1$ for $E \to 0$, and thus $\overline{\eta}(E)/\overline{\nu}(E)$ vanishes in this limit.

It is necessary to gain some experience concerning solutions of the integral equation. To this end we consider at first analytical solutions using simplified approximations to cross sections; this can be of interest particularly at the lower energies. Secondly, in § 5 we solve the integral equations numerically with more accurate cross sections, using electronic computations. We are then led to new asymptotic or approximate solutions, which may be checked by the numerical and analytical results. The present chapter may therefore be regarded as an exercise preliminary to the more precise treatment in § 5.

The simplest results obtain when we suppose that the differential cross section $d\sigma_n$ may be approximated by the power law scattering formula (1.3), corresponding to a potential proportional to r^{-s}. We can then arrive at analytical solutions of the various approximations to the integral equation. Let us start from approximation (E), i.e. (2.8). The homogeneous equation (2.8) for $\bar{\nu}$ becomes

$$(S_e + S_n) \cdot \bar{\nu}'(E) = \int_{T=o}^{E} \frac{d\sigma_n}{dT} dT \, \bar{\nu}(T), \tag{4.1}$$

where $\bar{\varphi}$ has been replaced by $\bar{\nu}$. We introduce (1.3) in (4.1), and multiply by $S_n^{-1} E^{1-1/s}$. Differentiating with respect to E we get a differential equation of second order in place of the integral equation (4.1),

$$(\xi(E) + 1)\, E^2 \bar{\nu}'' + \left\{ E\,\xi'(E) + \left(1 - \frac{1}{s}\right)(1 + \xi(E)) \right\} E \bar{\nu}' - \left(1 - \frac{1}{s}\right) \bar{\nu} = 0, \tag{4.2}$$

where $\xi(E) = S_e(E)/S_n(E)$. It is apparent that a differential equation was obtained from the original integral equation only because of the simple behaviour of the cross section (1.3), where the dependence of $d\sigma_n$ on E could be separated out as a factor.

Corresponding to (1.2) we shall assume that $S_e \propto E^{1/2}$, and since $S_n \propto E^{1-2/s}$ we get $\xi(E) \propto E^{2/s-1/2}$. It then turns out that the solutions of (4.2) are hypergeometric functions, of the kind $F(a, b;\ a+b;\ x)$, cf. Erdélyi et al. (1953). The complete solution of (4.2) is seen to be

$$\left.\begin{aligned} \bar{\nu}(E) = C_1 E \cdot F\left(\frac{2s}{4-s}, \frac{s+2}{4-s}; \frac{3s+2}{4-s}; -\xi(E)\right) + \\ + C_2 E^{\frac{1-s}{s}} \cdot F\left(\frac{2-2s}{4-s}, \frac{4-3s}{4-s}; \frac{6-5s}{4-s}; -\xi(E)\right), \end{aligned}\right\} \tag{4.3}$$

where C_1 and C_2 are arbitrary constants.

If we ask for the particular solution given by the normal boundary condition for $\bar{\nu}$ at $E = 0$, i.e. $\bar{\nu}(E)/E \rightarrow 1$ for $E \rightarrow 0$, we obtain $C_1 = 1$, $C_2 = 0$, if $s < 4$. Note that only for $s < 4$ does the present $\xi(E)$ tend to zero for $E \rightarrow 0$, and that this is the proper behaviour of $\xi(E)$.

If instead of (2.8) we start from the more correct equation (2.7), the cross section (1.3) is seen to lead to the equation

$$\frac{d}{dE}\left\{E^{1-1/s}\,\overline{\nu}'(E)\,\xi(E)\right\} = -\overline{\nu}''(E)\cdot E^{1-1/s} + $$
$$+\left(1-\frac{1}{s}\right)\int_0^E \frac{dT}{T^{1+1/s}}\cdot\left\{\overline{\nu}'(E-T)-\overline{\nu}'(E)+\overline{\nu}''(E)\,T\right\}.$$

The integrand on the right is large only for $T \approx E$. Making an underestimate of the integral (because $\overline{\nu}''(E)$ is always negative and increases with E) we then replace $T^{-1-1/s}$ by $E^{-1-1/s}$ in the integral. This gives the differential equation

$$E^2\cdot\overline{\nu}''\cdot\left(\xi+\frac{1}{2}+\frac{1}{2s}\right)+E\cdot\overline{\nu}'\cdot\left\{E\,\xi'+\left(1-\frac{1}{s}\right)(\xi+1)\right\}-\left(1-\frac{1}{s}\right)\overline{\nu} = 0. \tag{4.4}$$

This equation differs only little from (4.2), but is an underestimate of $\overline{\nu}$, as compared with the precise solution of (2.7) and (1.3). It is interesting that $\overline{\nu}$ from (4.2) is instead an overestimate of the solution of (2.7) and (1.3); this follows from $\overline{\nu}'(E)$ being a decreasing function of E. We have thus bracketed the solution of (2.7) between two approximate solutions. It turns out that (4.4) is generally a somewhat better approximation than (4.2). The solutions of (4.4) are seen to be hypergeometric functions, of the type

$$E\cdot F\left(\frac{2s}{(4-s)},\frac{s+2}{(4-s)};\frac{(4+s)\,\alpha+2s-2}{(4-s)\,\alpha};\ -\frac{\xi(E)}{\alpha}\right)\quad\text{and}$$
$$E^{\frac{1-s}{s\alpha}}\cdot F\left(\frac{2-2s}{(4-s)\,\alpha},\frac{(2-s)\,\alpha+2-2s}{(4-s)\,\alpha};\frac{(4-3s)\,\alpha+2-2s}{(4-s)\,\alpha};\ -\frac{\xi(E)}{\alpha}\right)$$

where $\alpha = \frac{1}{2}+\frac{1}{2s}$ is the coefficient of $\overline{\nu}''$ in the brackets in (4.4). The present solutions of (4.4) are similar to (4.3), and contain it as special case ($\alpha = 1$).

Region I. In region I, where $0 < E \lesssim E_c$, we may select a few suitable values of s, and study some of the approximate solutions. In doing this, we obtain not only a reasonable estimate of $\overline{\nu}(E)$, but also an insight in errors involved in some of the simplifications, (*A*) to (*E*), of the basic integral equation.

Let us consider the standard case, where $s = 2$ and $S_n = S_n^o$ is independent of energy, cf. (1.1) and (1.3). We put $\xi(E) = (E/E_c)^{1/2}$, and obtain from (4.2) and (4.3), with the boundary condition $\overline{\nu}(E)/E = 1$ at $E = 0$,

$$\overline{\nu}(E) = E_c\left\{-12+6\left[1+2\,(E_c/E)^{1/2}\right]\cdot\log\left(1+(E/E_c)^{1/2}\right)\right\}, \tag{4.5}$$

representing the solution of (2.8) – i.e. approximation (*E*) – for power law scattering with $s = 2$. The solution (4.5) can be used only at energies where E/E_c is somewhat less than unity. This limitation must be made because a decrease sets in in the actual function S_n at an energy somewhat lower than E_c, in most cases.

Let us consider in particular the limit of $(E/E_c) \ll 1$, where a more general approach is possible. In fact, in any one of the approximations (D) to (E') we get, when $s = 2$, a power series in $(E/E_c)^{1/2}$

$$\bar{\eta}(E) = E - \bar{\nu}(E) = \alpha_1 E^{3/2} E_c^{-1/2} - \dots \quad , \quad E \ll E_c, \tag{4.6}$$

where α_1 is a constant, the value of which depends on the approximation used. We compare four solutions of the case $s = 2$. Firstly, approximation (E) given by (4.5) leads to $\alpha_1 = 1$. Secondly, a series development of the solutions of the approximation (4.4) leads to $\alpha_1 = 16/13 = 1.23$. Thirdly, the more correct integral equation (2.7), i.e. approximation (D), may be solved by a series development, leading to $\alpha_1 = 4/(3\pi - 6) = 1.17$. These three values for α_1 give an indication of the accuracy of the various approximations. As expected, (cf. the discussion of (4.4)) the solution (4.5) is an overestimate and (4.4) an underestimate of $\bar{\nu}(E)$; (4.4) is a somewhat better approximation. A fourth case may be mentioned, i.e. approximation (E') given by equation (2.8'). It consists in including the next term in the series development of $\bar{\nu}(E - T_n) - \bar{\nu}(E)$, i.e. subtract $(1/2)\,\bar{\nu}''(E)\int d\sigma_n T_n^2$ on the left hand side of (4.1). We find here $\alpha_1 = 8/7 = 1.14$, so that approximation (E') is superior to (E).

Region II. In this region the function S_e remains the same, increasing as $E^{1/2}$. However, S_n begins to decrease and the scattering approaches the Rutherford scattering, though with a screening at a distance $\sim a$. For a qualitative orientation we again base our description on (1.3), so that we assume that S_n is proportional to a power of E, i.e. $E^{1-2/s}$. This approach is qualitatively less justified than in region I, but we can learn about the possible approximation methods for solving the basic integral equation.

Let us suppose that S_n is proportional to $E^{-1/2}$ for $E > E_0$, so that $s = 4/3$ in (1.3), and $\xi(E) = (S_e/S_n) = (E/E_b)$. Then, $E_b = (E_0 E_c)^{1/2}$ is the energy at which the two stopping cross sections become equal. Equation (4.2) for $\bar{\nu}$ now becomes

$$(4\,E^3 E_b^{-1} + 4\,E^2)\,\bar{\nu}'' + (5\,E^2 E_b^{-1} + E)\,\bar{\nu}' - \bar{\nu} = 0, \tag{4.7}$$

with the complete solution (cf. (4.3))

$$\left.\begin{aligned}\bar{\nu} = C_1 \cdot 5\, E_b \left\{ 1 - \frac{1}{4\sqrt{2}}\, \xi^{-1/4} \log \frac{\xi^{1/2}+\sqrt{2}\,\xi^{1/4}+1}{\xi^{1/2}-\sqrt{2}\,\xi^{1/4}+1} - \right.\\ \left. - \frac{1}{2\sqrt{2}}\, \xi^{-1/4} \operatorname{arctg} \frac{\sqrt{2}\,\xi^{1/4}}{1-\xi^{1/2}} \right\} + C_2\, \xi^{-1/4} E_b^{-1/4}.\end{aligned}\right\} \tag{4.8}$$

The solution is determined by the boundary conditions at the energy E_o, where we find $\bar{\nu}$ and $\bar{\nu}'$ from (4.5). Thus, C_1 is given by

$$C_1 = \frac{12}{5} x^{-2} + \frac{6}{5}(x+1)(x-2)\, x^{-3} \log(1+x) \simeq 1 - \frac{2}{5} x + \ldots, \tag{4.9}$$

where $x = E_o/E_b$ is less than unity for all values of $Z_1 = Z_2$. The expression for C_2 is more involved, but $C_2 < 0$. This shows that although $\bar{\nu}(E)$ increases with E, it remains below the value C_1, and it increases only slowly towards this limit. In region III, however, it turns out that $\bar{\nu}$ will go on increasing without an upper limit, although still quite slowly. The behaviour of (4.5) in region I and (4.8) in region II is shown by the dashed curve in Fig.s 5 and 6 for the case of $\varepsilon_c = 4.75$ ($k = 0.15$) and $x = 0.56$, where it is compared with a numerical estimate based on the more accurate scattering formula (1.4). It may be noted that the value of C_1 is not far from unity, and that C_2 is small. If we were to put $C_1 = 1$ and $C_2 = 0$, we would instead have the solution where $s = 4/3$, i.e. (4.7), is used down to zero energy, and apparently this is satisfactory as a rough estimate.

In region I the solution (4.3) of the equation (4.2) was an application of approximation (E) using the cross section (1.3). It might therefore seem that also in region II the equations (4.7) and (4.8) are equivalent to approximation (E). However, we change from one cross section $d\sigma_n$ in region I to another in region II. Since (4.2) and (4.7) were obtained by differentiation of (4.1), they should be supplemented by inhomogeneous terms if the cross section changes at low values of TE. This circumstance is disregarded in (4.7), (4.8) and (4.9), giving some deviation from (E).

Straggling in region I. An evaluation of the straggling in ν or η, $\Omega_\nu^2(E) = \Omega_\eta^2(E)$, from (3.3) is more involved than the estimate of $\bar{\nu}$ itself. Still, at low energies in region I, a series development may be made and the first term is readily obtained. If (1.3) is applied, it turns out that the relative straggling in η becomes a constant, independent of energy (and atomic number and mass) at low energies,

$$\sigma^2 = \frac{\Omega_\eta^2(E)}{\bar{\eta}^2(E)} = \text{const., for } \xi(E) \ll 1\,. \tag{4.10}$$

If we consider the standard case, $s = 2$ in (1.3) and $\xi = (E/E_c)^{1/2}$, we find at low energies that $\bar{\eta}$ is proportional to $E^{3/2}$, cf. (4.6). We solve (3.5) and get $\sigma^2 = 1/14$. We may also solve directly the more basic integral equation (3.4) for Ω_ν^2, which corresponds to equation (2.7) for $\bar{\eta}$ itself. Then we obtain $\sigma^2 = (3\,\pi/4) - (23/10) = 0.0562$, which is somewhat less than the previous value of σ^2.

If, instead of the relative straggling, we consider the absolute straggling Ω_η, we find that (3.5) gives closely the same as (3.4), being only about 4 percent less than (3.4). The approximation (E) is therefore considerably better for the straggling than for the value of the function $\bar{\eta}$ itself.

Since Ω_η^2 is expected to be more accurate than σ^2, we quote the value of Ω_η^2 obtained in approximation (E), i.e. (3.5), using (1.3)

$$\Omega_\eta^2(E) = \frac{s\,(s-1)\,(s+2)^2\,(11\,s^2+23\,s+6)}{4\,(3\,s+2)^3\,(2\,s+3)\,(2\,s-1)}\,(E\cdot\xi(E))^2, \quad \xi(E) \ll 1, \qquad (4.11)$$

which shows that the coefficient of $(E\cdot\xi(E))^2$ only varies from 0.071 to 0.109 when s increases from 2 to 3. The corresponding variation of σ^2 may be found from (4.3) and (4.11).

§ 5. Numerical and Asymptotic Solutions for $Z_1 = Z_2$

Numerical results.

The analytical solutions in § 4 give merely some guidance in the problem, because they are based on the power law scattering, which has quite limited applicability. A fairly complete and reasonably accurate solution of the case $Z_1 = Z_2$ may be obtained from representative values of the electronic stopping constant, k, together with the universal cross section given by (1.4) and Fig. 2. It is convenient to use the $\varepsilon - t$ variables in (1.4). The electronic stopping is then assumed to be $(d\varepsilon/d\varrho)_e = k\cdot\varepsilon^{1/2}$ in regions I and II. The homogeneous integral equation for $\bar{\nu}$ is

$$\left(\frac{d\varepsilon}{d\varrho}\right)_e\cdot\bar{\nu}'(\varepsilon) = \int_0^{\varepsilon^2}\frac{dt}{2\,t^{3/2}}\cdot f(t^{1/2})\left\{\bar{\nu}\left(\varepsilon-\frac{t}{\varepsilon}\right)-\bar{\nu}(\varepsilon)+\bar{\nu}\left(\frac{t}{\varepsilon}\right)\right\}, \qquad (5.1)$$

where $f(t^{1/2})$ is shown in Fig. 2. Note that (5.1) is equivalent to approximation (D).

The integral equation (5.1), with $(d\varepsilon/d\varrho)_e = k\cdot\varepsilon^{1/2}$, was solved by numerical methods on the electronic computer DASK. Actually, a slight modification of (5.1) was advantageous in the numerical computations; it gives a slight overestimate of $\bar{\nu}$ as compared to (5.1), and should be accurate within a few percent. When starting the solutions at small values of ε, the asymptotic behaviour of the cross section (1.4) was assumed to be $f(x) \propto x^{1/3}$, corresponding to power law scattering with $s = 3$. We could here use the analytical estimates in § 4. In the following, solutions are presented for $k = 0.10$, 0.15 and 0.20, which covers the range of variation of k for $Z_1 = Z_2$.

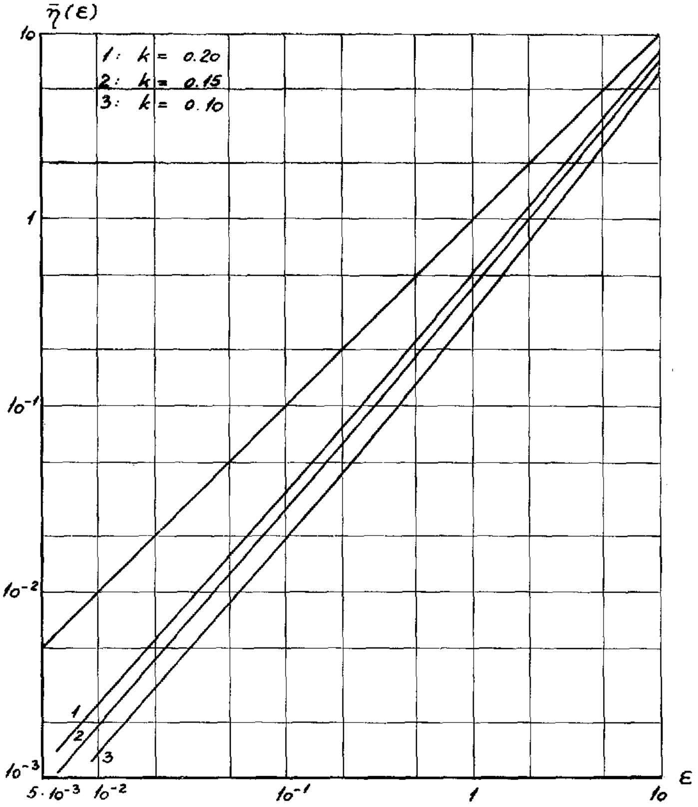

Fig. 3. The function $\bar{\eta}(\varepsilon)$ vs. ε at low values of ε, for $Z_1 = Z_2$ and in the three cases $k = 0.10, 0.15$ and 0.20. The curves were computed numerically from (5.1).

The results of the coded computations of $\bar{\nu}(\varepsilon)$ from (5.1), i.e. approximation (D), are shown in Fig.s 3 and 4 for the above three values of k. Fig. 3 represents low values of the energy variable ε. In this region it is preferable to give the function $\bar{\eta}(\varepsilon) = \varepsilon - \bar{\nu}(\varepsilon)$, because $\bar{\nu}(\varepsilon)$ is nearly equal to ε. Fig. 4 is a continuation of the curves up to $\varepsilon = 100$. The function $\bar{\nu}(\varepsilon)$

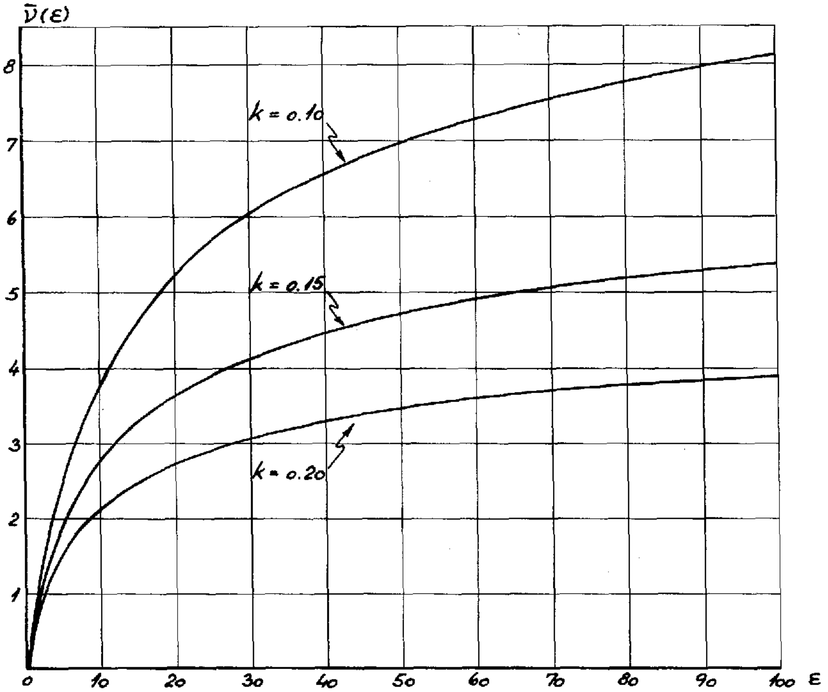

Fig. 4. The function $\bar{\nu}(\varepsilon)$ vs. ε for $0 < \varepsilon < 100$. The figure gives the continuation of the three solutions in Fig. 3.

increases initially as ε, but remains small compared to ε when ε is large. In region II, i.e. when $(d\varepsilon/d\varrho)_e = k \cdot \varepsilon^{1/2}$, $\bar{\nu}(\varepsilon)$ has an upper limit, as discussed below.

As a preliminary to the above calculations we made numerical calculations by hand in approximation (E), i.e. based on the homogeneous part of (2.8). It seems of interest to compare the two approximations. This is done in Fig.s 5 and 6, in the case of $k = 0.15$. The full-drawn curve in Fig. 5 is the accurate solution of (5.1). The dashed line is the analytical solution (4.5) for power law scattering, with $s = 2$. At $\varepsilon = 4.75$ this solution is continued by (4.8), corresponding to $s = 4/3$, cf. text in § 4. The accuracy of the power law solutions is seen to be moderate. Similarly, Fig. 6 shows $\bar{\nu}(\varepsilon)$ for $\varepsilon < 100$, in three approximations. The solid curve is the solution of (5.1). The analytical solution (4.8), for power law scattering with $s = 4/3$, is continued from Fig. 5, and shown by the dashed curve. This analytical solution is seen to become increasingly poor for large ε. The stipled curve represents the abovementioned computation by hand in approximation (E).

As expected, (E) is an overestimate of $\bar{\nu}$, by about 10 percent for high values of ε; this may be a tolerable accuracy for several purposes.

The average square fluctuation in ν, $\Omega^2(\varepsilon)$, may be computed from (3.4), i.e. approximation (D). In the coded computation we use $\varepsilon - t$ vari-

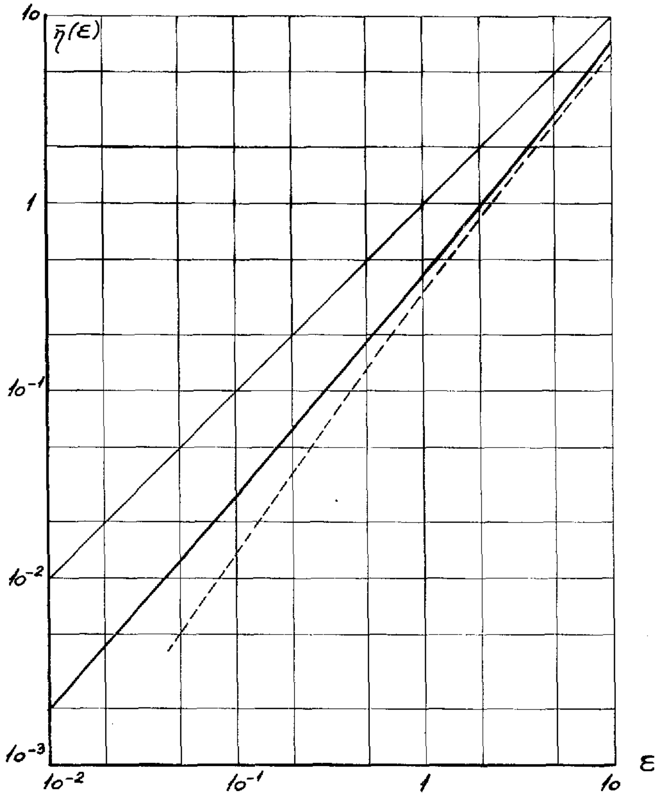

Fig. 5. Comparison of approximations for $Z_1 = Z_2$, $k = 0.15$ Curves show $\bar{\eta}(\varepsilon)$ vs. ε at low values of ε. Thick solid curve is solution of (5.1), like Fig. 3. Dashed line is power law formula (4.5), with $s = 2$. The curves approach the thin solid line $\bar{\eta} = \varepsilon$.

ables as in (5.1), and with $f(t^{1/2})$ given by Fig. 2. The equation contains inhomogeneous terms which may be computed from $\bar{\nu}(\varepsilon)$ in Fig.s 3 and 4. At $\varepsilon = 0$ the solutions were started from the analytical approximations in § 4, with $s = 3$. The results are shown in Fig. 7, for the three values of k used above, and relatively large values of ε. The figure gives $\Omega^2/\bar{\nu}^2$, the average square fluctuation divided by $\bar{\nu}^2$, and the resulting curves are seen to lie remarkably close to each other. It is instructive to compare various

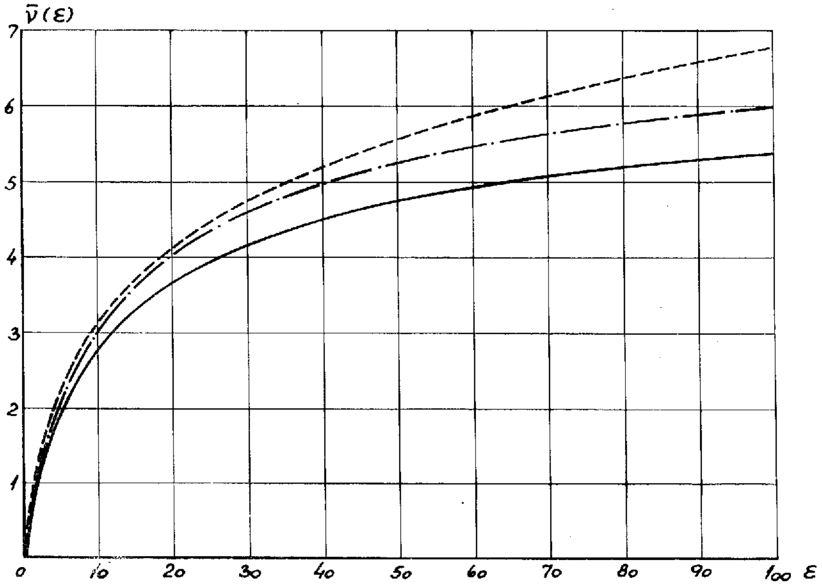

Fig. 6. Comparison of approximations for $Z_1 = Z_2$, $k = 0.15$. Curves show $\bar{\nu}(\varepsilon)$ vs. ε for $\varepsilon < 100$. The solid curve is solution of (5.1). Dashed curve is (4.8) continued from Fig. 5, corresponding to power law $s = 4/3$. Stipled curve was computed by hand in approximation (E).

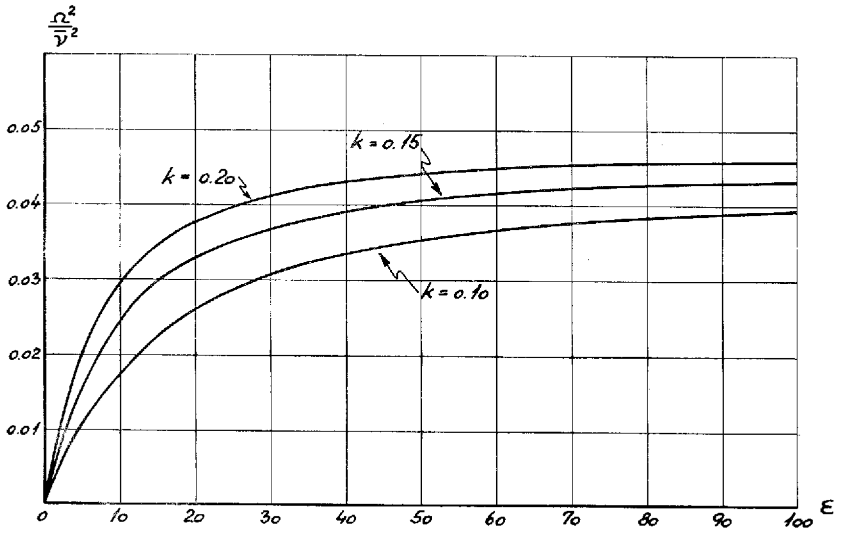

Fig. 7. Relative average square fluctuation in ν, $\Omega^2/\bar{\nu}^2$, for $k = 0.10, 0.15$ and 0.20. Coded computations in approximation (D).

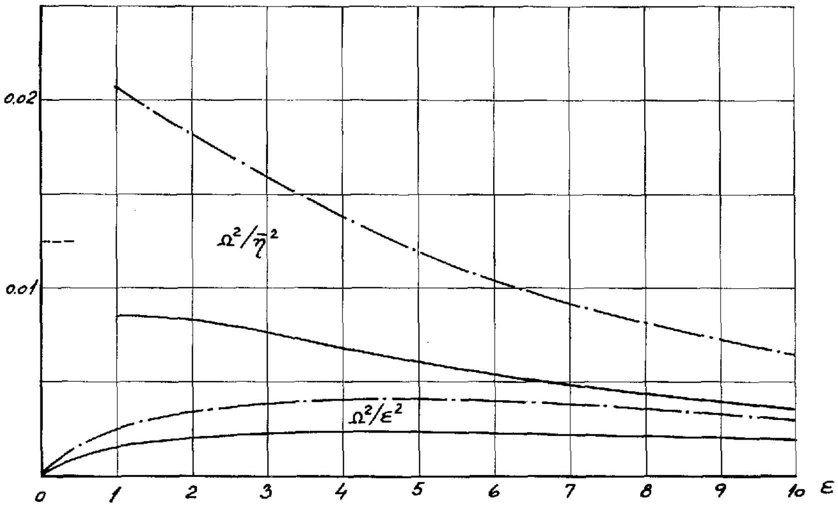

Fig. 8. $\Omega^2/\bar{\eta}^2$ (two upper curves) and Ω^2/ε^2 (two lower curves) for $k = 0.15$. Solid curves computed numerically in approximation (*D*), stipled curves in approximation (*E*).

approximations, as seen in Fig. 8 for $k = 0.15$. The solid curves represent approximation (*D*), as in Fig. 7. The stipled curves were computed by hand in approximation (*E*). The horizontal dashed line shows the point ($s = 3$), from which $\Omega^2/\bar{\eta}^2$ in approximation (*E*) was started at $\varepsilon = 0$. The difference between $\Omega^2/\bar{\eta}^2$ in approximations (*D*) and (*E*) is quite large, and here the errors in $\bar{\eta}$ and in Ω^2 seem to add, at low ε-values. We believe that the accuracy in Ω^2, at low values of ε, is not quite satisfactory in any of the approximations used.

One important reservation should be made as regards the above computations of $\bar{\nu}$ and $<(\nu-\bar{\nu})^2> = \Omega^2$. Apart from their definition as averages in the probability distribution $P(\nu)$, these two quantities acquire a simple meaning if $P(\nu)$ is approximately Gaussian, i. e. $P \sim C \cdot \exp\left\{-(\nu-\bar{\nu})^2/2\Omega^2\right\}$. However, sometimes the deviations from a Gaussian are noticeable. The probability distribution then has an asymmetric peak, with a most probable value ν^* slightly smaller than $\bar{\nu}$, and with a width at half maximum which may be considerably smaller than for the above Gaussian. There is also a tail towards high ν-values, decreasing with a power of ν of about -2 to -2.5, and having a cut-off at some high ν-value. Examples of this kind were studied in a recent paper (LINDHARD and NIELSEN (1962)). In any case, it depends on the experiment performed whether one may use the average values $\bar{\nu}$ and Ω^2, or take recourse to the probability distribution.

In a particle detector, where damage events due to single particles are recorded individually, one should normally consider the probability distribution. However, if many events are recorded together, like the damage by thousands of particles in a solid, the events collect into a Gaussian distribution, with average value $N \cdot \bar{\nu}$, and an average square fluctuation $N \cdot \Omega^2$, where N is the number of particles.

If the electronic stopping continued to rise as $k \cdot \varepsilon^{1/2}$, (region II), there would be an upper limit to $\bar{\nu}(\varepsilon)$. In the cases shown in Fig. 4 this upper bound may be obtained from (5.3); for $k = 0.15$ this leads to $\bar{\nu} < 7.8$. However, at an energy $\varepsilon_1 \sim 10^3$ the electronic stopping has a maximum and starts decreasing, so that approximately S_e/S_n tends to a constant $\sim 10^3$. Thus, in region III there is strictly no upper bound on $\bar{\nu}$, but its increase is extremely slow. We did not continue the coded computations into region III, partly because a new stopping parameter would be required, and partly because simple asymptotic equations take over, long before region III is reached.

Asymptotic equations.

Let us first consider a semi-empirical approximation to $\bar{\nu}$, which may be found from the numerical curves. In fact, from Fig. 4 it is seen that for large ε the function $\bar{\nu}$ is nearly reversely proportional to k, i.e. to the electronic stopping. This result cannot hold for $\varepsilon < 1$, where $\bar{\nu} \approx \varepsilon$. However, in this limit we found in § 4 that $\bar{\eta} = \varepsilon - \bar{\nu}$ is proportional to k, because the electronic stopping is small and a series development may be made of the function $\bar{\eta}$ in powers of k. A simple comprehensive formula joining the two results $\bar{\nu} \sim g_1(\varepsilon) k^{-1}$ and $\bar{\nu} \sim \varepsilon - k g_2(\varepsilon)$, is

$$\bar{\nu}(\varepsilon) = \frac{\varepsilon}{1 + k \cdot g(\varepsilon)}, \tag{5.2}$$

where $g(\varepsilon) \to 0$ for $\varepsilon \to 0$, and $g(\varepsilon) \to \varepsilon$ in region II. On the basis of the curves in Fig.s 3 and 4, we have estimated $g(\varepsilon)$ as shown in Fig. 9. It appears that (5.2) with Fig. 9 reproduces $\bar{\nu}(\varepsilon)$ within an accuracy of some percent, for all values of ε in regions I and II, and for the k-values of interest when $Z_1 = Z_2$.

A convenient approximation, valid for large ε, may be mentioned in connection with the numerical estimates. We note that for high energies E the differential cross section (1.4), as shown in Fig. 2, will be equal to the Rutherford cross section, $d\sigma_R$, except when $T \lesssim (E_0^2/E) \to 0$. If therefore we integrate a function of T, tending to zero as T, we may replace (1.4)

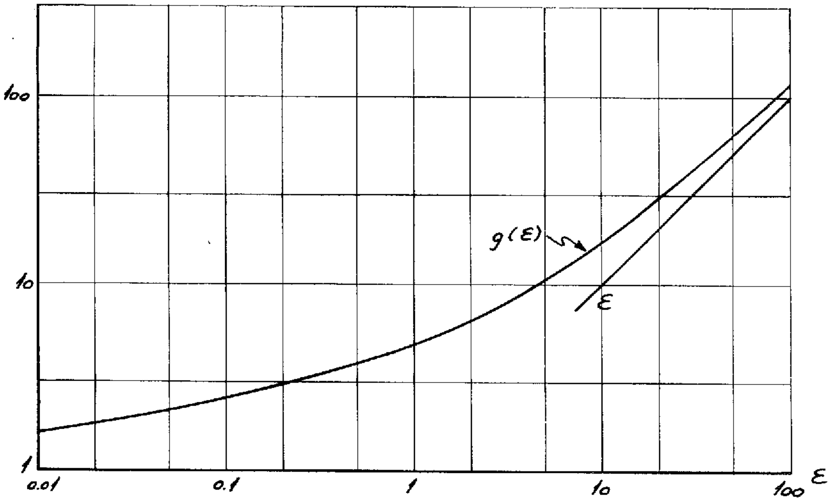

Fig. 9. The semi-empirical function $g(\varepsilon)$ in (5.2).

by the Rutherford cross section, integrated from the lower boundary $T = \lambda^2/E$, where the constant λ is determined by $\int_0 T d\sigma = \int_{\lambda^2/E} T d\sigma_R$. We might make this replacement in the accurate equation (2.7), but for the present purpose (4.1) is accurate enough. Since $\bar{\nu}(T)$ increases slowly at high T-values, we can replace the upper limit E by ∞ in the integral in (4.1) and find, expressed in the $\varepsilon - t$ variables,

$$\varepsilon \frac{d\varepsilon}{d\varrho} \bar{\nu}'(\varepsilon) = \varepsilon \int_{t_0}^{\infty} \frac{dt}{4t^2} \bar{\nu}(t/\varepsilon) = \frac{1}{4} \log \varepsilon + C, \tag{5.3}$$

where $t_0 = 0.60$, and C is a constant.

The formula (5.3) is a useful and rather accurate approximation, provided ε is larger than ~ 10. It may be readily integrated, without recourse to complicated coded computations. If we start using (5.3) at an energy ε_2, we may for instance fit $\bar{\nu}(\varepsilon_2)$ and $\bar{\nu}'(\varepsilon_2)$, the latter determining the constant C. We may normally disregard $(d\varepsilon/d\varrho)_n$ and write $d\varepsilon/d\varrho = (d\varepsilon/d\varrho)_e$. In region II we put $(d\varepsilon/d\varrho)_e = k \cdot \varepsilon^{1/2}$, and in this case (5.3) leads to an upper bound for $\bar{\nu}(\varepsilon)$, as mentioned on p. 31. We note furthermore that according to (5.3) the increase of $\bar{\nu}(\varepsilon)$ is proportional to k^{-1}, in agreement with (5.2).

An equation similar to (5.3) may be derived for the average straggling $\Omega^2(\varepsilon)$. For this purpose we consider equ. (3.4). Since the integrand on the right tends to zero as T^2 or faster, we may directly put $d\sigma = d\sigma_R$ for high energies and integrate from 0 to E, because the integral converges rapidly at $T = 0$. We may also simplify the right hand side, since clearly $\bar{\nu}(T)$ is the dominating term for small or moderate T, where the differential cross section is large. Because $\bar{\nu}^2(T)$ saturates we then have the simple limiting approximation

$$\varepsilon\left(\frac{d\varepsilon}{d\varrho}\right)\cdot\frac{d}{d\varepsilon}\Omega^2(\varepsilon) = \varepsilon\int_0^{\varepsilon^2}\frac{dt}{4\,t^2}\bar{\nu}^2(t/\varepsilon) = \psi(\varepsilon). \tag{5.4}$$

We observe that the right hand side of (5.4), $\psi(\varepsilon)$, tends to a constant for large ε. The magnitude of $\psi(\varepsilon)$ may be estimated roughly by putting (cf. (5.2)) $\bar{\nu}(x) = x\cdot(1+kx)^{-1}$, leading to $\psi(\varepsilon) = \bar{\nu}(\varepsilon)\cdot 4^{-1} \rightarrow k^{-1}4^{-1}$. Now, in region II we then obtain $(d\Omega^2/d\varepsilon) \simeq \bar{\nu}(\varepsilon)4^{-1}\cdot k^{-1}\varepsilon^{-3/2}$, leading us to expect that for large ε the function Ω^2 is proportional to k^{-2}. Actually, this result fairly well corresponds to the curves in Fig. 8. In the opposite limit of low ε-values we have found that $\Omega^2 \propto k^2$.

§ 6. Outline of Treatment for $Z_1 \neq Z_2$

From the previous discussion it appears that the most direct connection between experiments and theory may be achieved in the case of $Z_1 = Z_2$. Unfortunately, there are as yet no measurements of this kind.

A brief treatment may now be given of more involved cases. We consider problems where the incoming particle does not belong to the medium, but the medium still contains only one atomic species; we write briefly $Z_1 \neq Z_2$. As we shall see, our previous division into three energy regions can no longer be upheld. At the lowest energies the description remains comparatively simple, and experiments are available for comparison with theory.

We shall not consider cases where the medium contains more than one element. The formulation of accurate general solutions can here become quite complicated, but solutions of special cases may be worked out numerically. Several measurements are available.

Consider then an incoming particle with atomic number Z_1 different from Z_2. We assume that the case of $Z_1 = Z_2$ is already solved, as described in the preceding paragraphs, and the corresponding solution for the energy given to atomic motion is $\bar{\nu}(E)$. The unknown function for the case $Z_1 \neq Z_2$

is denoted as $\bar{r}_1(E)$. The integral equation for $\bar{r}_1$ is obtained from (2.3), where we introduce approximation (D),

$$\bar{r}_1'(E)\cdot S_{1e} = \int d\sigma_1 \left\{ \bar{r}_1(E-T) - \bar{r}_1(E) + \bar{r}(T) \right\}. \tag{6.1}$$

Here, S_{1e} is the electronic stopping cross section for the ion Z_1 in the medium Z_2, and $d\sigma_1$ is the differential cross section for an elastic nuclear collision between an ion Z_1 and an atom Z_2, with corresponding stopping cross section S_{1n}.

In (6.1) enters $\bar{r}(T)$, where $T \leq T_m = \gamma E$; $\gamma = 4\,M_1M_2/(M_1+M_2)^2$. Our previous division into three regions was characterized by the energies E_c and E_1, belonging to the atoms Z_2. Putting E_c and E_1 equal to the maximum recoil energy T_m we obtain for the particle Z_1 two characteristic energies $E_{2c} = \gamma^{-1}E_c$ and $E_{21} = \gamma^{-1}E_1$. However, the stopping cross sections S_{1e} and S_{1n} for the particle Z_1 give rise to a further subdivision. In fact, at energies lower than E_{1c} we may assume that S_{1e}/S_{1n} increases slowly, with a power of E between 1/2 and 1/6. At the energy E_{1c} the ratio S_{1e}/S_{1n} is comparable to 1. Next, above E_{1c} there is a decrease in S_{1n} while S_{1e} continues to rise as $E^{1/2}$ until the energy E_{11} is attained. For still higher energies S_{1e} decreases and the ratio S_{1e}/S_{1n} increases towards a constant $\sim 10^3$. Formally at least, we might then distinguish between five energy regions, separated by the energies E_{2c}, E_{1c}, E_{21} and E_{11}.

We limit the discussion to the lowest energy region. It is bounded upwards by either E_{1c} or E_{2c}. Approximate values of these energies are $E_{1c} \cong A_1^3(A_1+A_2)^{-2}$ $Z^{4/3}Z_1^{-1/3}\cdot 500$ eV, and $E_{2c} \cong (A_1+A_2)^2\cdot A_1^{-1}Z_2\cdot 125$ eV. When $Z_1 \gg Z_2$, E_{1c} will be larger than E_{2c}, while for $Z_2 \gg Z_1$ the energy E_{2c} becomes considerably larger than E_{1c}. For $Z_1 = Z_2$ the two energies are of course equally large.

Assume now that the energy is below E_{1c} and E_{2c}. We may then make the same approximation as in § 4 in region I. As an example we consider the standard case $s = 2$, leading to energy independent nuclear stopping cross sections, so that $S_{1e}/S_{1n} = (E/E_{1c})^{1/2}$ and $S_e/S_n = (E/E_c)^{1/2}$. For $\bar{r}(E)$ we can then apply approximation (4.6) with $\alpha_1 = 1$. The corresponding series development may be made in (6.1), i.e. in approximation (E). Using the expression (1.3) for $d\sigma$ we obtain

$$\bar{\eta}_1 = E - \bar{r}_1 = AE^{3/2}, \text{ for } E < E_{1c},\ E_{2c}, \tag{6.2}$$

where $A = \frac{2}{3}\left\{E_{1c}^{-1/2} + \frac{1}{2}\gamma^{1/2}E_c^{-1/2}\right\}$.

Next, we determine the straggling Ω_1^2 in η_1. With the same low energy approximation as in (4.10), we apply (3.5). Like in (4.10) the relative straggling in η_1 becomes a constant,

$$\Omega_1^2(E)/\bar{\eta}_1^2(E) = \frac{1}{14}\gamma\left\{\left(\frac{\gamma^{1/2}}{AE_c^{1/2}} - \frac{7}{4}\right)^2 + \frac{7}{16}\right\},\ E < E_{1c},\ E_{2c}. \tag{6.3}$$

The method actually used by us in solving equ. (6.1) is the following one. We introduce the $\varepsilon - \varrho - t$ variables described in § 1, and consider those regions where electronic stopping cross sections are proportional to $\varepsilon^{1/2}$. The problem then contains two empirical constants, k and k_1, i.e. the proportionality factors in electronic stopping for particles Z_2 in Z_2 and Z_1 in Z_2, respectively. The values of k and k_1 are estimated in (1.2). Two further parameters enter, one being the mass factor, $\gamma = 4M_1M_2/(M_1+M_2)^2$, and the other the ratio, λ, between the ε-units for the particle pairs (Z_1, Z_2) and (Z_2, Z_2). The solutions are then of type of $\bar{\nu}_1 = \bar{\nu}_1(\varepsilon;\, k,\, k_1;\, \lambda,\, \gamma)$ and $\Omega_1^2 = \Omega_1^2(\varepsilon;\, k,\, k_1;\, \lambda,\, \gamma)$. A programme was coded for electronic computation on this basis, and solutions have been obtained in a number of cases. Three sets of solutions of this kind are quoted below. Other solutions were utilized in a recent paper on damage in Si (DENNEY et al. (1962)).

The numerical solutions should be regarded with some reservation, and they are of limited applicability. Firstly, they apply only at the low energies where electronic stopping cross sections are proportional to $\varepsilon^{1/2}$. This can be remedied by continuing the solutions by means of asymptotic equations similar to (5.3) and (5.4), cf. (6.6). Secondly, the connection to an actual measurement is rather longwinded and uncertain. The usefulness of the average quantities $\bar{\nu}_1$ and Ω_1^2 can differ much from one set of (Z_1, Z_2) to another. In any case, the three examples in the following may illustrate some of the difficulties.

Ionization efficiency.

One important experimental observation is the number of ion pairs N_i produced by a certain incoming particle; in a solid state detector we let N_i represent the number of electron-hole pairs. We shall not discuss the detailed mechanism by which electrons create ion pairs, but only note that the energy per ion pair, $W_\beta = E_{\text{electron}}/\bar{N}_i$, is approximately constant for swift electrons.* In the present case of an arbitrary incoming particle it is therefore natural to consider the total energy η given to electronic motion, and expect that the average number of ions is approximately given by the relation

$$\bar{N}_i = \frac{\bar{\eta}(E)}{W_\beta}\,. \tag{6.4}$$

Evidently, if η fluctuates, N_i should fluctuate proportionally. An average square fluctuation in η, $\Omega^2(E)$, must therefore contribute to the average square fluctuation, $\overline{(\Delta N_i)^2}$, in N_i by the amount

$$\overline{(\Delta N_i)_\eta^2} = \Omega^2(E)/W_\beta^2\,, \tag{6.5}$$

---

* Experimental and theoretical discussions of W-values for electrons and α-particles are given in recent papers by JESSE (1961) and PLATZMAN (1961). The deviations of W_α/W_β from unity in polyatomic gases indicate one limitation in the accuracy of (6.4).

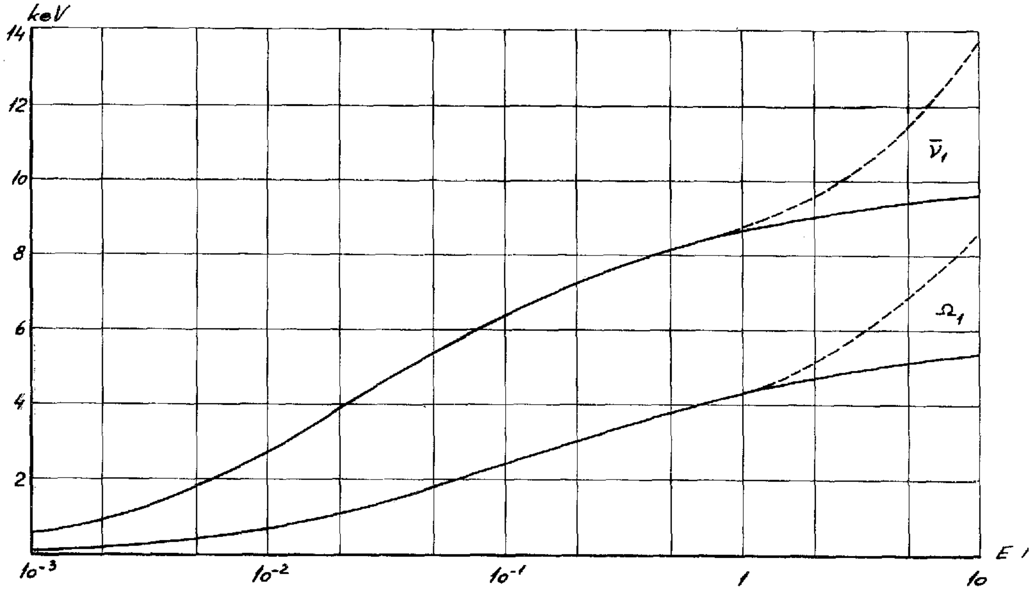

Fig. 10. Curves for $\bar{\nu}_1(E)$ and $\Omega_1(E)$ for α-particles in Si. Solid curves correspond to the coded computations. Dashed curves include corrections for decrease in electronic stopping, cf. (6.6).

but this is not the only cause of fluctuation of N_i. A direct statistical effect in ion pair production is that considered by Fano (1947), where the average square fluctuation was found to be $\overline{(\Delta N_i)^2_F} = F \cdot \overline{N}_i$, with $F \lesssim 0.5$, i.e. in some respects similar to a Poisson distribution. In many cases the fluctuation (6.5) dominates over the Fano effect.

In a treatment more precise than (6.4) and (6.5) one would introduce $\overline{N}_i$ directly as the variable $\overline{\varphi}$ in the basic integral equations. In fact, the basic case in production of ion pairs is an electron passing through a medium, and one must at first solve (2.2′) for $\overline{\varphi}_e(E) = \overline{N}_{ie}(E)$, i.e. the average number of ion pairs produced by an electron of energy E. Next, (2.1) is solved ($Z_1 = Z_2$) with respect to $\overline{N}_i(E)$, $\overline{N}_{ie}(E)$ being a source term. Thirdly, equ. (2.3) for $\overline{N}_{i1}(E)$ is solved. The Fano fluctuation is an estimate of the fluctuation in the first step only.

α-particles in Si.

Our first example of numerical computations illustrates the ionization by charged particles in a detector. We consider α-particles in Si, i.e. a solid state detector, but the results are quite similar to those for α-particles in A. In Fig. 10, the full-drawn curves show the behaviour of $\bar{\nu}_1(E)$ and $\Omega_1(E)$, as obtained from the coded computations mentioned above. Now, electronic stopping for α-particles in Si is proportional to velocity only up to about 0.7 MeV, where a maximum obtains, upon which the stopping decreases as $\sim v^{-1}$. The full-drawn curves in Fig. 10 are therefore underestimates at energies above 1 MeV. A correction can be made rather easily, since $\bar{\nu}(E)$ for Si ions in Si at the energies in question is given in e.g. Fig. 6, or by (5.1), so that the asymptotic equation is

$$\varepsilon\left(\frac{d\varepsilon}{d\varrho}\right)\cdot\bar{\nu}_1'(\varepsilon) = \frac{\lambda\varepsilon}{\gamma}\int_{t_0}^{\varepsilon^2}\frac{dt}{4t^2}\,\bar{\nu}\left(\frac{\gamma t}{\lambda\varepsilon}\right), \tag{6.6}$$

where the right hand side is known, and $t_0 = 0.60$. A similar treatment may be made for $\Omega_1^2(\varepsilon)$. In this manner the two dashed curves were obtained for $\bar{\nu}_1(E)$ and $\Omega_1(E)$ in Fig. 10. By means of (6.4) and (6.5) may be found the resulting effects on signal size, $\overline{N}_i$, and on signal fluctuation, $\overline{\Delta N_i^2}$. However, the fluctuation Ω_1 is so large that the distribution in ν_1 must differ considerably from a Gaussian. The quantities $\bar{\nu}_1$ and Ω_1 are then less relevant than the most probable value of ν_1, the width at half peak height, and the shape of the tail in the probability distribution. In a recent note (Lindhard and Nielsen (1962)) the latter quantities are obtained by a method much simpler than the above one.

Ionization by α-recoils.

The recoil nucleus in α-decay is a very heavy particle with an energy of only 100—200 keV. In this case $\bar{\eta}_1(E) \ll E$, and a conspicuous effect should be observed in the number of ion pairs, according to (6.4). Detailed measurements have been made by B. Madsen (1945), for Po, ThC and ThC′ α-recoils. In argon containing about 5 percent air, Madsen observed the average number of ion pairs, $\overline{N}_i$, and also the width of the distributions.

The corresponding coded computations of $\bar{\nu}_1(E)$ and $\Omega_1^2(E)$ for a heavy recoil particle in pure argon have been performed. The three recoil nuclei have practically the same atomic number, and differ only in energy. The resulting behaviour of $\bar{\eta}_1(E)/W_\beta$ is shown by the full-drawn curve in Fig. 11. In the figure is also shown the result, if power law scattering with $s = 2$ is assumed, as indicated by the dashed line. The three experimental points of Madsen are his values for $\overline{N}_i$, assuming $W_\alpha = W_\beta = 26.4$ eV, the energy per ion pair in pure argon. The points lie below the solid curve and, in view of the uncertainties, the agreement must be said to be satisfactory. From Madsen's curves the mean square relative fluctuation, $\overline{\Delta N_i^2}/\overline{N}_i^2$, may be estimated roughly. It is of order of $\overline{\Delta N_i^2}/\overline{N}_i^2 \sim 0.02$. This is considerably

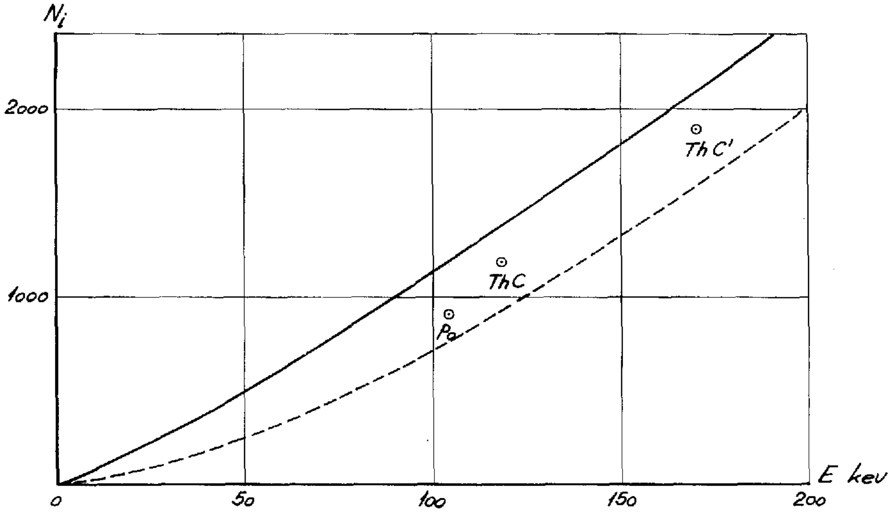

Fig. 11. Comparison with three α-recoil measurements by B. Madsen. Solid curve is $\bar{\eta}_1(E)/W_\beta$ computed numerically. Dashed curve corresponds to the power law approximation (6.3). Comparison assumes $W_\alpha = W_\beta$, but magnitude of this constant is not important.

larger than the numerically computed average square straggling, $\Omega_1^2/\bar{\eta}_1^2 \sim 0.002$, but in approximate agreement with (6.3), i.e. $s = 2$. The latter is possibly fortuitous, and further measurements in the region of extremely low velocities are desirable.

Ionization by fission fragments.

As a third example we may consider the ionization by fission fragments in various gases. The question of the ionization efficiency of fission fragments was studied experimentally by Schmitt and Leachman (1956), cf. also Utterback and Miller (1959). Schmitt and Leachman observed the variation of the number of ions, $\bar{N}_i$, with fragment energy in several gases. It turned out that $\bar{N}_i$ was not quite proportional to the energy of the fragment. They therefore considered the difference between E and the energy $E_\alpha = W_\alpha \cdot \bar{N}_i(E)$, where $W_\alpha \approx W_\beta$ is the energy per ion pair for natural α-particles. This difference, $\Delta = E - W_\alpha \bar{N}_i$, was called the ionization defect. Now, if (6.4) holds very accurately, and if $W_\alpha = W_\beta$, it is apparent that Δ becomes equal to the present function $\bar{\nu}_1(E)$. However, since the observed Δ's are only some 5 percent of E, and since in some cases already W_α can deviate from W_β by several percent, it is abundantly clear that a comparison between Δ and $\bar{\nu}_1$ is only qualitative, as long as the excitation and ionization cross sections for fission fragments have not been studied in detail.

The coded computations of $\bar{\nu}_1$ and Ω_1^2 were carried through for fission fragments in a number of substances, taking one representative of the median light group ($Z_1 = 39$, $A_1 = 94.7$, $E_{\text{initial}} = 98.9$ MeV), and one representative of the median heavy group ($Z_1 = 53$, $A_1 = 138.8$, $E_{\text{initial}} = 66.9$ MeV). Several results of this kind are given in a recent paper (LINDHARD and THOMSEN (1962)). Results are quoted in Table 1 for the two groups of fission fragments with initial velocities in Ne and A, as compared with the observations of Δ by SCHMITT and LEACHMAN. There is quantitative agreement, and more could hardly be expected. It is seen that $\bar{\nu}_1$ is systematically smaller than Δ, which is not surprising since the value to be used for W may be greater than W_α.

TABLE 1

	Ne		*A*	
	Δ (*MeV*)	$\bar{\nu}_1$ (*MeV*)	Δ (*MeV*)	$\bar{\nu}_1$ (*MeV*)
Heavy group	4.8 ± 0.7	2.5	5.5 ± 0.5	3.1
Light group	4.3 ± 1.0	1.6	5.1 ± 0.8	2.0

Fluctuations have not been studied experimentally. As examples of the numerical computations it may be mentioned that for the heavy fission fragment group with initial velocities in Ne and A the values of $\Omega_1/\bar{\nu}_1$ are 0.066 and 0.097, respectively.

In an interesting theoretical treatment of the ionization yields of fission fragments KNIPP and LING (1951) have used a differential-integral equation for the average ionization of similar type as (E) in the present paper. Moreover, they introduced the description by ionization defect Δ employed by SCHMITT and LEACHMAN. The estimates of atomic collision cross sections by KNIPP and LING were necessarily somewhat uncertain. They considered the case of fission fragments in argon. For argon in argon their maximum ionization defect Δ was 780 keV, while our upper bound on $\bar{\nu}_1$ in region II (cf. p. 31) gives 600 keV for argon in argon. For the two fission groups in argon their estimates of Δ are also somewhat larger than our values of $\bar{\nu}_1$. KNIPP and LING made use of the connection to MADSEN's measurements.

Production of lattice defects.

In the present context mention should be made of the damage produced in a crystal lattice by irradiation. A general survey of radiation damage in solids is given by BILLINGTON and CRAWFORD (1961). Consider a solid composed of one element only. We may let φ represent e.g. the number of vacancies N_v produced by a particle with $Z_1 = Z_2$. The discussion below applies just as well for the production of other lattice defects. In first approximation N_v should be proportional to the energy given to atomic motion, ν. The average value of N_v is therefore expected to obey an equation similar to (6.4)

$$\overline{N}_v = \frac{\overline{\nu}(E)}{U_v}, \tag{6.7}$$

where U_v may be regarded as an empirical constant. The relation (6.7) probably affords a more direct experimental check of the present results for $\overline{\nu}$ and $\overline{\eta}$ than does equ. (6.4). The reason is that in most cases $\overline{\nu} \ll E$ and $\overline{\eta} \approx E$, as in the ionization efficiency of fission fragments.

U_v can also be estimated theoretically from (2.5), i. e. approximation (B^{-1}), valid at low energies where no energy ends up in electronic motion. Having derived a constant U_v at such low energies, we have also justified the use of (6.7) at higher particle energies.

Several estimates have been made of the connection between U_v and atomic binding (Snyder and Neufeld (1955, 1956) and others, cf. Seitz and Koehler (1956), Billington and Crawford (1961)). It has become customary to use hard sphere ion-atom scattering, i.e. $d\sigma_n =$ const. dT. Our present cross sections in § 1 are much more forward peaked and lead to a higher value of the ratio between U_v and atomic binding.

The fluctuation in N_v, $\overline{(\Delta N_v)^2}$, has a contribution from the fluctuation in ν. We find analogously to (6.5), $\overline{(\Delta N_v)^2_\nu} = \Omega^2(E)/U_v^2$. The magnitude of the relative fluctuation in N_v may be read off directly from the curves in Fig. 7, for $Z_1 = Z_2$.

In approximation (B^{-1}), and with hard sphere ion-atom scattering, Leibfried (1958) has derived a fluctuation in N_v, $\overline{(\Delta N_v)^2_L} = 0.15\,\overline{N}_v$, analogous to the Fano ionization fluctuations. Already at quite low energies the fluctuation of Leibfried is completely overshadowed by the present fluctuations.

The above relations, together with our previous computations of $\overline{\nu}(E)$ and $\Omega^2(E)$, cover the question of $\overline{N}_v$ and its fluctuation for $Z_1 = Z_2$. If $Z_1 \neq Z_2$ some cases are represented by the examples in this section, and others by Lindhard and Thomsen (1962). An interesting further example is the damage produced by neutrons, where the production spectrum of recoils by neutrons, times $\overline{\nu}(E)$ from § 5, may be integrated to give the production of lattice defects.

Finally, it should again be emphasized that (6.7) is an approximation. If necessary, more accurate treatments may be made. Thus, let us consider the behaviour of $\overline{N}_v(E)$ at high particle energies. Here, an increasing fraction of the energy transfers to atoms are so small in magnitude that lattice bindings need not be disrupted. In fact, the logarithmic increase of the right hand side of (5.3) for increasing ε is due to such small energy transfers. In the evaluation of $\overline{N}_v$ we may therefore at a sufficiently high energy replace $\log \varepsilon$ by a constant, but this does not result in a large correction.

In conclusion we wish to express our deep gratitude to all who have encouraged us and assisted in this work. Miss Susann Toldi has given untiring assistance in the preparation of the manuscript.

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Note added in proof. In a recently published article by Abroyan and Zborovskii (Soviet Physics Doklady, **7**, 417 (1962)) the ionization pulse by potassium ions in a germanium detector is measured at ion energies ~ 1 keV. The authors find that the ratio β between the pulse for K ions and for electrons with the same energy is $\beta = 0.032$, 0.071, 0.114 and 0.135, for $E = 0.5$, 1, 3 and 8 keV, respectively. Now β should be equal to $\overline{\eta}/E$, and the simplified theoretical formula (6.2) gives $(\overline{\eta}/E) = 0.051\, E^{1/2}$, where E is measured in keV. This is in excellent agreement with the experimental values of β. However, numerical estimates corresponding to (5.2) are nearly a factor of 2 higher. In view of the smallness of β the results are promising in any case.

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