Multiple Elastic Scattering and Radiation Damping. I*

H. EKSTEIN
Armour Research Foundation of Illinois Institute of Technology, Chicago, Illinois
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The problem of potential scattering by a number of similar scatterers is reformulated so that the potential is eliminated from the equations and replaced by a function which characterizes the scattering properties of the individual scatterer. The resulting equations can be used for the more general case where the single-scattering process is not describable by a potential, e.g., absorption or—to a certain extent—inelastic scattering. A solution of the equations by iteration is considered and compared with Born's approximation. As an application, the second approximation for the scattering of thermal neutron by a small crystal is calculated.

I. INTRODUCTION

MOST papers on multiple scattering deal with the case where the coherence between individual scattering processes can be disregarded. This is true either when the wavelength is small in comparison with the distance between scatterers or when the individual scattering is essentially incoherent. The subject of this paper is the opposite end of the range, where elastic scattering and wave interference are of prime importance.

Most problems involving scattering of an incident particle by a scatterer are complicated many-body problems, in which often not even the correct form of the hamiltonian is known. To describe elastic scattering, an "effective potential" is usually introduced which is chosen so that it gives the observed scattering amplitudes. For the study of multiple scattering, the effective potentials of the scatterers are introduced into the Schrödinger equation. This paper formulates the multiple-scattering problem so that it contains not the effective potential but the scattering properties of the individual scatterers. Once the problem of potential scattering is restated in terms of the scattering properties of the individual scatterers, it is plausible that the equations remain approximately correct if the individual scattering problem is not really a potential problem. This is similar to the idea underlying the S-matrix theory. But since in our problem the scatterers are held at fixed finite distances, the S-matrix alone does not give sufficient information about the scatterer; it is necessary to know its behavior when the stream of incident particles issues from a source at a finite distance rather than from infinity, as well as the scattered amplitude at finite distances.

Another reason for this investigation is that the solution of the multiple scattering problem is often simplified by eliminating the potential from the equations, even if the potential is definitely known.

Most calculating methods are based on the smallness of the interaction. If the scatterers are, for instance, nearly impenetrable objects, the potential is very large so that the usual approximation methods fail. However, the scattering cross section of a single scatterer may be small, so that the problem in its restated form may be solved by expansion in terms of the single-scatterer cross section. The case of point-scatterers has been the subject of extensive work, first in the classical dispersion theory, and later in Ewald's rigorous lattice theory. Goldberger and Seitz[1] treated the refraction and diffraction of slow neutrons by nuclei in an analogous way. Foldy[2] studied the case of random atomic positions of point scatterers. The present paper generalizes these results for scatterers of finite size.

In Part I the general equations are derived, and the solution by iteration is investigated and compared with Born's approximation. The two methods are shown to be complementary. The results are applied to the calculation of the second approximation of the intensity of a thermal neutron beam scattered by a small crystal.

In Part II, the propagation of waves in an infinite medium is treated. It is found that the effect of radiation damping on multiple scattering is different from that assumed in previous work; in particular, for an infinite crystal the individual scattering amplitudes must be corrected for the lack of radiation damping, since no particles are lost by scattering to infinity in an indefinitely extended medium.

II. SINGLE SCATTERING IN MOMENTUM REPRESENTATION

The general formalism of scattering in momentum representation has been presented by Møller.[3] For the simplest case of nonrelativistic scalar particles, the Schrödinger equation is

$$[(-\hbar^2/2m)\nabla^2+v-E]\psi=0, \tag{1}$$

with the additional requirement that the asymptotic form of the wave function be

$$\psi\sim e^{ikz}+F(\theta,\phi)e^{ikr}/r. \tag{2}$$

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[1] M. L. Goldberger and F. Seitz, Phys. Rev. **71**, 294 (1947).
[2] L. L. Foldy, Phys. Rev. **67**, 107 (1945).
[3] C. Møller, Kgl. Danske Videnskab. Selskab. Mat.-fys. Medd. **23**, No. 1 (1945); **22**, No. 19 (1946).

Let

$$u(\mathbf{k})=\frac{-2m}{\hbar^2(2\pi)^3}\int v(\mathbf{x})\exp(-i\mathbf{k}\cdot\mathbf{x})d\mathbf{x}, \quad (3)$$

$$f(\mathbf{k})=\frac{-2m}{\hbar^2(2\pi)^3}\int v\psi(\mathbf{x})\exp(-i\mathbf{k}\cdot\mathbf{x})d\mathbf{x}, \quad (4)$$

$$k_0^2=2m/\hbar^2=E. \quad (5)$$

Then the equivalent of Eqs. (1) and (2) is

$$f(\mathbf{k})-\int_h \frac{u(\mathbf{k}-\mathbf{k}')}{k'^2-k_0^2}f(\mathbf{k}')d\mathbf{k}'=u(\mathbf{k}-\mathbf{k}_0), \quad (6)$$

where $\mathbf{k}_0$ is the propagation vector of the incident wave. The symbol h (for hook-integral) below the integral sign has the following meaning: in polar coordinates k', θ', ϕ', the path of integration with respect to k' is to be indented at $k'=k_0$ and deviated into the lower half of the complex k' plane. Explicitly,

$$\int_h \frac{u(\mathbf{k}-\mathbf{k}')}{k'^2-k_0^2}f(\mathbf{k}')d\mathbf{k}'$$

$$=\frac{i\pi k_0}{2}\int_s u(\mathbf{k}-\mathbf{k}')f(\mathbf{k}')d\Omega+P\int\frac{u(\mathbf{k}-\mathbf{k}')}{k'^2-k_0^2}f(\mathbf{k}')d\mathbf{k}', \quad (7)$$

where the first integral or the right-hand side extends only over the sphere $\mathbf{k}'^2=k_0^2$ and P stands for the principal value of the second integral. The direct significance of $f(\mathbf{k})$ is given by

$$\psi_{sc}(\mathbf{r})\sim(2\pi^2/r)\exp(ik_0r)f(k_0\mathbf{r}/|r|), \quad (8)$$

which states that the asymptotic value of the scattered wave ψ_{sc} is proportional to the value of f at the point where the vector $\mathbf{r}$ intersects the sphere $\mathbf{k}^2=k_0^2$. To exhibit the meaning of Eq. (6) in coordinate space, it can be re-transformed, giving term by term

$$-\frac{2m}{\hbar^2}v\psi-\frac{(2m)^2}{4\pi\hbar^4}v\int\frac{\exp(ik_0r_{12})}{r_{12}}v(\mathbf{r}_2)\psi(\mathbf{r}_2)d\mathbf{r}_2$$

$$=-\frac{2m}{\hbar^2}v\exp(i\mathbf{k}_0\cdot\mathbf{r}), \quad (9)$$

i.e., the well-known integral equation of scattering,[4] multiplied by $(-2mv/\hbar^2)$.

When the potential has spherical symmetry, the introduction of polar coordinates k, θ, ϕ makes possible a separation of variables. With the usual notation, let

$$f(\mathbf{k})=\sum_l f_l(k)P_l(\cos\theta) \quad (10)$$

and one obtains the set of one-dimensional integral equations[5]

$$f_l(x)-2\pi\int_h\frac{y^2dy}{y^2-k_0^2}f_l(y)K_l(x,y)=\frac{2l+1}{2}K_l(x,k_0), \quad (11)$$

where

$$K_l(x,y)=\int_{-1}^{+1}P_l(t)u[(x^2+y^2-2xyt)^{\frac{1}{2}}]dt. \quad (12)$$

To exhibit the connection between the kernels K_l and the potential v, one can substitute the definition (3) for u, which reduces to

$$u(k)=\frac{1}{2\pi^2k}\int_0^\infty v(r)\sin krdr \quad (13)$$

and use the expansion theorem[6]

$$\frac{\sin r(x^2+y^2-2xyt)^{\frac{1}{2}}}{(x^2+y^2-2xyt)^{\frac{1}{2}}}=\pi\sum_0^\infty\frac{(m+\frac{1}{2})}{(xy)^{\frac{1}{2}}}J_{m+\frac{1}{2}}(rx)J_{m+\frac{1}{2}}(ry)P_m(t) \quad (14)$$

to obtain

$$K_l(x,y)=\frac{-m}{\pi\hbar^2(xy)^{\frac{1}{2}}}\int_0^\infty rv(r)J_{l+\frac{1}{2}}(rx)J_{l+\frac{1}{2}}(ry)dr. \quad (15)$$

It is possible to separate the influence of radiation damping as follows:[7] by the definition (7) of the symbol h, one can write instead of Eq. (11):

$$f_l(x)-2\pi P\int_0^\infty\frac{y^2dy}{y^2-k_0^2}f_l(y)K_l(x,y)$$

$$=K_l(x,k_0)\left[\frac{2l+1}{2}+i\pi^2k_0f_l(k_0)\right]. \quad (16)$$

Now consider the auxiliary equation

$$g_l(x)-2\pi P\int_0^\infty\frac{y^2dy}{y^2-k_0^2}g_l(y)K_l(x,y)=\frac{2l+1}{2}K_l(x,y), \quad (17)$$

which involves only real quantities; hence, g_l is real. Then,

$$f_l(x)=g_l(x)\left(1+\frac{2}{2l+1}i\pi^2k_0f_l(k_0)\right) \quad (18)$$

and in particular, for $x=k_0$

$$f_l(k_0)=\frac{g_l(k_0)}{1-i\pi^2k_0g_l(k_0)2/(2l+1)} \quad (19)$$

Equation (17) can be thought as having been derived

[4] N. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions* (Oxford University Press, London, 1949), p. 116.

[5] V. Fock, Z. Physik **98**, 145 (1935); M. Lévy, Proc. Roy. Soc. (London) **A204**, 145 (1950).

[6] G. N. Watson, *Bessel Functions* (Cambridge University Press, London, 1944), p. 366.

[7] H. Ekstein, Phys. Rev. **75**, 1322 (1949).

by separating a three-dimensional equation similar to Eq. (6) but containing the principal value instead of the hook-integral. This equation may be considered as describing a scattering problem in which radiation damping is absent. Equation (19) then is the degenerate one-dimensional form of Heitler's integral equation[8] which shows the influence of radiation damping on the actual solution.

The connection with the usual formula

$$\psi_{sc}(r)\sim\frac{\exp(ik_0r)}{2ik_0r}\sum P_l(\cos\theta)(2l+1)[\exp(2i\delta_l)-1] \quad (20)$$

is established by comparing with Eqs. (8), (10), and (18). One finds

$$f_l(k_0)=\frac{2l+1}{4\pi^2ik_0}[\exp(2i\delta_l)-1], \quad (21)$$

$$g_l(k_0)=\frac{2l+1}{2\pi^2k_0}\tan\delta_l. \quad (22)$$

$g_l(k_0)$ is unbounded, because the homogeneous equation corresponding to Eq. (17) may have solutions. This is understood by the observation that a system without radiation damping can have nonvanishing solutions without a source at infinity.

For the study of multiple scattering, we will have to consider the case where the source of incident particles is at a finite distance R. The solution of this problem is the Green's function $G(\mathbf{r},\mathbf{R})$ which satisfies the differential equation:

$$\left(\frac{-\hbar^2}{2m}\nabla^2+v-E\right)G(\mathbf{r},\mathbf{R})=\delta(\mathbf{r}-\mathbf{R}) \quad (23)$$

and if the required asymptotic form represents outgoing waves only, the integral equation

$$G(\mathbf{r},\mathbf{R})+\frac{2m}{4\pi\hbar^2}\int\frac{\exp[ik_0|\mathbf{r}-\mathbf{r}'|]}{|\mathbf{r}-\mathbf{r}'|}v(\mathbf{r}')G(\mathbf{r}',\mathbf{R})d\mathbf{r}'=-\frac{2m}{4\pi\hbar^2}\frac{\exp(ik_0|\mathbf{r}-\mathbf{R}|)}{|\mathbf{r}-\mathbf{R}|}. \quad (24)$$

For calculations in momentum representation, it is more convenient to use the solution of the related equation

$$\chi(\mathbf{r},\boldsymbol{\kappa})+\frac{2m}{4\pi\hbar^2}\int\frac{\exp(ik_0|\mathbf{r}-\mathbf{r}'|)}{|\mathbf{r}-\mathbf{r}'|}v(\mathbf{r}')\chi(\mathbf{r}',\boldsymbol{\kappa})d\mathbf{r}'=\exp(i\boldsymbol{\kappa}\cdot\mathbf{r}). \quad (25)$$

The connection between G and χ is established by noticing that

$$\int\frac{\exp(ik_0|\mathbf{r}-\mathbf{R}|)}{|\mathbf{r}-\mathbf{R}|}\exp(i\boldsymbol{\kappa}\cdot\mathbf{R})d\mathbf{R}=\exp(i\boldsymbol{\kappa}\cdot\mathbf{r})\frac{4\pi}{\kappa^2-k_0^2}. \quad (26)$$

Hence, by multiplying Eq. (24) by $\exp(i\boldsymbol{\kappa}\cdot\mathbf{R})$ and integrating with respect to the parameter $\mathbf{R}$, it is shown that

$$\chi(\mathbf{r},\boldsymbol{\kappa})=-\frac{\hbar^2(\kappa^2-k_0^2)}{2m}\int G(\mathbf{r},\mathbf{R})\exp(i\boldsymbol{\kappa}\cdot\mathbf{R})d\mathbf{R}. \quad (27)$$

If G is considered known, χ is also known. In momentum representation, we consider the equation

$$\alpha(\mathbf{k},\boldsymbol{\kappa})-\int_h\frac{u(\mathbf{k}-\mathbf{k}')}{k'^2-k_0^2}\alpha(\mathbf{k}',\boldsymbol{\kappa})d\mathbf{k}'=u(\mathbf{k}-\boldsymbol{\kappa}) \quad (28)$$

of which Eq. (6) is a special case. The transformation of Eq. (25) into momentum space (after multiplication by $(-2mv/\hbar^2)$) leads directly to Eq. (28) if

$$\alpha(\mathbf{k},\boldsymbol{\kappa})=\frac{-2m}{\hbar^2(2\pi)^3}\int v\chi(\mathbf{r},\boldsymbol{\kappa})\exp(-i\mathbf{k}\cdot\mathbf{r})d\mathbf{r}. \quad (29)$$

In the theory of multiple scattering (Part II) we will have to consider an analog of Eq. (28) from which radiation damping has been eliminated:

$$\beta(\mathbf{k},\boldsymbol{\kappa})-P\int\frac{u(\mathbf{k}-\mathbf{k}')\beta(\mathbf{k}',\boldsymbol{\kappa})}{k'^2-k_0^2}d\mathbf{k}'=u(\mathbf{k}-\boldsymbol{\kappa}). \quad (30)$$

If the potential has spherical symmetry, separation of variables is again possible, leading to the set of one-dimensional integral equations

$$\alpha_l(k)-2\pi\int_h^\infty\frac{y^2dy}{y^2-k_0^2}\alpha_l(y)K_l(k,y)=\frac{2l+1}{2}K_l(k,\kappa) \quad (31)$$

and

$$\beta_l(k)-2\pi P\int_0^\infty\frac{y^2dy}{y^2-k_0^2}\beta_l(y)K_l(k,y)=\frac{2l+1}{2}K_l(k,\kappa). \quad (32)$$

In the case where the wave function has several components, the scattering problem can be treated in a similar manner. In particular, for the scattering of electromagnetic waves by an object of dielectric constant $\epsilon(\mathbf{r})$ we have[9]

$$\mathbf{f}(\mathbf{k})+\mathbf{k}\times\mathbf{k}\times\int_h\frac{u(\mathbf{k}-\mathbf{k}')}{k'^2-k_0^2}\mathbf{f}(\mathbf{k}')d\mathbf{k}'=-\mathbf{k}\times\mathbf{k}\times\mathbf{E}_0u(\mathbf{k}-\mathbf{k}_0) \quad (33)$$

[8] W. Pauli, *Meson Theory of Nuclear Forces* (Interscience Publishers, Inc., New York, 1948), p. 45.

[9] H. Ekstein, Phys. Rev. **62**, 255 (1942).

analogous to Eq. (7). The asymptotic value of the scattered field is connected to $\mathbf{f}$ by

$$\mathbf{E}_{sc}\sim(1/r)\exp(ik_0r)2\pi^2\mathbf{f}(k_0\mathbf{r}/|\mathbf{r}|) \tag{34}$$

similar to Eq. (8). The potential u is defined by

$$u(\mathbf{k})=\frac{1}{(2\pi)^3}\int\frac{\epsilon-1}{\epsilon}\exp(-i\mathbf{k}\cdot\mathbf{r})d\mathbf{r} \tag{35}$$

similar to Eq. (3). In Eq. (33), $k_0^2=\omega^2/c^2$ and $\mathbf{E}_0$ is the field intensity of the incident wave. The variable $\mathbf{f}$ is connected to the polarization $\mathbf{P}$ by

$$\mathbf{f}=(2\pi)^{-3}\int\exp(-i\mathbf{k}\cdot\mathbf{r})\nabla\times\nabla\times\mathbf{P}dr. \tag{36}$$

Most of the results obtained for the scalar case can be generalized for the case of many components, but this paper will mainly be concerned with the scalar case.

III. MULTIPLE SCATTERING: GENERAL EQUATIONS

We consider N similar scatterers at positions $\mathbf{r}=\mathbf{r}_n$. The total potential V is

$$V=\sum_n^N v(\mathbf{r}-\mathbf{r}_n). \tag{37}$$

To obtain the generalization of Eq. (3) we form

$$\int\sum v(\mathbf{r}-\mathbf{r}_n)\exp(-i\mathbf{k}\cdot\mathbf{r})d\mathbf{r}$$
$$=\sum\exp(-i\mathbf{k}\cdot\mathbf{r}_n)\int v(\mathbf{r})\exp(-i\mathbf{k}\cdot\mathbf{r})d\mathbf{r}, \tag{38}$$

so that the quantity $U(\mathbf{k})$ to use instead of $u(\mathbf{k})$ for multiple scattering is

$$U=u\sum\exp(-i\mathbf{k}\cdot\mathbf{r}_n). \tag{39}$$

If we designate by $F(\mathbf{k})$ the equivalent of $f(\mathbf{k})$ in multiple scattering, Eq. (6) becomes

$$F(\mathbf{k})-\int_h\frac{d\mathbf{k}'}{k'^2-k_0^2}\sum\exp[-i\mathbf{r}_n\cdot(\mathbf{k}-\mathbf{k}')]u(\mathbf{k}-\mathbf{k}')F(\mathbf{k}')$$
$$=u(\mathbf{k}-\mathbf{k}_0)\sum\exp[-i\mathbf{r}_n\cdot(\mathbf{k}-\mathbf{k}_0)]. \tag{40}$$

We define a set of functions $F_n(\mathbf{k})$ by the equations

$$F_n(\mathbf{k})-\int_h\frac{d\mathbf{k}'}{k'^2-k_0^2}\exp[-i\mathbf{r}_n\cdot(\mathbf{k}-\mathbf{k}')]u(\mathbf{k}-\mathbf{k}')F(\mathbf{k}')$$
$$=u(\mathbf{k}-\mathbf{k}_0)\exp[-i\mathbf{r}_n\cdot(\mathbf{k}-\mathbf{k}_0)]. \tag{41}$$

By summing Eq. (41) with respect to n, one sees that

$$F=\sum_n^N F_n. \tag{42}$$

Substitution of Eq. (42) into the second term of (41) gives

$$F_n(\mathbf{k})-\int_h\frac{d\mathbf{k}'}{k'^2-k_0^2}\exp[-i\mathbf{r}_n\cdot(\mathbf{k}-\mathbf{k}')]u(\mathbf{k}-\mathbf{k}')F_n(\mathbf{k}')$$
$$=u(\mathbf{k}-\mathbf{k}_0)\exp[-i\mathbf{r}_n\cdot(\mathbf{k}-\mathbf{k}_0)]+\sum_{m\neq n}\int\frac{d\mathbf{k}'}{k'^2-k_0^2}$$
$$\times\exp[-i\mathbf{r}_n\cdot(\mathbf{k}-\mathbf{k}')]u(\mathbf{k}-\mathbf{k}')F_m(\mathbf{k}'). \tag{43}$$

If, for the moment, the quantities on the right-hand side are considered as known, Eq. (43) is an inhomogeneous integral equation which can be solved in terms of the function $\alpha(\mathbf{k},\boldsymbol{\kappa})$ as follows: Let

$$G_n=\exp(i\mathbf{r}_n\cdot\mathbf{k})F_n, \tag{44}$$

so that

$$G_n(\mathbf{k})-\int_h\frac{d\mathbf{k}'}{k'^2-k_0^2}u(\mathbf{k}-\mathbf{k}')G_n(\mathbf{k}')$$
$$=u(\mathbf{k}-\mathbf{k}_0)\exp(i\mathbf{r}_n\cdot\mathbf{k}_0)+\sum_{m\neq n}\int_h\frac{d\mathbf{k}'}{k'^2-k_0^2}$$
$$\times\exp[i(\mathbf{r}_n-\mathbf{r}_m)\cdot\mathbf{k}']u(\mathbf{k}-\mathbf{k}')G_m(\mathbf{k}'). \tag{45}$$

Let $G_n^{(m)}$ be defined as the formal solution of

$$G_n^{(m)}(\mathbf{k})-\int_h\frac{d\mathbf{k}'}{k'^2-k_0^2}u(\mathbf{k}-\mathbf{k}')G_n^{(m)}(\mathbf{k}')$$
$$=\int_h\frac{dk'}{k'^2-k_0^2}\exp[i(\mathbf{r}_n-\mathbf{r}_m)\cdot\mathbf{k}']u(\mathbf{k}-\mathbf{k}')G_m(\mathbf{k}') \tag{46}$$

and

$$G_n^{inc}-\int_h\frac{d\mathbf{k}'}{k'^2-k_0^2}u(\mathbf{k}-\mathbf{k}')G_n^{inc}(\mathbf{k}')$$
$$=u(\mathbf{k}-\mathbf{k}_0)\exp(i\mathbf{r}_n\cdot\mathbf{k}_0), \tag{47}$$

so that

$$G_n=\sum_m G_n^{(m)}+G_n^{inc}. \tag{48}$$

By multiplying Eq. (28) by

$$\frac{\exp[i(\mathbf{r}_n-\mathbf{r}_m)\cdot\boldsymbol{\kappa}]G_m(\boldsymbol{\kappa})}{\kappa^2-k_0^2} \tag{49}$$

and integrating with respect to the parameter $\boldsymbol{\kappa}$, one obtains

$$G_n^{(m)}(\mathbf{k})=\int_h\frac{d\boldsymbol{\kappa}}{\kappa^2-k_0^2}\exp[i(\mathbf{r}_n-\mathbf{r}_m)\cdot\boldsymbol{\kappa}]G_m(\boldsymbol{\kappa})\alpha(\mathbf{k},\boldsymbol{\kappa})d\boldsymbol{\kappa}, \tag{50}$$

so that

$$G_n(\mathbf{k})=\alpha(\mathbf{k},\mathbf{k}_0)\exp(i\mathbf{r}_n\cdot\mathbf{k}_0)$$
$$+\sum_{m\neq n}\int_h\frac{d\boldsymbol{\kappa}}{\boldsymbol{\kappa}^2-k_0^2}\exp[i(\mathbf{r}_n-\mathbf{r}_m)\cdot\boldsymbol{\kappa}]G_m(\boldsymbol{\kappa})\alpha(\mathbf{k},\boldsymbol{\kappa}) \tag{51}$$

or, returning to the original notation,

$$F_n(\mathbf{k})=\alpha(\mathbf{k},\mathbf{k}_0)\exp[-i\mathbf{r}_n(\mathbf{k}-\mathbf{k}_0)]$$
$$+\sum_{m\neq n}\int_h \frac{d\boldsymbol{\kappa}}{\kappa^2-k_0^2}\exp[-i\mathbf{r}_n(\mathbf{k}-\boldsymbol{\kappa})]\alpha(\mathbf{k},\boldsymbol{\kappa})F_n(\boldsymbol{\kappa}). \quad (52)$$

Equation (52) together with Eq. (42) is a restatement of the multiple scattering problem from which the original potential has been eliminated, and only the function α characterizing the properties of the individual scatterer has been left. It is now possible to drop the restriction to potential scattering and consider α as solution of a much more general problem. For instance, the original interaction hamiltonian may not be diagonal in coordinate representation, or it may be non-hermitian so that it describes particle absorption. Inelastic scattering processes may be described in part by this formalism, by considering all inelastically scattered particles as lost, so that the elastic phase δ_e becomes complex. Of course, the present equations do not account for the particles which have been inelastically scattered at least once. This generalization is clearly approximate also in another respect; every inelastic process changes the state of the scatterer, whereas in our formalism the scatterers have definite time-independent properties. One can assume that the present approximation will be adequate as long as only a small part of the scatterers has been excited. Clearly, the present approximation does not cover such cases as Compton-scattering, which is essentially inelastic.

From the viewpoint of mathematical convenience, if a definite potential is either known or assumed, Eq. (52) is useful when the potential is very large. One may think of impenetrable spheres or very deep potential holes where the large numerical values of U prevents the usual approximation methods, whereas $\alpha(\mathbf{k},\boldsymbol{\kappa})$ may be quite small.

To illustrate the physical meaning of Eq. (52), the equivalent of the preceding calculation in coordinate representation will be given.

If the potential is given by Eq. (37), the integral equation for scattering, multiplied by V is

$$V\psi+\frac{2m}{\hbar^2 4\pi}V\int\frac{\exp(ik_0r_{12})}{r_{12}}V(\mathbf{r}_2)\psi(\mathbf{r}_2)d\mathbf{r}_2=V\exp(i\mathbf{k}_0\cdot\mathbf{r}). \quad (53)$$

Let

$$V\psi=P \quad (54)$$

and define a set of functions $P_n=\psi(\mathbf{r})v(\mathbf{r}-\mathbf{r}_n)$:

$$P_n+\frac{2m}{4\pi\hbar^2}v(\mathbf{r}-\mathbf{r}_n)\int\frac{\exp(ik_0r_{12})}{r_{12}}P(\mathbf{r}_2)d\mathbf{r}_2$$
$$=v(\mathbf{r}-\mathbf{r}_n)\exp(i\mathbf{k}_0\cdot\mathbf{r}). \quad (55)$$

Summation with respect to n shows that

$$\sum_n P_n=P. \quad (56)$$

On the other hand, if Eq. (24) is multiplied by v and the notation

$$p(\mathbf{r},\mathbf{R})=v(\mathbf{r})G(\mathbf{r},\mathbf{R}) \quad (57)$$

is used, we have

$$p(\mathbf{r},\mathbf{R})+\frac{2m}{4\pi\hbar^2}v(\mathbf{r})\int\frac{\exp(ik_0r_{12})}{r_{12}}p(\mathbf{r}_2,\mathbf{R})d\mathbf{r}_2$$
$$=-\frac{2m}{4\pi\hbar^2}v(\mathbf{r})\frac{\exp(ik_0|(\mathbf{r}-\mathbf{R}|)}{|\mathbf{r}-\mathbf{R}|}. \quad (58)$$

By the procedure used in the preceding calculation in momentum space, one shows by comparison of Eqs. (55) and (58) that

$$P_n=\sum_{m\neq n}\int p(\mathbf{r}-\mathbf{r}_n,\mathbf{R})P_m(\mathbf{R}+\mathbf{r}_n)d\mathbf{R}+p(\mathbf{r}-\mathbf{r}_n,\mathbf{k}_0). \quad (59)$$

Here, $p(\mathbf{r},k_0)$ means the solution of Eq. (58) if the source is removed to infinity; i.e., $\exp(i\mathbf{k}_0\cdot\mathbf{r})$ is substituted for $1/|\mathbf{r}-\mathbf{R}|[\exp(ik_0|\mathbf{r}-\mathbf{R}|)]$. Equation (59) restates the multiple scattering problem in terms of $p(\mathbf{r},\mathbf{R})$ which is essentially the Green's function of the individual scattering problem. The meaning of Eq. (59) can be seen more clearly if, after summation over n, the original notation is used:

$$v(\mathbf{r}-\mathbf{r}_n)\psi(\mathbf{r})=v(\mathbf{r}-\mathbf{r}_n)\sum_{m\neq n}\int G(\mathbf{r}-\mathbf{r}_n,\mathbf{R})v(\mathbf{R}+\mathbf{r}_n-\mathbf{r}_m)$$
$$\times\psi(\mathbf{R}+\mathbf{r}_n)d\mathbf{R}+v(\mathbf{r}-\mathbf{r}_n)G(\mathbf{r}-\mathbf{r}_n,\mathbf{k}_0). \quad (60)$$

IV. SOLUTION BY ITERATION

The most obvious method for solving Eq. (52) is iteration. In the first approximation, we disregard all integrals on the right-hand side. In the second approximation, the values of F_n so obtained are substituted into the integrals and so forth. It is usually more convenient to consider this solution as a power series in terms of a parameter. For this purpose, let α_0 be a number representative of the order of magnitude of $\alpha(\mathbf{k},\boldsymbol{\kappa})$. For instance,

$$\alpha_0=\alpha(\mathbf{k}_0,\mathbf{k}_0) \quad (61)$$

or

$$\alpha_0=\left[(1/4\pi)\int\alpha^2(\mathbf{k},\mathbf{k}_0)d\Omega\right]^{\frac{1}{2}}, \quad (62)$$

where the integration extends over a sphere $k^2=k_0^2$. Then we can define a dimensionless function $\bar{\alpha}$ by

$$\alpha=\alpha_0\bar{\alpha}. \quad (63)$$

α_0 has the dimension of a length. If the solution of Eq.

(52) is written as a power series in α_0,

$$F_n=\sum_{l=1} \alpha_0{}^l F_n{}^{(l)}, \tag{64}$$

substitution into Eq. (52) and comparison of coefficients shows that

$$F_n{}^{(1)}=\bar{\alpha}(\mathbf{k}, \mathbf{k}_0) \exp[-i\mathbf{r}_n\cdot(\mathbf{k}-\mathbf{k}_0)] \tag{65}$$

and, for $l\neq 1$,

$$F_n{}^{(l)}=\sum_{m\neq n} \int_h \frac{d\boldsymbol{\kappa}}{\kappa^2-k_0{}^2} \exp[-i\mathbf{r}_n\cdot(\mathbf{k}-\boldsymbol{\kappa})]\bar{\alpha}(\mathbf{k}, \boldsymbol{\kappa})F_m{}^{(l-1)}. \tag{66}$$

In first approximation, we obtain after summation

$$F^{(1)}(\mathbf{k})=\bar{\alpha}(\mathbf{k}, \mathbf{k}_0) \sum \exp[-i\mathbf{r}_n(\mathbf{k}-\mathbf{k}_0)] \tag{67}$$

and, for the scattered wave, by Eq. (8)

$$\psi_{sc}\sim(2\pi^2/r) \exp(ik_0r)\alpha(k_0\mathbf{r}/r, \mathbf{k}_0) \sum\exp[-i\mathbf{r}_n\cdot(\mathbf{k}-\mathbf{k}_0)], \tag{68}$$

i.e., the sum of all waves scattered by the individual scatterers under the influence of the primary wave alone. This is, of course, what one has to expect in the first approximation. It is clear now that our expansion is just the usual expansion into primary, secondary, tertiary, etc., waves, which is usually made for infinitely small scatterers. The expansion (64) is not restricted in this respect. This expansion can be expected to be useful when the number of scattering units is small. Actually, it will be shown that its first term is, under certain practical conditions, sufficient even when N exceeds 10^{15}. However, for extended media other methods must be used which will be discussed in the second part of this paper.

The expansions (64, 65, 66) can be compared to Born's approximation, which is obtained by direct iteration of Eq. (40). Let us again define a parameter such that

$$u=u_0\bar{u}, \tag{69}$$

where $\bar{u}$ is dimensionless, and u_0 has the dimension of a length. For instance,

$$u_0=u(0). \tag{70}$$

We have then the expansion

$$F=\sum_{l=1} u_0{}^l F^{(l)} \tag{71}$$

and

$$F^{(1)}=\bar{u}(\mathbf{k}-\mathbf{k}_0) \sum \exp[-i\mathbf{r}_n(\mathbf{k}-\mathbf{k}_0)], \tag{72}$$

$$(l\neq 1) \quad F^{(l)}=\int_h \frac{d\mathbf{k}'}{k'^2-k_0{}^2} \sum \exp[-i\mathbf{r}_n\cdot(\mathbf{k}-\mathbf{k}')] \times\bar{u}(\mathbf{k}')F^{(l-1)}(\mathbf{k}'). \tag{73}$$

The convergence of the two series will depend on the value of the parameters α_0 and u_0, respectively, and on the rapidity of decrease of $\bar{\alpha}$ and $\bar{u}$, respectively, for large values of $\mathbf{k}'$. When the potential is very large, as for impenetrable spheres, u_0 is also very large, whereas α_0 may be quite small. To obtain an idea of the magnitude of α_0, let us consider the case of very small scatterers. If we use the definition (61), then, by Eqs. (28) and (6)

$$\alpha_0=\alpha(\mathbf{k}_0, \mathbf{k}_0)=f(\mathbf{k}_0) \tag{74}$$

and since for small scatterers only S-scattering is important,

$$f(\mathbf{k}_0)=f_0(k_0)=\frac{1}{4\pi^2ik_0}[\exp(2i\delta_0)-1] \tag{75}$$

by Eqs. (10) and (21). If, in addition, δ_0 is small, we have

$$\alpha_0\approx\frac{\delta_0}{2\pi^2k_0}, \tag{76}$$

so that α_0 is of the order of $(1/2\pi^2)$ times the scattering length. Thus, where the potential is large but the individual scattering length is small, the expansion (64–66) is preferable to the Born approximation.

To discuss the second element mentioned above, we may consider the extreme case where the scatterers are represented by delta-functions. Then, the second Born approximation diverges already for the single scatterer; it is easy to verify that this holds for $F^{(2)}$ in Eq. (73). However, Eq. (66) gives

$$F_n{}^{(2)}=\int_h \frac{d\boldsymbol{\kappa}}{\kappa^2-k_0{}^2}\bar{\alpha}(\boldsymbol{\kappa}, \mathbf{k}_0)\bar{\alpha}(\mathbf{k}, \boldsymbol{\kappa}) \exp[-i\mathbf{r}_n\cdot(\mathbf{k}-\boldsymbol{\kappa})] \times\sum_m \exp[-i\mathbf{r}_m\cdot(\boldsymbol{\kappa}-\mathbf{k}_0)]-\exp[-i\mathbf{r}_n(\mathbf{k}-\mathbf{k}_0)] \tag{77}$$

and by summation

$$F^{(2)}=\int_h \frac{d\boldsymbol{\kappa}}{\kappa^2-k_0{}^2}\bar{\alpha}(\boldsymbol{\kappa}, \mathbf{k}_0)\bar{\alpha}(\mathbf{k}, \boldsymbol{\kappa}) \times[S(\mathbf{k}-\boldsymbol{\kappa})S(\boldsymbol{\kappa}-\mathbf{k}_0)-S(\mathbf{k}-\mathbf{k}_0)], \tag{78}$$

where

$$S(\mathbf{k})=\sum_n \exp(-i\mathbf{r}_n\cdot\mathbf{k}). \tag{79}$$

This equation holds in general; if, in particular, the scatterer becomes vanishingly small, $\bar{\alpha}$ becomes a constant (equal to one, if α_0 is chosen as in Eqs. (61) or (62)). But $F^{(2)}$ still converges, because

$$S(\mathbf{k}-\boldsymbol{\kappa})S(\boldsymbol{\kappa}-\mathbf{k}_0)-S(\mathbf{k}-\mathbf{k}_0) =\sum_{m\neq n} \exp[-i\mathbf{r}_n(\mathbf{k}-\boldsymbol{\kappa})+i\mathbf{r}_m(\mathbf{k}_0-\boldsymbol{\kappa})] \tag{80}$$

has oscillating terms only. This oscillating behavior is sufficient to make the integral converge, as one can easily verify. The corresponding formula in Born's

approximation is

$$F^{(2)}=\int_h \frac{d\kappa}{\kappa^2-k_0^2}\bar{u}(\kappa-\mathbf{k}_0)\bar{u}(\mathbf{k}-\kappa)S(\mathbf{k}-\kappa)S(\kappa-\mathbf{k}_0), \quad (81)$$

which is divergent when $\bar{u}$ becomes a constant. We may conclude, in general, that the expansion (64–66) is preferable when the potential is large or the scatterers small.

On the other hand, one can see intuitively that in the case of largely overlapping scatterers the Born approximation will be preferable; in this case, the interaction of scatterers, disregarded in Eq. (67), is of major importance. Therefore, it would be probably impractical to subdivide the total potential into a sum of individual terms and proceed according to Eqs. (64–66) in the case of electron scattering by a small metal crystal. To illustrate the point by an extreme example: if the scattering by a small homogeneous body is to be calculated, one could arbitrarily subdivide the body into smaller homogeneous cubes, calculate their individual scattering amplitudes α and use the expansion (64), but this would clearly be impractical, even though the expansion finally may converge to the correct result.

Comparison of first approximation (67) with the first Born approximation (72) admits the following simple interpretation: given a number of scatterers with potential v, one defines an "effective potential" $\alpha(\mathbf{k}, \kappa)$ in momentum space, and proceeds by iteration of the scattering equation (40) [where $\alpha(\mathbf{k}, \mathbf{k}')$ has been substituted for $u(\mathbf{k}-\mathbf{k}')$]. In particular, for very small scatterers, the effective potential is the constant α_0. In the latter case, one can even define a potential in coordinate space which is a delta-function, whereas in general the transformation into coordinate space of an equation of the type (40) with $\alpha(\mathbf{k}, \mathbf{k}')$ substituted for $u(\mathbf{k}-\mathbf{k}')$ would lead to an integro-differential equation; in other words, the interaction matrix $\alpha(\mathbf{k}, \mathbf{k}')$ is no longer diagonal in coordinate representation.

For the case of slow neutron scattering by nuclei, the above interpretation is widely used in scattering calculations: when more than one kind of nucleus exists, one can make the obvious generalization and replace each nucleus by a delta-function with appropriate constant factor, essentially the scattering length.

However, this interpretation holds only for the first approximation; the higher terms are different, as shown for instance by comparison between Eqs. (78) and (81) (where $\bar{\alpha}$ is to be substituted for $\bar{u}$). A similar result was obtained by Breit[10] in connection with the scattering of a neutron by a bound proton: Fermi's replacement of the actual interaction by an effective delta-function is correct only if one uses Born's *first* approximation with the effective potentials.

However, a somewhat modified rule for the equivalent potential for small scatterers can be stated as follows:

[10] G. Breit, Phys. Rev. **71**, 215 (1947).

The integrand (78) consists of terms

$$\frac{1}{\kappa^2-k_0^2}\exp(-i\mathbf{r}_{mn}\cdot\kappa),$$

which contribute very little beyond a limit $|\kappa_m|\gg k_0$, $|\kappa_m|\gg 1/r_{mn}$, since the denominator has become almost constant, and a large number of periods of the oscillatory function cancel each other. Hence, the integral can be cut off at this limit. On the other hand, the constant term $S(\mathbf{k}-\mathbf{k}_0)$ contributes only N terms as against the first term in brackets which contributes N^2 terms. Thus, if the number of scatterers is not too small, the second term is negligible in the domain where all terms contribute about evenly. Therefore, $F^{(2)}$ can be written

$$F^{(2)}\approx\alpha_0^2\int_h^{|\kappa_m|}\frac{d\kappa}{\kappa^2-k_0^2}S(\mathbf{k}-\kappa)S(\kappa-k_0); \quad (82)$$

and this has the same form as Born's second approximation, with a cutoff $|\kappa_m|\gg k_0, 1/r_{mn}$. It can be shown similarly that the higher approximations can be written formally like terms of the Born approximation with a cutoff of the same order.

Thus we can formulate the following heuristic rule: replace the actual potential by the "effective potential" α_0 and proceed by Born's approximation, cutting off all integrals at some value $\kappa\gg 1/r_{nm}, k_0$. In many cases, as in the following application, the result is quite insensitive toward the exact point of cutoff.

V. SCATTERING OF THERMAL NEUTRONS BY SMALL CRYSTALS (SECOND APPROXIMATION)

The nuclear scattering of neutrons by crystals is well understood in the two extreme ranges of very small and very large crystals.[1,11] In addition, the theory of an infinitely extended plane-parallel plate of finite thickness has been adapted from the dynamical theory of x-rays.[1] No results for three-dimensional crystals of intermediate size are available. In this section, the preceding results will be used to calculate in second approximation the intensity scattered by a spherical crystal, for a special orientation of the primary ray with respect to the crystal.

Because of the small size of the nuclei, $\bar{\alpha}$ can be set equal to one. We shall consider a simple Bravais lattice; a generalization for a composite lattice would be obvious. The function $S(\mathbf{k})$ can be written

$$S=\sum c_n\exp(-i\mathbf{a}_n\cdot\mathbf{k}), \quad (83)$$

where $\mathbf{a}_n$ are the lattice vectors and c_n is unity inside, and zero outside the sphere of radius ρ. By Poisson's sum formula[12]

$$S=\sum_m s(\mathbf{k}-2\pi\mathbf{A}_m), \quad (84)$$

[11] G. C. Wick, Physik. Z. **38**, 403, 689 (1937).

[12] S. Bochner, *Vorlesungen über Fouriersche Integrale* (Leipzig, 1932), p. 203.

where $\mathbf{A}_m$ are the reciprocal lattice vectors, and s is the fourier transform of the function $c(\mathbf{r})$ which interpolates the discrete values c_n:

$$s(\mathbf{k})=(1/v)\int c(\mathbf{r})\exp(-i\mathbf{k}\cdot\mathbf{r})d\mathbf{r}$$

$$=(1/v)\int_0^\rho r^2\exp(-i\mathbf{k}\cdot\mathbf{r})drd\Omega$$

$$=\frac{4\pi}{k^3v}(\sin k\rho-k\rho\cos k\rho)=\frac{-4\pi}{vk}\frac{d}{dk}\left(\frac{\sin k\rho}{k}\right), \quad (85)$$

v being the volume of the unit cell.[13]

We consider the value of the second approximation for a direction close to the incident beam ($\mathbf{k}=\mathbf{k}_0+\mathbf{p}$) in the case when the crystal is exactly in reflecting position; i.e., one reciprocal lattice point satisfies the condition

$$(\mathbf{k}_0+2\pi\mathbf{A}_1)^2-k_0^2=0. \quad (86)$$

We have

$$S(\mathbf{k}-\boldsymbol{\kappa})=S(\mathbf{k}_0-\boldsymbol{\kappa})+\mathbf{p}\cdot\nabla S(\mathbf{k}_0-\boldsymbol{\kappa})$$
$$=\sum s(\mathbf{k}_0-\boldsymbol{\kappa}-2\pi\mathbf{A}_m)+\mathbf{p}\cdot\sum\nabla s(\mathbf{k}_0-\boldsymbol{\kappa}-2\pi\mathbf{A}_m). \quad (87)$$

In the integral (78) this is multiplied by $S(\boldsymbol{\kappa}-\mathbf{k}_0)=\sum s(\mathbf{k}_0-\boldsymbol{\kappa}-2\pi\mathbf{A}_m)$. Since the function s decreases rapidly from its maximum value at the origin, only the immediate neighborhood of those points $\boldsymbol{\kappa}$ will be of importance which make the argument of one of the terms vanish. But the gradient of s at that point vanishes by Eq. (85), so that the second term in (87) is negligible. Thus, the value of $F^{(2)}$ in the neighborhood of the forward direction is approximately constant, and we have

$$F^{(2)}=\int_h\frac{d\boldsymbol{\kappa}}{\kappa^2-k_0^2}[|S(\mathbf{k}-\boldsymbol{\kappa})|^2-S(0)]. \quad (88)$$

The range of values $|\mathbf{p}|$ for which $F^{(2)}$ is constant can be estimated by determining the point at which $s(k)$ begins to decrease noticeably from its peak value. By Eq. (85), the first zero is the first root of

$$\tan k\rho=k\rho.$$

Thus, Eq. (88) may be considered correct for a range of the order of $|\mathbf{p}|\rho\leq 2$.

We consider now $F^{(2)}$ for values of $\mathbf{k}$ close to the reflecting point, i.e., $\mathbf{k}=k_0+2\pi\mathbf{A}_1+\mathbf{p}$. From the geometry it can be seen that this case is symmetric to the previous one, so that Eq. (88) holds also for the neighborhood of the reflecting direction, and for the same range. Of the terms in the sum (84), only the two with $m=0$ and $m=1$ are important, because the corresponding reciprocal points are on the Laue sphere $\kappa^2=k_0^2$. All other contributions are much smaller, and we shall take them into account in a summary manner, by using the average value of $|S|^2$ over a cell of the reciprocal lattice, rather than the exact function. Since, by Eq. (83), S is periodic in momentum space, we can use Parseval's theorem to obtain

$$\langle|S|^2\rangle=v\int_{\text{cell}}|S|^2d\mathbf{k}=\sum|c_n|^2=N. \quad (89)$$

By inspection of Eq. (83) this can be seen to be also the value of $S(0)$, so that the contributions of the two terms in the integrand cancel for the more remote reciprocal lattice points. This example illustrates the general theory of the preceding section: we would have obtained the same result by cutting off the integral and disregarding the contributions of all points $\mathbf{A}_m$, $m\neq 0, 1$. However, the naive use of Born's approximation would have led to a divergent integral. It is true that taking into account the finite nuclear radius one would obtain a function $\bar{\alpha}$ decreasing asymptotically so that the integral would converge; but then, the Born approximation would be incorrect (in most cases far too large) although finite.

To evaluate the contribution of the two remaining reciprocal lattice points, we set

$$\mathbf{k}_0+2\pi\mathbf{A}_1=\boldsymbol{\kappa}_1, \quad (90)$$

and remember that the point $\boldsymbol{\kappa}=\boldsymbol{\kappa}_1$ is exactly on the Laue sphere. By Eq. (84)

$$|S(\mathbf{k}_0-\boldsymbol{\kappa})|^2=|s(\boldsymbol{\kappa}-\mathbf{k}_0)+s(\boldsymbol{\kappa}-\boldsymbol{\kappa}_1)|^2$$
$$\approx|s(\boldsymbol{\kappa}-\mathbf{k}_0)|^2+|s(\boldsymbol{\kappa}-\boldsymbol{\kappa}_1)|^2, \quad (91)$$

since, owing to the rapid decrease of s, the overlap is negligible. In carrying out the integration, the sphere $\kappa^2=k_0^2$ can be replaced by its tangent plane, because the range of s is small against the radius k_0. The two contributions to $|S|^2$ have spherical symmetry with respect to the two points $\mathbf{k}_0$ and $\boldsymbol{\kappa}_1$, respectively, which are both situated on the sphere. Hence, the principal value contributes nothing to the integral (88), and we are left with

$$F^{(2)}=\frac{\pi i}{2k_0}\int d\sigma[|s(\boldsymbol{\kappa}-\mathbf{k}_0)|^2+|s(\boldsymbol{\kappa}-\boldsymbol{\kappa}_1)|^2-S(0)], \quad (92)$$

the integral being extended over the sphere of radius k_0. In using the tangent plane approximation for the second term, we choose as new origin for a system of plane polar coordinates r, ϕ the point $\boldsymbol{\kappa}=\boldsymbol{\kappa}_1$, so that

$$\int d\sigma|s(\boldsymbol{\kappa}-\boldsymbol{\kappa}_1)|^2=2\pi\int_0^\infty rdrs^2(r)$$
$$=2\pi\left(\frac{4\pi}{v}\right)^2\int_0^\infty\frac{dr}{r}\left[\frac{d}{dr}\left(\frac{\sin\rho r}{r}\right)\right]^2. \quad (93)$$

[13] This is a simplified derivation of a result obtained previously by A. L. Patterson, Phys. Rev. **56**, 972 (1939), and H. Ekstein, Cahiers phys. **B**, 33 (1942).

This integral can be calculated by differentiation with respect to the parameter ρ, giving

$$\int d\sigma |s(\kappa-\kappa_1)^2 = 2\pi(4\pi/v)^2(\rho^4/4). \tag{94}$$

The first term gives obviously the same contribution, so that

$$F^{(2)} = 2i(2\pi^2/v)^2(\rho^4/k_0) - i2\pi^2 k_0 N. \tag{95}$$

The second term is entirely negligible; this illustrates the rule of the preceding section; we would have obtained the same result by merely cutting off and dropping the term $S(0)$.

The second approximation is here entirely due to radiation damping. As a consequence, the second term in the expansion of $|\psi_{sc}|^2$, proportional to $\alpha_0{}^3$, vanishes for real α_0, as one sees immediately by forming the square modulus of $\alpha_0 F^{(1)} + \alpha_0{}^2 F^{(2)}$. Therefore, it is necessary to calculate the third approximation $F^{(3)}$ in order to obtain the first nonvanishing correction to the scattered intensity.

For this calculation, we use the rule stated in Sec. IV to limit the integration to the neighborhood of the sphere $\kappa^2 = k_0{}^2$. We have

$$F^{(3)} = \int_h \frac{d\kappa}{\kappa^2 - k_0{}^2} S(\kappa_1 - \kappa) F^{(2)}(\kappa), \tag{96}$$

where we consider only the exact Laue reflecting direction. Again, we have only the contributions of the neighborhood of κ_1 and $\mathbf{k}_0$; and again, because of the symmetry with respect to the tangent plane of the Laue sphere, the principal value is negligible. According to the previous result, $F^{(2)}$ is approximately constant for a distance $r\rho \approx 2$ from either $\kappa = \kappa_1$ or $\mathbf{k}_0$. For this range, we can use the peak value

$$s(0) = 4\pi\rho^3/3v$$

to approximate S. Hence, by analogy to Eq. (92)

$$F^{(3)} \approx \frac{2\pi i}{2k_0} F^{(2)} \frac{4\pi}{v} \frac{\rho^3}{3} \int_0^{2/\rho} 2\pi r dr = -\frac{2^6\pi^7\rho^5}{k_0{}^2 v^3}, \tag{97}$$

the factor 2 being due to the contribution of the two lattice points. For the absolute square of the amplitude, the argument of the complex number α_0 is of importance. According to Eqs. (74) and (75), α_0 is, strictly speaking, never real, not even in the case of pure potential scattering, because of radiation damping, and even less when absorption is present. However, for small absorption and small phase δ_0, the imaginary part is small, of second order. In this case, according to Eqs. (64), (67), (95), and (97)

$$|F|^2 = \alpha_0{}^2 \frac{(4\pi)^2\rho^6}{9v^2} - \alpha_0{}^4 \frac{7\cdot 2^6\pi^8\rho^3}{9v^4 k_0{}^2}. \tag{98}$$

By introducing the number of atoms per cm^3

$$n = 1/v, \tag{99}$$

the scattering length

$$a = 2\pi^2\alpha_0, \tag{100}$$

and the wavelength

$$\lambda = 2\pi/k_0, \tag{101}$$

Eq. (98) simplifies:

$$|F|^2 = \left(\frac{2an\rho^3}{3\pi}\right)^2 [1 - (7/4)(an\lambda\rho)^2]. \tag{102}$$

In a typical case, $n = 3\times 10^{22}$, $\lambda = 1.5\times 10^{-8}$, $a = 10^{-12}$, with a particle diameter $2\rho = 10\mu$, the second term amounts only to 9 percent. Thus, the range of validity of the first approximation is larger than is frequently assumed in cautious estimates.[14] This fact is caused by the vanishing of the term proportional to $\alpha_0{}^3$. It is true that our calculation concerns only the intensity in exact Laue position, whereas for comparison with experiment an integration over all crystal orientations would be necessary. However, it is probable that the exact Laue orientation is the "worst" case with respect to the importance of higher order terms.

That the corrective term is negative is what one would expect: for sufficiently large crystals the intensity must become proportional to ρ^2 rather than to ρ^6. Hence, if the crystal is large enough so that the second term matters, the intensity must be smaller than if this term had been omitted.

[14] Fermi, Sturm, and Sachs, Phys. Rev. **71**, 589 (1947).