PHYSICAL REVIEW VOLUME 85, NUMBER 4 FEBRUARY 15, 1952

Multiple Scattering of Waves. II. The Effective Field in Dense Systems*

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(Received October 30, 1951)

The multiple scattering of waves interacting with a system of particles is treated by a self-consistent approach. Scattering processes are described by operators that permit anisotropy, absorption, and creation. The scattering system may be randomly, partially, or completely ordered.

The propagation constant k' of the coherent wave in the scatterer medium differs from the vacuum constant k by $(k')^2=k^2+4\pi ncf(\mathbf{k}', \mathbf{k}')$, where n is the scatterer density and f is an operator whose matrix elements $f(\mathbf{b}, \mathbf{a})$ represent the scattering amplitude in direction **b** for a wave incident in direction **a** on a single scatterer bound by the forces of its neighbors. The parameter c, defined by $cf(\mathbf{k}', \mathbf{k}')=\int \exp(-i\mathbf{k}'\cdot\mathbf{r})f \times\psi_e(\mathbf{r})d\mathbf{r}$, is a measure of the ratio of the effective field $\psi_e(\mathbf{r})$ to the average field.

An integral equation is found for $\psi_e(\mathbf{r})$ with the help of a "quasi-crystalline" approximation. A variational expression is then found for c that becomes exact for point scatterers.

A comparison is made of finite and infinite scattering systems. The extinction theorem is proven. The macroscopic viewpoint is found to be applicable to small systems whose size is large compared to the scatterer potential range, and the range of scatterer position correlations.

I. INTRODUCTION

EWALD[1] in 1916 developed a fairly complete theory of optical dispersion in crystals based on the multiple scattering of light by atoms acting as induced dipoles. Foldy[2] has applied a similar self-consistent scattering calculation to obtain the index of refraction for scalar waves travelling in a medium of randomly distributed, isotropic scatterers. The author[3] in 1949 generalized the self-consistent procedure to include (1) anisotropic scattering in addition to the monopole and dipole cases, (2) inelastic scattering, including the creation and absorption of particles, and (3) scattering systems that are randomly, partially, or completely ordered.

The results obtained by the self-consistent procedure were an equation for the total (coherent) wave in terms of the effective field with one particle held fixed, an equation for the effective field with one particle fixed in terms of the field with two particles fixed, etc. A solution of these equations by an iteration procedure using the incident wave as starting function would lead to an expansion in waves that were singly scattered, doubly scattered, triply scattered, etc. Such a procedure is poorly converging because it assumes that the effective field is similar to the incident wave, whereas it has the propagation constant of the total wave.

The author therefore suggested a procedure similar to that of Lorentz—assuming that the effective field (with one scatterer fixed) bears a simple relation to the total field—for point scatterers a proportionality constant is sufficient. In this way, the first of the set of equations described can be used to obtain an equation for the index of refraction. The succeeding equations must then be used to obtain the relationship between the effective and the coherent fields.

The equation obtained by the author for the index of refraction, containing as it does, the unknown relation between the effective and coherent fields has been criticized[4] as an "approximation." This is by no means the case. The determination of the effective field was merely considered to be a problem of sufficient intricacy to warrant separate discussion.

We intend to show in this paper that a good approximation can be obtained for the effective field by using the second in the set of equations mentioned. Additional accuracy can, of course, be obtained by using the third equation, and then higher order equations. We have decided to publish results at this point, using only two equations, because the accuracy involved is equivalent to the use of the Lorentz-Lorenz formula for nonpolar liquids. A detailed treatment of the electrostatic problem using a self-consistent procedure by Brown[5] indicates (in addition to the experimental evidence), that the corrections to the Lorentz-Lorenz formula in nonpolar liquids are small.

II. FORMULATION

In previous work[3] (see I-3.7 and I-3.8) it was shown that a self-consistent description of the total field $\psi(\mathbf{r}; \mathbf{1}, \mathbf{2}, \cdots \mathbf{N})$ and the effective field $\psi^j(\mathbf{r}; \mathbf{1}\cdots \mathbf{N})$ could be given by the equations

$$\psi(\mathbf{r})=\phi(\mathbf{r})+\textstyle\sum_s(E-H)^{-1}T(\mathbf{s})\psi^s(\mathbf{r}), \tag{2.1}$$

$$\psi^j(\mathbf{r})=\phi(\mathbf{r})+\textstyle\sum_{s\neq j}(E-H)^{-1}T(\mathbf{s})\psi^s(r), \tag{2.2}$$

where the symbols $\mathbf{1}, \mathbf{2}, \cdots \mathbf{i}, \mathbf{j}, \mathbf{s}\cdots \mathbf{N}$ refer to the positions of the scatterers (which are omitted for simplicity in ψ and ψ^j). The energy and Hamiltonian of the wave are E and H. The transition operator[6] $T(\mathbf{s})$

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[*] This work supported in part by the ONR.

[1] P. P. Ewald, Ann. Physik **49**, 1, 117 (1916).

[2] L. L. Foldy, Phys. Rev. **67**, 107 (1945).

[3] M. Lax, Phys. Rev. **77**, 756 (1950). For a detailed account see Revs. Modern Phys. **23**, October (1951) hereafter referred to as I.

[4] H. Ekstein, *Multiple Elastic Scattering and Radiation Damping II*, ONR report, Armour Research Foundation, Chicago; see also Phys. Rev. **83**, 721 (1951).

[5] W. F. Brown, J. Chem. Phys. **18**, 1193, 1206 (1950).

[6] For properties of the transition operator T see I or M. Lax, Phys. Rev. **78**, 306 (1950). A detailed discussion is given by B. A. Lippmann and J. Schwinger, Phys. Rev. **79**, 469 (1951).

describes the scattering produced when the wave interacts with a single scatterer at **s**. (Strictly speaking, the scatterer is not fixed at **s** but merely bound by the forces exerted by other particles in the system. This point will be established in paper III of this series.)

In principle, one should solve Eqs. (2.1) and (2.2) for a fixed set of scatterer positions and then average $\psi(\mathbf{r};\mathbf{1},\cdots\mathbf{N})$ against the quantum-mechanical distribution of scatterer positions. The resulting average $\langle\psi(\mathbf{r})\rangle$ will be the coherent wave. Such a procedure is analogous to the Born-Oppenheimer calculation of electron wave functions in molecules: the wave functions are calculated for fixed nuclear configurations; then the nuclei are allowed to move.

The solution of Eqs. (1) and (2) for an arbitrary, fixed set of scatterer positions is quite difficult unless one is willing to resort to iteration methods. Instead, we can follow Foldy's[2] procedure of averaging first and then solving. Using the methods of I-Secs. IV and V, the averages of (1) and (2) are:

$$\langle\psi(\mathbf{r})\rangle=(E-H)^{-1}\int n(\mathbf{s})d\mathbf{s}T(\mathbf{s})\langle\psi^s(\mathbf{r})\rangle_s, \tag{2.3}$$

$$\langle\psi^j(\mathbf{r})\rangle_j=(E-H)^{-1}\int n(\mathbf{j}\,|\,\mathbf{s})d\mathbf{s}T(\mathbf{s})\langle\psi^s(\mathbf{r})\rangle_{sj}, \tag{2.4}$$

$$\langle\psi^j(\mathbf{r})\rangle_{ji}=(E-H)^{-1}\int n(\mathbf{ji}\,|\,\mathbf{s})d\mathbf{s}T(\mathbf{s})\langle\psi^s(\mathbf{r})\rangle_{sji}. \tag{2.5}$$

Subscripts denote variables held fixed in a given averaging process. Particle variables have been suppressed when their presence is obvious. For example, $\langle\psi^s(\mathbf{r})\rangle_s$, the effective field holding particle s fixed, clearly depends on the position of that particle and should be written in full $\langle\psi^s(\mathbf{r};\,\mathbf{s})\rangle_s$.

The incident wave $\phi(\mathbf{r})$ has been omitted from Eqs. (3)–(5). This is permissible for infinite systems. A discussion of this point and of finite systems will be presented in Sec. VI. The density of scatterers at s is given by $n(\mathbf{s})$ if no information is available, by $n(\mathbf{j}\,|\,\mathbf{s})$ if a scatterer is known to be at **j**, and by $n(\mathbf{ji}\,|\,\mathbf{s})$ if scatterers are known to be at **j** and **i**. For a set of fixed scatterers, e.g., a crystal, these density functions are given by

$$n(\mathbf{s})=\sum\delta(\mathbf{s}-\mathbf{s}^0), \tag{2.6}$$

$$n(\mathbf{j}\,|\,\mathbf{s})=-\delta(\mathbf{s}-\mathbf{j})+\sum\delta(\mathbf{s}-\mathbf{s}^0), \tag{2.7}$$

and for a liquid they are averages of thes eexpressions with symbols to the left of the vertical bar held fixed. For a liquid $n(\mathbf{s})=n=$ a constant and

$$w(\mathbf{s})=n(0\,|\,\mathbf{s})/n \tag{2.8}$$

is the usual pair correlation function normalized to unity at large distances.

In the crystalline case, Eqs. (3) and (4) constitute a complete description of the problem since no additional information can be gained by holding additional particles fixed. Thus for any fixed set of scatterers, $\langle\psi^s\rangle_{sj}$ does not differ from $\langle\psi^s\rangle_s$ so that (4) involves only effective fields of a single type. Thus no approximations are required to treat the crystalline case.

In the case of a liquid or gas, the field on the right-hand side (RHS) of any equation has one more particle held fixed than the left-hand side (LHS). A suitable approximate procedure is then to take one such equation and modify the RHS by dropping an index on one field variable. The solution of this equation, with the help of the preceding equations in the series, can be used to determine the index of refraction. The accuracy of such a procedure will depend on the equation chosen. If the Nth equation were used, where all particles are held fixed, then no approximation is involved whatever.

III. THE INDEX OF REFRACTION

In this section, an equation for the index of refraction will be developed starting from (2.3) without the use of any approximations. Instead, we shall make use of the general properties of the transition operator and the various fields under displacements.

The operator $T(\mathbf{s})$ differs from the corresponding operator $T(0)$ for a scatterer at the origin by a displacement transformation of the usual form:

$$T(\mathbf{s})=\exp(-i\mathbf{p}\cdot\mathbf{s})T(0)\exp(i\mathbf{p}\cdot\mathbf{s}), \tag{3.1}$$

where $\mathbf{p}=-i\boldsymbol{\nabla}$ is the momentum operator in units $\hbar=1$. The corresponding statement in matrix rotation

$$T_{ba}(\mathbf{s})=\exp[i(\mathbf{a}-\mathbf{b})\cdot\mathbf{s}]T_{ba}(0) \tag{3.2}$$

was established in Eq. I-(3.4), where **a** and **b** are the initial and final propagation constants previously written $\mathbf{k}_a$ and $\mathbf{k}_b$.

In a manner similar to that used in deriving the properties of Bloch waves in crystals, it can be shown that $\psi(\mathbf{r};\mathbf{1},\cdots\mathbf{N})$ and $\psi^s(\mathbf{r};\mathbf{1},\cdots\mathbf{N})$ are multiplied by a factor $\exp(i\mathbf{k}'\cdot\mathbf{d})$ if all the variables $\mathbf{r}$, $\mathbf{1}$, $\cdots\mathbf{N}$ are subject to the same displacement **d**. For a liquid, **d** is an arbitrary displacement; for an ideal crystal, **d** is a lattice displacement. It follows from these general considerations that

$$\begin{aligned}\exp(i\mathbf{p}\cdot\mathbf{s})\langle\psi^s(\mathbf{r};\,\mathbf{s})\rangle_s&=\langle\psi^s(\mathbf{r}+\mathbf{s};\,\mathbf{s})\rangle_s\\&=\exp(i\mathbf{k}'\cdot\mathbf{s})\langle\psi^s(\mathbf{r};\,0)\rangle_s.\end{aligned} \tag{3.3}$$

The propagation constant k' is, as yet, unknown. The use of these translational properties, however, permits (2.3) to be rewritten in the simpler form:

$$\begin{aligned}\langle\psi(\mathbf{r})\rangle&=[E-H(\mathbf{p})]^{-1}DT(0)\psi_e(\mathbf{r}),\\D&=\int n(\mathbf{s})d\mathbf{s}\exp[i(\mathbf{k}'-\mathbf{p})\cdot\mathbf{s}],\end{aligned} \tag{3.4}$$

where we abbreviated the effective field $\langle\psi^s(\mathbf{r};\,0)\rangle_s$ by $\psi_e(\mathbf{r})$.

The matrix elements of D in the liquid case are then given by

$$D_{ba}=n\delta(\mathbf{b},\,\mathbf{a})\delta(\mathbf{k}',\,\mathbf{a}), \tag{3.7}$$

where $\delta(\mathbf{b}, \mathbf{a})$ is a Kronecker delta that equals unity when $\mathbf{b}=\mathbf{a}$, and zero otherwise. In the crystalline, use must be made of the periodic density (2.6) and

$$D_{ba}=n\delta(\mathbf{b}, \mathbf{a})\textstyle\sum_K \delta(\mathbf{k}'+\mathbf{K}, \mathbf{a})F(\mathbf{K})/Z, \tag{3.8}$$

where the $\mathbf{K}$ are the reciprocal lattice vectors, Z is the number of particles per unit cell, and $F(\mathbf{K})$ is the cell structure factor:

$$F(\mathbf{K})=\textstyle\sum_{j \text{ in cell}} \exp[i\mathbf{K}\cdot(\mathbf{j}-\mathbf{i})] \tag{3.9}$$

taken relative to a particular atom i in the cell. The average of $F(\mathbf{K})$ over the positions i in the cell is given by

$$\langle F(\mathbf{K})\rangle=|F(\mathbf{K})|^2/Z. \tag{3.10}$$

The total or coherent wave is given by

$$\psi(\mathbf{r})=\textstyle\sum_b \phi_b(\mathbf{r})(\phi_b(\mathbf{r}), \psi(\mathbf{r})), \tag{3.11}$$

where the $\phi_b(r)=\exp(i\mathbf{b}\cdot\mathbf{r})$ constitute a set of plane waves normalized in a box of unit volume. For the liquid and crystalline cases, respectively, we obtain:

$$\langle\psi(\mathbf{r})\rangle=[E-H(\mathbf{k}')]^{-1}U(\mathbf{k}', \mathbf{k}') \exp(i\mathbf{k}'\cdot\mathbf{r}), \tag{3.12}$$

$$\psi(\mathbf{r})=\sum_K \frac{U(\mathbf{k}'+\mathbf{K}, \mathbf{k}')}{E-H(\mathbf{k}'+\mathbf{K})}\left|\frac{F(\mathbf{K})}{Z}\right|^2 e^{i(\mathbf{k}'+\mathbf{K})\cdot\mathbf{r}}, \tag{3.13}$$

where

$$U(\mathbf{b}, \mathbf{k}')=n(\phi_b(\mathbf{r}), T(0)\psi_e(\mathbf{r})). \tag{3.14}$$

In the crystalline case, no averaging symbol should be used since no average has been taken.

Thus we have established that for the liquid, the coherent wave is a plane wave, and in the crystal a plane wave plus plane waves in all the possible Bragg reflection directions. In fact, (3.13) has the Bloch form of a plane wave $\exp(i\mathbf{k}'\cdot\mathbf{r})$ times a function with the crystal periodicity. If the periodic factor is replaced by its space average, i.e., $\mathbf{K}=0$ part, we obtain the macroscopically observable part of the solution. Since $F(0)=Z$, the macroscopic average of (3.13) is identical in form to (3.12). Therefore, the macroscopic average coherent field can for both the crystalline and liquid cases be denoted, without ambiguity, by the same symbol $\langle\psi(\mathbf{r})\rangle$. In both cases, then, $\langle\psi(\mathbf{r})\rangle$ is obtained by replacing $n(\mathbf{s})$ by a constant in (3.4).

Since Eqs. (2.3)–(2.6) are homogeneous, the normalization of $\langle\psi(\mathbf{r})\rangle$ can be chosen at our convenience to be:

$$\langle\psi(\mathbf{r})\rangle=\exp(i\mathbf{k}'\cdot\mathbf{r}) \tag{3.15}$$

for both liquid and crystalline cases. With this choice of normalization the index of refraction in both cases is given by

$$H(\mathbf{k}')=E-U(\mathbf{k}', \mathbf{k}'). \tag{3.16}$$

If in (3.14) the effective field $\psi_e(\mathbf{r})$ is replaced by the plane wave $\langle\psi(\mathbf{r})\rangle$, then we obtain $U(\mathbf{k}', \mathbf{k}')=nT_{k'k'}$ and the elementary result that the index of refraction is determined by the forward scattered amplitude. Deviations from this result depend on the extent to which the effective field differs from the macroscopic average field and can be referred to as effective field corrections. The author has previously suggested[3] that these corrections be taken into account by using the formula:

$$H(\mathbf{k}')=E-ncT_{k'k'}, \tag{3.17}$$

where c is a measure of the ratio of the effective field $\psi_e(\mathbf{r})$ to the average field $\langle\psi(\mathbf{r})\rangle$.

For point isotropic scatterers, the matrix element $U(k', k')$ depends only on the value of $\psi_e(\mathbf{r})$ at the origin, so that c can be interpreted as $\psi_e(0)/\langle\psi(0)\rangle$. For point dipole scatterers $c=\nabla\psi_e(0)/\nabla\langle\psi(0)\rangle$. For non-point scatterers, the matrix (3.14) depends on the properties of $\psi_e(\mathbf{r})$ over a region. The correctly weighted ratio of effective to average fields is in all cases $c=U(\mathbf{k}', \mathbf{k}')/(nT_{k'k'})$ or:

$$c=(\phi_{\mathbf{k}'}, T\psi_e)/(\phi_{\mathbf{k}'}, T\langle\psi\rangle). \tag{3.18}$$

For Schrödinger type waves, $E=(\hbar k)^2/(2m)$ and $H(k')=(\hbar k')^2/(2m)$, so that (3.17) can be rewritten in the form:

$$(k')^2=k^2+4\pi ncf(\mathbf{k}', \mathbf{k}'), \tag{3.19}$$

where $f(\mathbf{b}, \mathbf{a})$ is the scattering amplitude in direction $\mathbf{b}$ for a wave $\mathbf{a}$ incident on a bound single scatterer. The scattering amplitude operator is proportional to the transition operator and may be defined by:[3]

$$f=-2\pi mT/h^2. \tag{3.20}$$

IV. THE QUASI-CRYSTALLINE APPROXIMATION

In the preceding section, the calculation of the index of refraction was reduced to a determination of the effective field, using only (2.3) and the translation properties of the fields. With the help of the translational requirement

$$\langle\psi^s(\mathbf{r}+\mathbf{s}; \mathbf{s}, \mathbf{j})\rangle_{js}=\exp(i\mathbf{k}'\cdot\mathbf{s})\langle\psi^s(\mathbf{r}; 0, \mathbf{j}-\mathbf{s})\rangle_{sj} \tag{4.1}$$

the effective field according to (2.4) is given by:

$$\psi_e(\mathbf{r})=\int n(\mathbf{j}|\mathbf{s}) \exp[i(\mathbf{k}'-\mathbf{p})\cdot(\mathbf{s}-\mathbf{j})] \times(E-H)^{-1}T(0)\langle\psi^s(\mathbf{r}; 0, \mathbf{j}-\mathbf{s})\rangle_{js}d\mathbf{s}. \tag{4.2}$$

This result has again been obtained without making approximations. And $\langle\psi^s\rangle_{sj}$ should be investigated with the help of (2.5). In this way, each effective field can be expressed in terms of an effective field with one more particle held fixed. The accuracy of the result depends on how many of the Eqs. (2.3), (2.4), (2.5), etc. are used.

An iteration procedure, applied to (2.2), is equivalent to choosing for $\psi_e(\mathbf{r})$ a plane wave $\exp(i\mathbf{k}\cdot\mathbf{r})$ with the vacuum propagation constant k, and then inserting this result into the formula (3.14) for the index of refraction. A double iteration procedure is approximately equivalent to replacing $\langle\psi^s\rangle_{sj}$ by $\exp(i\mathbf{k}\cdot\mathbf{r})$, inserting this result into (4.2) and then inserting the resulting $\psi_e(\mathbf{r})$ into (3.14). Such a procedure is essentially an expansion in powers of the scattering amplitude.

Instead, we shall suggest an approximation:

$$\langle\psi^s(\mathbf{r};\mathbf{s},\mathbf{j})\rangle_{sj}\simeq\langle\psi^s(\mathbf{r};\mathbf{s})\rangle_s \tag{4.3}$$

that is (1) at least as good as the double iteration procedure, (2) is not strictly an expansion in powers of the scattering amplitude, and (3) is most accurate for dense systems where multiple scattering corrections are most important.

Equation (4.3) may be referred to as the quasi-crystalline approximation since it is strictly valid in the crystalline case. This approximation is tacitly made in many treatments of homogeneous media,[7,8] since the notation used does not distinguish between various types of effective fields. The quasi-crystalline assumption is equivalent to the neglect of the fluctuation of the effective field as $\mathbf{s}$ due to a deviation of particle j from its average position. The success of this assumption is based on the approximate validity of the cellular model for liquids. Certainly further investigation of this assumption is necessary. Because of their usefulness, however, we shall present here the results obtained by a multiple scattering treatment using the quasi-crystalline approximation.

The assumption (4.3) is equivalent to neglecting the difference between $\langle\psi^s(\mathbf{r};0,\mathbf{j}-\mathbf{s})\rangle_{sj}$ and the effective field $\psi_e(\mathbf{r})$. If $n(\mathbf{j}|\mathbf{s})$ is written in the form:

$$n(\mathbf{j}|\mathbf{s})=n+n(0|\mathbf{s}-\mathbf{j})-n, \tag{4.4}$$

the effective field is found to obey the integral equation:

$$\psi_e(\mathbf{r})=\langle\psi(\mathbf{r})\rangle+(E-H)^{-1}GT(0)\psi_e(\mathbf{r}), \tag{4.5}$$

where

$$G(\mathbf{p}-\mathbf{k}')=\int[n(0|\mathbf{r})-n]\exp[i(\mathbf{k}'-\mathbf{p})\cdot\mathbf{r}]d\mathbf{r}. \tag{4.6}$$

Equations (4.5) and (4.6) are strictly valid for crystals providing the pair correlation function is interpreted in agreement with (2.7).

For a crystal, (4.5) and (2.7) can readily be combined to verify that the effective field $\psi_e(\mathbf{r})$ is equal to the total field (3.13) minus the field emitted by the scatterer at the origin. For a liquid (4.5) may be interpreted as saying that the effective field differs from the total field by the scattering produced by the hole $n-n(0|\mathbf{r})$ left by the scatterer whose center is at $\mathbf{r}=0$.

In the limiting case of point scatterers in a liquid, the hole $n-n(0|\mathbf{r})$ approaches zero and it is very tempting to say that G approaches zero so that according to (4.5) the effective field can be represented accurately by the average field $\exp(i\mathbf{k}'\cdot\mathbf{r})$. That this is not generally the case follows from a consideration of the case of scattering of electromagnetic waves by induced dipoles. There, the effective field correction factor $(\epsilon+2)/3$ arises precisely because the field within a hole, no matter how small, differs from the field in the external medium.

It is therefore necessary to investigate the solution of (4.5) for each particular problem and make approximations, if necessary, in the solution but not in the kernel of the integral equation. For present purposes, we are not interested in a complete evaluation of the effective field but merely in the matrix element

$$U(\mathbf{k}',\mathbf{k}')=n(\varphi,T\psi_e).$$

In order to obtain a variation expression for $U(\mathbf{k}',\mathbf{k}')$, methods were developed for integral equations in which neither the kernel $L=(E-H)^{-1}G$ nor the perturbing operator $V=T(0)$ were Hermitian.[6] With an appropriate transcription of notation, the variational expression for U_{ba} is given by:

$$U_{ba}=\frac{n({}^1\psi_e{}^b,T(0)\phi_a)(\phi_b,T(0)\psi_e{}^a)}{({}^1\psi_e{}^b,[T(0)-T(0)(E-H)^{-1}GT(0)]\psi_e{}^a)}, \tag{4.7}$$

where $\psi_e{}^a$ is the effective field when the average field is $\exp(i\mathbf{a}\cdot\mathbf{r})$. The fields ${}^1\psi_e(\mathbf{r})$ are solutions[6] of an equation adjoint to (4.5). If the guess

$${}^1\psi_e{}^{k'}(\mathbf{r})\simeq\psi_e{}^{k'}(\mathbf{r})\simeq c\exp(i\mathbf{k}'\cdot\mathbf{r}) \tag{4.8}$$

is inserted into (4.7), the diagonal matrix element of U is given by:

$$\begin{gathered}U(\mathbf{k}',\mathbf{k}')\simeq nT_{k'k'}(1-J)^{-1},\\ J=(T_{k'k'})^{-1}\textstyle\sum_b T_{k'b}(E-E_b)^{-1}G(\mathbf{b}-\mathbf{k}')T_{bk'}.\end{gathered} \tag{4.9}$$

One of the advantages of the variational method (4.7) is that U is insensitive to the choice of c. For point scatterers, therefore, (4.9) is exact. The integral Eq. (4.5), in fact, reduces for point scatterers to a linear equation for the constant c. For scatterers that are small but not point scatterers, (4.9) should be quite accurate.

The ratio of the effective field to the average field (3.18), can be written according to (4.9) and (3.20) in terms of scattering amplitudes:

$$\begin{gathered}c=(1-J)^{-1},\\ J=\int\frac{f(k',b)f(b,k')}{f(k',k')}\,\frac{G(\mathbf{b}-\mathbf{k}')}{b^2-k^2}\,\frac{d\mathbf{b}}{2\pi^2}.\end{gathered} \tag{4.10}$$

V. BOUNDARY CONDITIONS AT INFINITY

In scattering problems it is customary to introduce a boundary condition that describes radiation travelling outward at infinity. This boundary condition is included in our formalism provided we understand the operator $(E-H)^{-1}$ everywhere to mean[9]

$$(E-H)^{-1}=P(E-H)^{-1}-i\pi\delta(E-H) \tag{5.1}$$

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[7] M. Born, *Optik* (Julius Springer, Berlin, 1933), p. 313 ff.

[8] L. Rosenfeld, *Theory of Electrons* (North-Holland Publishing Company, Amsterdam, 1951), Chapter VI.

[9] P. A. M. Dirac, *Principles of Quantum Mechanics* (Oxford University Press, London, 1947), third edition, Section 50; see also reference 6.

where P stands for the principle valued reciprocal. The transition operator T for a single scatterer with potential V is in fact the solution of the equation

$$T=V+V(E-H)^{-1}T, \tag{5.2}$$

with the above boundary condition. Because of this condition the operator T is nonhermitian and $T_{k'k'}$ is complex. Thus, if we would neglect the correction factor c, the index of refraction would have an imaginary part determined by the imaginary part of the forward scattered amplitude—i.e., by the total cross section, scattering plus absorption.[6]

Ekstein[4] has recently suggested that for an infinite system, the radiation condition should be replaced by a standing wave condition, i.e., that $(E-H)^{-1}$ be interpreted as the principal valued reciprocal. This is equivalent to replacing T of (5.2) by a new operator K satisfying

$$K=V+VP(E-H)^{-1}K. \tag{5.3}$$

If no true absorption is present, V is Hermitian, and because of (5.3) K is Hermitian.

Since no explicit use has been made in our paper of the radiation condition (5.1), all of our equations can be applied with either boundary condition. An examination of (4.7) and (4.9), assuming T is Hermitian (i.e., replaced by K) and using principal-valued reciprocals, demonstrates that under these circumstances the diagonal matrix elements of U are real. Thus Ekstein's boundary condition is equivalent to asserting that when no true absorption is present, the index of refraction for an infinite system is real.

Let us now examine the consequences of the usual radiation condition (5.1). For this purpose we need to evaluate the diagonal matrix element of U. A slight generalization of the cross-section theorem[6] to Eq. (4.5) leads to the relation:

$$\begin{aligned}\mathrm{Im}U_{aa}=&\,\mathrm{Im}(\psi_e^a, T\psi_e^a)\\ &-\pi \textstyle\sum_b G_{ba}|(\phi_b, T\psi_e^a)|^2\delta(E_b-E_a).\end{aligned} \tag{5.4}$$

To understand this result, introduce the approximation (4.8) valid for point scatterers and rearrange terms:

$$\begin{aligned}\mathrm{Im}U_{aa}=&\,|c|^2[\mathrm{Im}T_{aa}+\pi \textstyle\sum_b |T_{ba}|^2\delta(E_b-E_a)]\\ &-\pi|c|^2 \textstyle\sum_b[1+G(\mathbf{b}-\mathbf{a})]|T_{ba}|^2\delta(E_b-E_a).\end{aligned}$$

Multiplication of (5.5) by $-2/\hbar$ converts each term into a transition probability. The term in $\mathrm{Im}T_{aa}$ is the total transition probability for the single scattering problem (aside from the factor $|c|^2$). The second terms in $|T_{ab}|^2$ is the negative of the transition probability for scattering. The sum of these two terms is then the absorption probability. The term in $(1+G_{ba})$ is the transition probability for scattering modified by the position correlation between a given atom and its neighbors. In short, the second line is what is usually referred to as the fluctuation scattering. Both lines are corrected by a factor $|c|^2$ signifying the enhancement of the scattering power due to the effective field correction.

If the transition probability is divided by the incident flux $\mathrm{Re}(\hbar k')/m$ to obtain cross sections, (5.5) can be written in the form:

$$4\pi\,\mathrm{Im}(fc)/\mathrm{Re}(k')=|c|^2(\sigma_{\mathrm{abs}}+\sigma_{\mathrm{fl}}), \tag{5.6}$$

where σ_{abs} in the total cross section for true absorption, and σ_{fl} is the total scattering cross section due to density fluctuations:

$$\sigma_{\mathrm{fl}}=\int d\sigma_{\mathrm{sc}}(1+G_{ba}). \tag{5.7}$$

Here f is an abbreviation for the forward scattered amplitude $f(\mathbf{k}', \mathbf{k}')$. The imaginary part of the index of refraction determined by (3.19) and (5.6) is found to produce an attenuation in agreement with that predicted by a direct calculation of the fluctuation scattering[3] I-(6.20).

Thus the use of the radiation boundary condition has led to the physically reasonable result that even in the absence of true absorption the coherent beam will attenuate at a rate determined by scattering due to density fluctuations in the medium. For a gas, these fluctuations are large, $G_{ba}\simeq 0$, and the fluctuation cross section is essentially equal to the scattering cross section. Thus the attenuation for a gas is determined by the total cross section corrected by the factor $|c|^2$. For the liquid and solid states, fluctuations are greatly reduced, since the density fluctuation is proportional to the compressibility I-(1.14). Thus G is negative, the fluctuation cross section is small, and the attenuation will be more nearly determined by the absorption cross section. In any case, to a good approximation, the attenuation constant is given by

$$\tau=n|c|^2(\sigma_{\mathrm{abs}}+\sigma_{\mathrm{fl}}). \tag{5.8}$$

VI. FINITE SCATTERING SYSTEMS

Some question has been raised by Ekstein[2] as to the proper manner of treating infinite scattering systems. In this paper, the questionable procedure has been adopted of omitting the incident wave in setting up the self-consistent Eqs. (2.3)–(2.5) for an infinite system. It seems necessary, therefore, to investigate the index of refraction for a finite scattering system and compare the result with the previous calculation for an infinite system. An important by-product of this investigation will be an answer to the question: how small can a system be and still obey the "macroscopic" coherent wave equation for an infinite system. This question is of some interest in view of the recent application of a macroscopic viewpoint to describe diffraction of high energy neutrons by nuclei.[10]

Equation (2.3) can be modified to describe finite systems by adding the incident wave $\phi(\mathbf{r})$ and limiting the integration over $\mathbf{s}$ to a region bounded by the surface S. Rewriting these results in the space representation

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[10] Fernbach, Serber, and Taylor, Phys. Rev. **75**, 1352 (1949).

with the help of (3.1) and (3.20), (2.3) takes the form:

$$\langle\psi(\mathbf{r})\rangle=\phi(\mathbf{r})+\int d\mathbf{r}'\int_S n(\mathbf{s})G(\mathbf{s})\chi(\mathbf{s})d\mathbf{s}, \tag{6.1}$$

$$\begin{aligned}\chi(\mathbf{s})&=f\langle\psi^s(\mathbf{r}'+\mathbf{s};\,\mathbf{s})\rangle_s;\\ G(\mathbf{s})&=[\exp(ik|\mathbf{r}-\mathbf{r}'-\mathbf{s}|)/|\mathbf{r}-\mathbf{r}'-\mathbf{s}|].\end{aligned} \tag{6.2}$$

Equation (6.1) describes the macroscopic average field in the crystalline as well as liquid cases provided $n(\mathbf{s})$ is regarded as a constant in both cases. Outside the surface S, $\langle\psi(\mathbf{r})\rangle$, like $\phi(\mathbf{r})$, is a solution of the homogeneous unperturbed wave equation since all the "sources" are within S. (More precisely, these sources are within S plus a thin boundary layer whose thickness depends on the spatial extent of the operator f. For point scatterers, this layer vanishes.)

Inside the surface S, the field $\langle\psi(\mathbf{r})\rangle$ will not be a plane wave because of diffraction effects. If the concept of a medium is to be at all applicable, the average field must be representable as a sum of plane waves of various orientations and propagation constant k':

$$\langle\psi(\mathbf{r})\rangle=\sum M(\mathbf{k}')\exp(i\mathbf{k}'\cdot\mathbf{r}). \tag{6.3}$$

The translational consideration (3.3) must now be replaced by the more general condition

$$\langle\psi^s(\mathbf{r}'+\mathbf{s};\,\mathbf{s})\rangle_s=\sum M(\mathbf{k}')\exp(i\mathbf{k}'\cdot\mathbf{s})\psi_e(\mathbf{k}',\mathbf{r}), \tag{6.4}$$

where $\psi_e(\mathbf{k}',\mathbf{r})$ is the effective field for an average field in direction $\mathbf{k}'$. Since the operator f does not act on s, $\chi(\mathbf{s})$ is a solution of the medium wave equation. With the help of the replacement

$$\chi(\mathbf{s})=-(k')^{-2}\nabla_s^2\chi(\mathbf{s}), \tag{6.5}$$

and Green's second identity, the volume integral in (6.1) can be written as the usual integral over all space plus a correction term in the form of a surface integral:

$$\begin{aligned}\int G(\mathbf{s})\chi(\mathbf{s})d\mathbf{s}&=4\pi[(k')^2-k^2]^{-1}[\chi(\mathbf{r}-\mathbf{r}')-I],\\ I&=\int[\chi(\mathbf{s})(\partial G/\partial n)-G(\partial\chi/\partial n)]dS,\end{aligned} \tag{6.6}$$

where the derivatives are outward normal to the surface S.

With the help of (6.3) and (6.4) we may verify that

$$\int\chi(\mathbf{r}-\mathbf{r}')d\mathbf{r}'=\langle\psi(\mathbf{r})\rangle g, \tag{6.7}$$

$$g=\int\exp(-i\mathbf{k}'\cdot\mathbf{r}')f\psi_e(\mathbf{k}',\mathbf{r}')d\mathbf{r}'. \tag{6.8}$$

Finally the average field can be written in the form:

$$\begin{aligned}\langle\psi(\mathbf{r})\rangle=4\pi ng[(k')^2-k^2]^{-1}\langle\psi(\mathbf{r})\rangle+\phi(\mathbf{r})\\ -n\int dS[(\partial G(\mathbf{s})/\partial n)\int d\mathbf{r}'f\langle\psi^s(\mathbf{r}'+\mathbf{s};\,\mathbf{s})\rangle_s\\ -G(\mathbf{s})\int d\mathbf{r}'(\partial/\partial n)f\langle\psi^s(\mathbf{r}'+\mathbf{s};\,\mathbf{s})\rangle_s].\end{aligned} \tag{6.9}$$

The surface integral may be interpreted as the field due to a set of sources on the surface (or in a thin layer) whose field within the region is like $\phi(\mathbf{r})$ a solution of the unperturbed wave equation. The only way (6.9) can be satisfied inside the system is for the surface term to cancel the incident wave and for

$$(k')^2=k^2+4\pi ng. \tag{6.10}$$

The first statement constitutes the "extinction" theorem: the unperturbed incident wave is extinguished within the medium by waves induced at the boundary of the system. This theorem justifies the procedure adopted earlier in the paper of omitting the incident wave and neglecting boundary effects.

The second statement is equivalent to the validity of the previous index of refraction formula (3.19), since g is formally equivalent to $cf(\mathbf{k}',\mathbf{k}')$. The only question to be investigated is whether the effective field entering into the definition of g is the same as the one previously used for an infinite system.

Applying to (2.4), for the effective field, a procedure similar to the above calculation of the average field, we obtain:

$$\langle\psi^j(\mathbf{r};\,\mathbf{j})\rangle_j=\phi(\mathbf{r})+\int d\mathbf{r}'\int_S n(\mathbf{j}|\mathbf{s})G(\mathbf{s})\chi(\mathbf{s})d\mathbf{s}, \tag{6.11}$$

where we have made of the quasi-crystalline approximation (4.3). Writing $n(\mathbf{j}|\mathbf{s})=n+n(\mathbf{j}|\mathbf{s})-n$ and using (6.1) the effective field obeys the equation

$$\langle\psi^j(\mathbf{r};\,\mathbf{j})\rangle_j=\langle\psi(\mathbf{r})\rangle+\int d\mathbf{r}'\int_S[n(\mathbf{j}|\mathbf{s})-n]G(\mathbf{s})\chi(\mathbf{s})d\mathbf{s}. \tag{6.12}$$

This equation would reduce to the previous Eq. (4.5) for the effective field provided the integral over $\mathbf{s}$ could be extended over all space. However $n(\mathbf{j}|\mathbf{s})-n$ vanishes quite rapidly for large $|\mathbf{s}-\mathbf{j}|$. Thus if the region of integration is large compared to the region of importance of the correlation density $n(\mathbf{j}|\mathbf{s})-n$, the "macroscopic" index of refraction will be valid. For liquid type systems, this condition is easily satisfied, since it merely requires that the system be large in size compared to the interparticle separation. Nonideal, vibrating lattices obey a similar restriction. Ideal lattices require further investigation of the convergence involved in the sum implied by (6.12). Convergence can certainly be secured in the ideal case by using a system large compared to the wavelength as well as the interparticle separation. This wavelength condition is sufficient, but probably not necessary.

Another restriction on the use of a macroscopic viewpoint is that the region should be large compared to the boundary layer associated with the surface S because of the finite range of the scatterer potentials.

A third restriction on the above discussion has been the use of a constant density. This restriction can be removed by introducing an index of refraction that varies with position because of density changes. Such a procedure can be useful, for example, in treating a nucleus as a system, since for this case the density is not completely uniform.

When the restrictions mentioned above are met, the continuity of $\langle\psi(\mathbf{r})\rangle$ and its gradient in (6.1) across the surface S justifies the usual procedure of finding an external solution and an internal solution, and matching them at the boundary.

VII. NEUTRON SCATTERING IN LIQUIDS AND CRYSTALS

The results of the preceding sections can be applied to neutron scattering in the low energy range by replacing the operator f_{op} by $f\delta(\mathbf{q})$ where f is the bound scattered amplitude for scattering of neutrons by the nucleus in question [see Eq. (3.20)]. This is equivalent to replacing the matrix $f(\mathbf{b},\mathbf{a})$ by the constant amplitude f. Thus the usual index of refraction formula (3.19) is applicable with $c=(1-J)^{-1}$ where J according to (4.10) can be written as:

$$J=f\int(b^2-k^2)^{-1}G(\mathbf{b}-\mathbf{k}')d\mathbf{b}/(2\pi^2),\qquad(7.1)$$

with $G(\mathbf{p}-\mathbf{k}')$ given by (4.6). Utilizing the radiation condition

$$(k^2-b^2)^{-1}=P(k'-b^2)^{-1}-i\pi\delta(k^2-b^2),\qquad(7.2)$$

we have

$$J=-f[A+ik(1-E)],\qquad(7.3)$$

where

$$A=P\int(k^2-b^2)^{-1}G(\mathbf{b}-\mathbf{k}')d\mathbf{b}/(2\pi^2)\qquad(7.4)$$

$$=n\int r^{-1}\cos kr[1-w(\mathbf{r})]\cos(\mathbf{k}'\cdot\mathbf{r})d\mathbf{r},\qquad(7.5)$$

and

$$E=1+\int G(\mathbf{b}-\mathbf{k}')d\Omega_b/4\pi\qquad(7.6)$$

$$=\int d\Omega_b/4\pi\left\{1+n\int e^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{r}}[w(\mathbf{r})-1]d\mathbf{r}\right\}.\qquad(7.7)$$

The index of refraction Eq. (3.19) can now be written in the form:

$$(k')^2=k^2+4\pi n|c|^2[f-ik|f|^2+A^*|f|^2+ik|f|^2E^*].\qquad(7.8)$$

If we neglect the fact that k' may have a small imaginary part, A and E will be real. E can be recognized as the ratio by which the effective scattering cross section is modified by interference due to correlation of scatterer pairs. In the long wavelength limit, E can be interpreted as proportional to the mean square fluctuation in number of particles [I-(6.23) and I-(1H4)]:

$$E(0)=\langle(\Delta N)^2\rangle/\langle N\rangle=-n(kT)(\partial\ln V/\partial P)_T.\qquad(7.9)$$

Thus E is equal to the relative compressibility of the liquid or solid to a perfect gas at the same pressure and temperature. In other words, the fluctuation scattering is small in a liquid or solid (vanishing in an ideal nonvibrating crystal) and the imaginary part of $(k')^2$ is determined by $\mathrm{Im}(f-ik|f|^2)$, which vanishes unless true absorption is present.[4]

The long wavelength approximation for A is:

$$A(0)=n\int[1-w(\mathbf{r})]d\mathbf{r}/r.\qquad(7.10)$$

The rigid sphere model (valid at low densities) indicates that $A(0)=2\pi na^2$. In other words, $A(0)$ is of order a^{-1} and its effect as a correction is of order f/a, the ratio of scattering amplitude to size of scatterer. For neutron scattering, where only the nucleus is effective but a is of atomic size, $f/a\sim10^{-4}$.

A detailed evaluation of E in the short wavelength limit has been given by Placzek, Nijboer, and van Hove,[11] in the approximation $\mathbf{k}'\simeq\mathbf{k}$. The average of E over all orientations of $\mathbf{k}$ has been denoted in their paper by σ_{tot}. and $1+G(\mathbf{k}-\mathbf{b})$ is designated $\sigma(\mathbf{h})$ where $\mathbf{h}=(\mathbf{k}-\mathbf{b})/2\pi$. Their results may be summarized by:

$$\int Ed\Omega_k/4\pi=\sigma_{\mathrm{tot}}=1-(\lambda^2/8\pi)n^{\frac{2}{3}}I,\qquad(7.11)$$

where I is a pure number defined by

$$I=n^{-\frac{2}{3}}\int[1-\sigma(\mathbf{h})]d\mathbf{h}/h,\qquad(7.12)$$

when the integration is extended over a sphere in h space of radius $2/\lambda$. They approximate (8.12) by extending the integration over all $\mathbf{h}$ space, and then revert to ordinary space:

$$I\simeq n^{\frac{1}{3}}\int[1-w(\mathbf{r})]d\mathbf{r}/\pi r^2.\qquad(7.13)$$

They can establish (a) $I<3$, (b) for close-packing $I\simeq2.88$, (c) for rigid spheres of radius a, $I=4an^{\frac{1}{3}}K$, and $K=1-0.6488\gamma$ for $\gamma\ll1$, and $K\simeq0.64\gamma^{-\frac{1}{3}}$ for $\gamma\sim1$, where $\gamma=na^3/\sqrt{2}$ is a measure of the closeness of packing such that γ cannot exceed unity. Placzek *et al.*[11] give numerical results for I for ideal lattices and for vibrating lattices.

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[11] Placzek, Nijboer, and van Hove, Phys. Rev. **82**, 392 (1951).

For ideal lattices and arbitrary wavelength, A can be written in the form of a poorly converging series in reciprocal space:

$$-A=\lim_{r\to 0}\left[4\pi n\sum_{\mathbf{K}\neq 0}\frac{\cos(\mathbf{k}'-\mathbf{K})\cdot\mathbf{r}}{(\mathbf{k}'-\mathbf{K})^2-k^2}\left|\frac{F(\mathbf{K})}{Z}\right|^2-\frac{\cos kr}{r}\right]. \tag{7.14}$$

This may be converted into a sum of two rapidly converging series, one in ordinary space and one in reciprocal space with the help of the device originally introduced by Ewald:[1]

$$[(\mathbf{k}'-\mathbf{K})^2-k^2]^{-1}$$

$$=\int_0^\eta+\int_\eta^\infty \exp\{[k^2-(\mathbf{k}'-\mathbf{K})^2]t\}dt. \tag{7.15}$$

The resulting series are:

$$\begin{aligned}-A=4\pi n\sum_{\mathbf{K}\neq 0}&\frac{\exp\{[k^2-(\mathbf{k}'-\mathbf{K})^2]\eta\}}{(\mathbf{k}'-\mathbf{K})^2-k^2}\left|\frac{F(\mathbf{K})}{Z}\right|^2\\ &-4\pi n[(k')^2-k^2]^{-1}[1-\exp\eta(k^2-k'^2)]\\ &+\textstyle\sum_{j\neq 0}\cos(\mathbf{k}'\cdot\mathbf{j})G(k,\mathbf{j})\\ &+\lim_{r\to 0}[G(k,\mathbf{r})-r^{-1}],\end{aligned} \tag{7.16}$$

where

$$G(k,\mathbf{r})=\tfrac{1}{2}\pi^{-\frac{1}{2}}\int_0^\eta \exp[k^2t-r^2/(4t)]dt/t^{\frac{3}{2}}. \tag{7.17}$$

The sum over $\mathbf{j}$ is taken over all lattice points, except $\mathbf{j}=0$. For $j^2/\eta\gg 1$, $G(k,\mathbf{j})$ can be approximated by:

$$\begin{aligned}G(k,\mathbf{j})\simeq 2(\eta/\pi)^{\frac{1}{2}}\{1-[2\eta+(2k\eta)^2]/j^2\}\\ \times\exp[k^2\eta-j^2/(4\eta)].\end{aligned} \tag{7.18}$$

The $\mathbf{j}=0$ term requires special consideration:

$$\lim_{r\to 0}[G(k,r)-r^{-1}]$$

$$=-(\pi\eta)^{-\frac{1}{2}}+\tfrac{1}{2}\pi^{-\frac{1}{2}}\int_0^\eta[\exp(k^2t)-1]dt/t^{\frac{3}{2}}. \tag{7.19}$$

In the limiting case of long wavelengths, A reduces to the more familiar form:

$$\begin{aligned}-A(0)\simeq 4\pi n\sum_{\mathbf{K}\neq 0}|F(\mathbf{h})/Z|^2[\exp(-K^2\eta)/K^2]\\ +\sum_{j\neq 0}G(0,\mathbf{j})-4\pi n\eta-(\pi\eta)^{-\frac{1}{2}},\end{aligned} \tag{7.20}$$

$$rG(0,r)=(2/\sqrt{\pi})\int_x^\infty \exp(-u^2)du;\quad x=\tfrac{1}{2}r\eta^{-\frac{1}{2}}. \tag{7.21}$$

Rapidity of convergence can be secured for the two series by choosing, for example, $\eta=a^2/(4\pi)$, where a is a typical lattice constant. In any case A will have the order of magnitude of $(1/a)$ except in the immediate neighborhood of a Bragg reflection.

It should be emphasized that the scattering amplitude operator f has been defined in terms of the transition operator T by (3.20). And the transition operator is to be obtained by solving a one-body interaction problem: namely, a scattering problem in which the wave interacts with a single scatterer while the latter is subject to the forces of its neighbors—i.e., a scatterer that is neither completely bound nor completely free.

The one-body interaction problem was first considered by Fermi[12] in treating the scattering of neutrons by protons bound in a molecule. A more accurate treatment by Breit[13] using integral equation methods led to corrections of the order of 0.3 percent. A variational approach to the same problem by Lippmann and Schwinger[14] led to results in agreement with Breit. Fermi's result for elastic scattering can be written in the form [reference 14, Eq. (2.21)]:

$$T_{ba}=\int T_{ba}(\mathbf{s})p(\mathbf{s})d\mathbf{s}, \tag{7.22}$$

where $p(\mathbf{s})$ is the probability of finding the scatterer at position $\mathbf{s}$ in the molecule and $T_{ba}(\mathbf{s})$ is the transition operator for a free scatterer at $\mathbf{s}$. Of course f is still related to T by (3.20), but the free scattering length a obeys a similar relation with the neutron mass m replaced by the corresponding reduced mass μ relative to the scattering nucleus, so that $f=(am/\mu)$. Aside from this change in scattering amplitudes that does not affect T, the primary effect of the binding is taken into account by calculating the appropriate interference sum over the distribution of scatterer positions. This interference sum is automatically included in our original formulation (2.3)–(2.5).

The results of this section on the neutron index of refraction can therefore be understood to be correct in Fermi approximation if for f we use the scattering amplitude appropriate to bound scatterers. The small corrections obtained by Breit can be included if the scattering amplitude is modified to include the small effect of tightness of binding. The modified scattering amplitude $f(\mathbf{b},\mathbf{a})$ will, however, be slightly anisotropic, and a rigorous calculation, even for the neutron case, can be made only by returning to the general anisotropic formulas (3.19) and (4.10).

VIII. SUMMARY

In previous work[3] the author has treated the multiple scattering of waves by a system of particles using a self-consistent approach. In this treatment, the use of transition operators permitted the individual scattering

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[12] E. Fermi, Ricerca sci. **7**, Part 2, 13 (1936).

[13] G. Breit, Phys. Rev. **71**, 215 (1947); G. Breit and P. R. Zilsel, Phys. Rev. **71**, 232 (1947); Breit, Zilsel, and Darling, Phys. Rev. **72**, 576 (1947).

[14] B. H. Lippmann and J. Schwinger, Phys. Rev. **79**, 469 (1950).

processes to possess anisotropy and includes the possibility of absorption or creation of waves in a generalized scattering act. The scattering system was described by a quantum-mechanical distribution function in configuration space. The final results depended largely on the density of scatterers and the pair correlation density of scatterers. The treatment was sufficiently general to handle scattering systems that are randomly, partially, or completely ordered, i.e., gases, liquids, imperfect and ideal crystals.

One of the principal results of the self-consistent approach was an adequate definition of the coherent wave and a proof that the latter obeys a suitable wave equation, i.e., a proof that a distribution of scatterers can, for this purpose, be represented by a medium. Most calculations[7,8] proceed by assuming the existence of such a "medium" equation.

The propagation constant k' associated with the medium equation was found to differ from the corresponding vacuum constant k by

$$(k')^2=k^2+4\pi ncf(\mathbf{k}',\mathbf{k}'), \tag{8.1}$$

where n is the scatterer density and f is an operator whose matrix elements $f(\mathbf{b},\mathbf{a})$ represent the scattering amplitude with propagation vector $\mathbf{b}$ for a wave incident in direction $\mathbf{a}$ on a bound scatterer.

The parameter c is a measure of the ratio of the effective field $\psi_e(\mathbf{r})$ to the macroscopic average field $\langle\psi(\mathbf{r})\rangle$. For point isotropic scatters $c=\psi_e(0)/\langle\psi(0)\rangle$ and for point dipole scatterers, c is simply the ratio of gradients at the origin. In this paper, we have demonstrated that a valid general formula for c including finite scatterers is

$$c=\int \exp(-i\mathbf{k}'\cdot\mathbf{r})f\psi_e(\mathbf{r})d\mathbf{r}\bigg/\int \exp(-i\mathbf{k}'\cdot\mathbf{r})f\langle\psi(\mathbf{r})\rangle d\mathbf{r}. \tag{8.2}$$

Following the procedure described in *I*, a set of equations [(2.3)–(2.5)] were developed expressing the coherent field $\langle\psi(\mathbf{r})\rangle$ in terms of the effective field $\langle\psi^s(\mathbf{r})\rangle_s$ with one particle fixed, and the latter in terms of the effective field $\langle\psi^s(\mathbf{r})\rangle_{sj}$ with two particles fixed, etc. This infinite sequence of equations was broken by the quasi-crystalline approximation:

$$\langle\psi^s(\mathbf{r})\rangle_{sj}\simeq\langle\psi^s(\mathbf{r})\rangle_s. \tag{8.3}$$

An integral Eq. (4.5) was thus obtained for the effective field. This integral equation reduces to a linear equation for point scatterers. Using (4.5), a variational expression (4.10) [see also (8.2)] was developed for c, valid for finite scatterers and exact for point scatterers.

The preceding results were obtained using an infinite scattering system with the radiation boundary condition (5.1). The imaginary part of the index of refraction was found to lead to an attenuation constant (5.8) produced by the cross section for true absorption plus the cross section for fluctuation scattering, each enhanced by a factor $|c|^2$. This result is in exact agreement with a direct calculation of the attenuation I-(6.20).

In Sec. VI, a comparison was made between finite and infinite scattering systems. A general proof was given for the extinction theorem: the unperturbed incident wave is extinguished within the medium by waves induced at the boundary of the system.

An investigation was made of the validity of applying the macroscopic medium viewpoint to small scattering systems. This procedure was found applicable for systems whose size is large (1) compared to the range of the potential presented by a single scatterer to the wave and (2) compared to the distance over which correlations in scatterer positions are significant. (For ideal crystals, the last condition is too stringent.) These conditions can be relaxed somewhat by making direct use of (6.9) and (6.12).

In Sec. VII, applications are made to neutron scattering. It is emphasized that the scattering amplitudes to be used must be those of a scatterer bound by interaction with its neighbors. It is demonstrated (7.22) that the corrections used by Fermi are automatically included in this paper if $T(\mathbf{s})$ is the transition operator for a free scatterer. However, additional small corrections[13,14] must be included by making a small change in the operator $T(\mathbf{s})$. This point will be considered in more detail in a subsequent paper.