Scattering by Many-Body Systems in Terms of Two-Body Collision Parameters

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The scattering of a particle by a system of N particles is described without approximation by a set of equations not containing the interaction Hamiltonian, but an infinite set of two-body collision parameters which can be obtained from solving two-body problems. These equations, obtained with the assumption of two-body potential interaction between particles, can be applied to the case where the scattering particles are themselves complex systems, provided that the relevant two-body collision parameters are known or inferred from experiment. In the simplest case where the only relevant parameter is the scattering length, the first approximation is Fermi's result for the scattering of slow neutrons by protons. The "impulse approximation" is shown to be an approximate form of the present first approximation. It is shown that previous approximation schemes, in general, fail to give convergent higher approximations for the limiting case of point scatterers, whereas the present equations give convergent higher terms. It can be concluded that the latter are particularly appropriate for short-range interaction. The matrix α which contains all necessary two-body collision parameters is expressed in terms of solutions of the ordinary free two-body scattering problem. The result is applied to derive a revised theory of refraction and diffraction of slow neutrons in crystals by including the effect of zero-point motion of the nuclei and the electrostatic interaction between neutrons and electrons.

I. INTRODUCTION

THE usual starting point in treating the scattering of an incident particle by a system of many particles is the total Hamiltonian of the composite system. One assumes then that the solutions of the unperturbed scatterer are known and determines the effect of the incident particle by perturbation calculus.

If the particles composing the scatterer are not simple but complex systems in themselves, such as nuclei or atoms, this direct approach becomes not only prohibitively complicated but it is often barred by ignorance of the correct Hamiltonian as in the case of nuclei.

An alternative approach to the multiple scattering problem is used in classical dispersion theory and in Ewald's theory of electromagnetic lattice waves. The individual scatterers are represented by point-dipoles characterized by their polarizability. The total field is composed by individual wavelets, each of which is expressed in terms of the effective field, i.e., the field emitted by all other scatterers, evaluated at the location of one scatterer. The remarkable feature of this method is its ability to be generalized for the case where the individual scatterers are not simple dipoles but atoms or ions. One uses the results derived for the simple case by simply substituting the appropriate polarizability for the atoms; these may be either calculated or observed.

Another example of this approach is given by Fermi's calculation of scattering of slow neutrons by bound protons.[1] The equations describing the scattering is first approximated by an equation which does not contain the interaction potential but the scattering length. The result is then applied to the more general case of complex nuclei where the interaction cannot be described by a two-body potential. By simply substituting the empirical scattering length of the nucleus, a complex many-body problem becomes tractable.

These examples suggest that one could apply the same method to a wider field if it were possible to take the first step rigorously, i.e., to restate the scattering problem for a system of many simple particles in terms of two-body collision parameters rather than interaction potentials. Clearly, it will not be possible, in general, to characterize the scatterers by only one two-body collision parameter as in the two cases mentioned. One must be prepared to deal with an infinite set of two-body collision parameters replacing the interaction potential. One may hope that it will be possible to eliminate, in a given case, all but a few of these parameters as unessential.

This step was taken in a previous paper[2] for the case of static scattering centers. In the present paper the procedure is applied to the general case of a system of bound particles.

The transformation of the many-body Schrödinger equation into a set of equations which contain only two-body collision parameters is done without approximation; the solution, of course, is possible only by successive approximation.

While in the case of simple scattering particles the new equations are thus rigorously equivalent to the Schrödinger equation, the approximate solutions of the two equations are not identical. It is found that the equations presented here are particularly useful for scatterers with short-range interaction. This result is not surprising in view of the similar circumstance in the case of fixed scatterers studied previously.[2]

II. THE TRANSFORMED INTEGRAL EQUATION

We consider the interaction of a colliding particle with kinetic energy W_c and momentum-spin variables k, with a system of N particles interacting among themselves by an interaction Hamiltonian V which may include an external potential but does not act on

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

[2] H. Ekstein, Phys. Rev. **83**, 721 (1951).

the incident particle. The Schrödinger equation is

$$\left(W_c+\sum_{i=1}^{N} W_i+V+U-E\right)\Psi=0, \tag{1}$$

where W_i is the kinetic energy ot the ith particle, and U describes the interaction between the incident and all target particles. The "initial" state of the system is described by the wave function Ψ_0 which is a normalized solution of

$$(W_c+\sum W_i+V-E)\Psi_0=0, \tag{2}$$

describing a plane wave of incident particles. The total solution consists of the sum of Ψ_0 and ψ, the scattered wave which vanishes for large values of r, the coordinate of the incident particle. Equation (1) becomes

$$(W_c+\sum W_i+V+U-E)\psi=-U\Psi_0. \tag{3}$$

We assume that U describes two-body forces only, so that it can be decomposed into

$$U=\sum_{i=1}^{N} U_i, \tag{4}$$

where every U_i acts only on the positional and spin-coordinates of the incident and of the ith target particle. Since we deal with a multiple scattering problem, we decompose the scattered wave ψ into waves scattered by the individual target particles as follows:

$$(W_c+\sum W_i+V-E)\psi_i+U_i\psi=-U_i\Psi_0, \tag{5}$$

and it is clear that

$$\sum\psi_i=\psi, \tag{6}$$

so that Eq. (5) can be written as

$$(W_c+\sum W_n+U_i-E)\psi_i=-U_i\Psi_0-V\psi_i-\sum_{j\neq i} U_i\psi_j. \tag{7}$$

We seek to restate the scattering problem in terms of the solution of a two-body problem which involves only U_i. If the right-hand side of Eq. (7) is temporarily considered as a known function h, then the solution of the equation

$$(W_c+\sum W_n+U_i-E)\psi_i=h, \tag{8}$$

can be expressed in terms of the resolvent kernel K_i,

$$(W_c+\sum W_n-E)\psi_i=(1+K_i)h, \tag{9}$$

and the compatibility of the two equations requires that

$$K_i+U_i(W_c+\sum W_n-E)^{-1}K_i = -U_i(W_c+\sum W_n-E)^{-1}, \tag{10}$$

and

$$K_i(W_c+\sum W_n-E)+K_iU_i=-U_i. \tag{11}$$

Again, K_i is a unit operator with respect to variables other than those describing the incident and ith particles.

To give a definite meaning to the inverse operators appearing in Eq. (10), it is remembered that in scattering problems the solution containing outgoing waves is obtained by adding a small positive imaginary constant to the energy, and letting it vanish after integrations are performed.[3] We shall assume tacitly that this is done in all subsequent equations.

We now choose a definite representation in which the momentum- and spin-variables of all particles k and $p_1\cdots p_N$ are diagonal. In this representation all kinetic energy terms are numbers, and U_i is a unit operator with respect to all variables except those of the colliding and the ith particle. In Eq. (8) and the subsequent equations all but these variables may be considered as constant parameters. With the notation

$$\bar{E}(p_1\cdots p_{i-1}, p_{i+1}\cdots p_N)=E-\textstyle\sum_{n\neq i} W_n, \tag{12}$$

and

$$\gamma_i=K_i(W_c+W_i-\bar{E}), \tag{13}$$

where W_c and W_i are definite functions of k and p_i, respectively, Eq. (10) can be written

$$\gamma_i+U_i(W_c+W_i-\bar{E})^{-1}\gamma_i=-U_i. \tag{14}$$

Equation (14) is now a statement of a two-body problem. By Eqs. (19), (11), and (13) we obtain for Eq. (7)

$$(W_c+\sum W_n+V-E)\psi_i=\gamma_i\Psi_0+\textstyle\sum_{j\neq i}\gamma_i\psi_j -\gamma_i(W_c+\sum W_n-E)^{-1}V\psi_i. \tag{15}$$

In order to obtain the asymptotic form of the wave function in coordinate space, we transform to that representation in which the energy of the unperturbed scatterer and the momentum of the incident particle are diagonal, i.e., we expand the present wave functions $\psi_i(k, p)$

$$\psi_i(k, p)=\sum\varphi_l(p)\psi_{i,l}(k), \tag{16}$$

where the φ_l are eigenfunctions of the scatterer's Hamiltonian

$$(\sum W_n+V-E_l)\varphi_l(p)=0. \tag{17}$$

The total scattered wave function $\sum_i\psi_{i,l}(k)$ is then the probability amplitude for finding the incident particle scattered into a state k and simultaneously, the scatterer in the state l. One obtains in the usual manner from Eq. (15)

$$(W_c+E_l-E)\psi_{i,l}(k)-\sum_m\sum_{j\neq i}\int(k|\gamma_{i,lm}|k')\psi_{j,m}(k')dk' -\sum_m\int(k|\bar{\gamma}_{i,lm}|k')\psi_{i,m}(k')dk'=(k|\gamma_{i,l0}|k_0), \tag{18}$$

with

$$\gamma_{i,lm}=(\varphi_l, \gamma_i\varphi_m), \tag{19}$$

and

$$\bar{\gamma}_{i,lm}=\left(\varphi_l, \gamma_i\frac{\sum W_n-E_m}{W_c+\sum W_n-E}\varphi_m\right). \tag{20}$$

[3] C. Møller, Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd. **23**, No. 1 (1945); **22**, No. 19 (1946).

In coordinate space the asymptotic value of the wave function $\psi_l(\mathbf{r})$ is[4]

$$\psi_l(\mathbf{r})\sim-(2\pi)^{\frac{1}{2}}\frac{\exp(ik_lr)}{r}k_l\left(\frac{dk}{dE}\right)_{k=k_l}F_l\left(\frac{k_l}{r}\mathbf{r}\right), \quad (21)$$

where

$$F_l(k)=-(W_c+E_l-E)\psi_l(k), \quad (22)$$

and k_l is defined by

$$W_c(k_l)+E_l=E. \quad (23)$$

With this notation Eq. (18) can be written

$$F_{i,l}(k)-\sum_m\sum_{j\neq i}\int(k|\gamma_{i,lm}|k')\frac{F_{j,m}(k')}{W_c(k')+E_m-E}dk'$$
$$-\sum_m\int(k|\bar{\gamma}_{i,lm}|k')\frac{F_{i,m}(k')}{W_c(k')+E_m-E}dk'$$
$$=-(k|\gamma_{i,l0}|k_0), \quad (24)$$

and

$$\sum_i F_{i,l}=F_l. \quad (25)$$

Equations (24) and (25) restate the scattering problem in terms of two-body collision parameters. Only the knowledge of the unperturbed wave functions φ_l and of the two-body matrices γ_i is necessary to write down Eq. (24) explicitly.

The integral Eq. (14) for γ_i can be simplified by separating off the total momentum of the two particles, as usual in two-body problems. To satisfy the conservation of momentum the interaction Hamiltonian U_i must be of the form

$$(kp_i|U_i|k'p_i')=(\kappa|U_i|\kappa')\delta(\mathbf{K}-\mathbf{K}'), \quad (26)$$

where $\mathbf{K}$ is the total momentum and κ is some relative momentum together with spin variables. By the form of Eq. (14) it is clear that γ_i can also be factored

$$(kp_i|\gamma_i|k'p_i')=-(\kappa|\alpha_i|\kappa')\delta(\mathbf{K}-\mathbf{K}'), \quad (27)$$

and the integral equation for α_i is

$$\alpha_i+U_i[W(\kappa)+W(K')-\bar{E}]^{-1}\alpha_i=U_i, \quad (28)$$

where $W(\kappa)$ is that part of W_c+W_i which depends on the relative momentum κ and $W(K')$ the remainder. Equation (28) involves only three momentum coordinates like the problem of scattering by a fixed center of force.

In the remainder of this section the preceding equations will be written down more explicitly for the case of scalar nonrelativistic particles with potential interaction. Let m and m_i be the mass of the incident and the ith scatterer particle, respectively. We choose obviously for relative momentum coordinate the momentum conjugate to the relative distance of the two particles

$$\kappa=(m_i\mathbf{k}+m\mathbf{p}_i)/(m+m_i), \quad (29)$$

and

$$\mathbf{K}=\mathbf{k}+\mathbf{p}_i. \quad (30)$$

Then,

$$W(\kappa)=\hbar^2\kappa^2/2\mu_i, \quad (31)$$

and

$$W(K)=\hbar^2K^2/2(m+m_i), \quad (32)$$

where μ_i is the reduced mass. The momentum representation of the potential U_i becomes

$$(\mathbf{k}\mathbf{p}_i|U_i|\mathbf{k}'\mathbf{p}_i')=U_i(\boldsymbol{\kappa}-\boldsymbol{\kappa}')\delta(\mathbf{K}_i-\mathbf{K}_i'), \quad (26a)$$

where

$$U_i(\boldsymbol{\kappa})=(2\pi)^{-3}\int\exp(-i\boldsymbol{\kappa}\cdot\mathbf{r})u_i(\mathbf{r})d\mathbf{r}. \quad (33)$$

The integral equation for the matrix α_i becomes

$$(\boldsymbol{\kappa}|\alpha_i|\boldsymbol{\kappa}')+\int\frac{U_i(\boldsymbol{\kappa}-\boldsymbol{\kappa}'')(\boldsymbol{\kappa}''|\alpha_i|\boldsymbol{\kappa}')}{W(\kappa'')+W(K_i)-\bar{E}}d\boldsymbol{\kappa}''$$
$$=U_i(\boldsymbol{\kappa}-\boldsymbol{\kappa}'), \quad (28a)$$

in which K_i is considered as a constant parameter. If the potential has spherical symmetry, separation of variables in Eq. (28a) leads to a set of one-dimensional integral equations.[2] Alternatively, the matrix α_i can be constructed from the Green's function which satisfies the differential equation

$$[-(\hbar^2/2\mu_i)\nabla^2+u_i-\bar{E}+W(K_i)]G_i(\mathbf{r},\mathbf{R})$$
$$=-\delta(\mathbf{r}-\mathbf{R}), \quad (34)$$

as follows:[2,5]

$$(\boldsymbol{\kappa}|\alpha_i|\boldsymbol{\kappa}')=\frac{\bar{E}-W(K_i)-W(\kappa')}{(2\pi)^3}\int d\mathbf{r}d\mathbf{R}$$
$$\times\exp(i\boldsymbol{\kappa}'\cdot\mathbf{R}-i\boldsymbol{\kappa}\cdot\mathbf{r})u_i(\mathbf{r})G_i(\mathbf{r},\mathbf{R}). \quad (35)$$

The matrices $\gamma_{i,lm}$ and $\bar{\gamma}_{i,lm}$ are explicitly

$$(\mathbf{k}|\gamma_{i,lm}|\mathbf{k}')=-\int\varphi_l^*(\mathbf{p})\left(\frac{m_i\mathbf{k}-m\mathbf{p}_i}{m+m_i}|\alpha_i|\frac{m_i\mathbf{k}'-m\mathbf{p}_i'}{m+m_i}\right)$$
$$\times\delta(\mathbf{k}+\mathbf{p}_i-\mathbf{k}'-\mathbf{p}_i')\varphi_m(\mathbf{p}_i'\mathbf{p}_n)d\mathbf{p}'d\mathbf{p}, \quad (19a)$$

and

$$(\mathbf{k}|\bar{\gamma}_{i,lm}|\mathbf{k}')=-\int\varphi_l^*(\mathbf{p})\frac{W(p_i'p_n)-E_m}{W(k'p_i'p_n)-E}$$
$$\times\left(\frac{m_i\mathbf{k}-m\mathbf{p}_i}{m+m_i}|\alpha_i|\frac{m_i\mathbf{k}'-m\mathbf{p}_i'}{m+m_i}\right)$$
$$\times\delta(\mathbf{k}+\mathbf{p}_i-\mathbf{k}'-\mathbf{p}_i')\varphi_m(\mathbf{p}_i'\mathbf{p}_n)d\mathbf{p}_i'd\mathbf{p}. \quad (20a)$$

[4] W. Pauli, *Meson Theory of Nuclear Forces* (Interscience Publishers, New York, 1948). We have added a minus sign missing in the text.

[5] In reference 2 a minus sign on the right-hand side of Eq. (23) was omitted erroneously.

The notation $p_i'p_n$ means explicitly $\mathbf{p}_1\cdots\mathbf{p}_{i-1}\mathbf{p}_i'$ $\mathbf{p}_{i+1}\cdots\mathbf{p}_N$, i.e., n stands for all but the ith momentum. Further,

$$W(k'p_i'p_n)=\frac{\hbar^2}{2}\left(\frac{k'^2}{m}+\frac{p_i'^2}{m_i}+\sum_{n\neq i}^{N}\frac{p_n^2}{m_n}\right), \quad (36)$$

and the analogous expression with omission of k'^2/m holds for $W(p_i'p_n)$. Equation (21) becomes

$$\psi_l(\mathbf{r})\sim\frac{-(2\pi)^{\frac{1}{2}}m}{\hbar^2 r}\exp(ik_l r)F_l\left(\frac{k_l}{r}\mathbf{r}\right). \quad (21a)$$

III. DISCUSSION OF THE FIRST APPROXIMATION

We consider first the scattering of a scalar particle by another particle bound by an external potential. If the range of the interaction force is very small, Eq. (26a) shows that U becomes constant. Hence, by Eq. (28a), α becomes also constant.[6] In this case the collision of two free particles in the center-of-mass system is described by the asymptotic wave function

$$\Psi\sim(2\pi)^{-\frac{3}{2}}\exp(i\mathbf{k}_0\cdot\mathbf{r})-\frac{(2\pi)^{\frac{1}{2}}\exp(ik_0r)}{\hbar^2 r}\alpha, \quad (37)$$

as can be seen by applying Eqs. (21a) and (24) to the simple case of scattering by a fixed center of force. By comparing with the usual definition of the scattering length

$$\Psi\sim\exp(i\mathbf{k}_0\cdot\mathbf{r})-\frac{\exp(ik_0r)}{r}a, \quad (38)$$

one has

$$\alpha=\hbar^2a/(2\pi)^2\mu. \quad (39)$$

By Eqs. (24), (19a), and (21a) we have for the first approximation of the bound scatterer

$$\psi_l\sim-\frac{m}{\mu}a(2\pi)^{-\frac{3}{2}}\frac{\exp(ik_lr)}{r}\int\varphi_i^*(\mathbf{p})\,\varphi_0(\mathbf{k}-\mathbf{k}_0+\mathbf{p})d\mathbf{p}, \quad (40)$$

where

$$\mathbf{k}=k_l\mathbf{r}/r.$$

In coordinate representation the integral is

$$\int\varphi_l^*(\mathbf{r})\exp[-i\mathbf{r}\cdot(\mathbf{k}-\mathbf{k}_0)]\varphi_0(\mathbf{r})d\mathbf{r},$$

and it is clear that Eq. (40) is identical with Fermi's result for the scattering of neutrons by one bound proton.[1]

Similarly, for N scatterers with scattering lengths a_i, one obtains

$$\psi_l\sim-(2\pi)^{-\frac{3}{2}}\frac{m\exp(ik_lr)}{r}\sum_i^N\frac{a_i}{\mu_i}\int\varphi_l^*(\mathbf{r})\times\exp[-i\mathbf{r}_i\cdot(\mathbf{k}-\mathbf{k}_0)]\varphi_0(\mathbf{r})d\mathbf{r}, \quad (41)$$

the obvious generalization of Fermi's result for N bound scatterers.

We now turn to the more general case where the two-body collision cannot be described merely by a constant a. It is shown in Sec. V that, in general, for small scattering cross section

$$(\boldsymbol{\kappa}|\,\alpha\,|\boldsymbol{\kappa}')\approx(\boldsymbol{\kappa}|\,f\,|\boldsymbol{\kappa}').$$

The matrix f describes the ordinary free scattering problem where "initially" both particles are described by plane waves. $\boldsymbol{\kappa}'$ is the relative "initial" momentum. We obtain for the first approximation

$$\psi_l\sim-\frac{(2\pi)^{\frac{1}{2}}m\exp(ik_lr)}{\hbar^2\quad r}\sum_i\int\varphi_i^*(\mathbf{p})\times\left(\frac{m_i\mathbf{k}-m\mathbf{p}_i}{m+m_i}|f_i|\frac{m_i\mathbf{k}_0-m\mathbf{p}_i'}{m+m_i}\right)\times\delta(\mathbf{k}+\mathbf{p}_i-\mathbf{k}_0-\mathbf{p}_i')\,\varphi_0(\mathbf{p}_i'\mathbf{p}_n)d\mathbf{p}d\mathbf{p}_i'. \quad (42)$$

This equation has an intuitive meaning; it represents the probability amplitude for an initial momentum $\mathbf{p}_i'$, times the probability amplitude for a momentum $\mathbf{p}_i$ in the final state, multiplied by the scattering function for the free two-body collision of particles $\mathbf{k}_0$, $\mathbf{p}_i'\rightarrow\mathbf{k}$, $\mathbf{p}_i$ with the restriction of momentum conservation integrated over all initial and final momenta. It shows that in the first approximation the particles are considered free in the following restricted sense: The total process $0\rightarrow l$ can be represented as a sum of elementary free collisions, although ultimately the scattering particle may remain in a bound state l. In classical language the interaction force U is so much larger than the binding force V that during the collision the two particles behave as if they were free, but immediately after the collision the binding force predominates again and may retain the particle in its original or another bound orbit.

For the scattering of slow neutrons by bound nuclei Eq. (42) can be further simplified. We notice first that it is necessary here to use the generalization from simple particles to composite particles discussed in the introduction. If the scatterer is very small in comparison to $1/k_0$, the scattering length would be a constant if the scattering were due to a potential but not when the scatterer itself is a complex system. For example, the scattering of slow neutrons by nuclei may well be velocity-dependent. Hence, in this case α is not defined by Eq. (28) but by a more general equation describing the scattering of a neutron by a free nucleus, an

[6] The potential does not behave like any obvious delta-function, since this does not lead to a limiting value for α. In the case of a square well the potential becomes infinite and the radius zero in such a manner that the product potential$\times$(radius)^2 retains a constant value. The author is indebted to Dr. G. Wentzel for this remark.

equation which we cannot correctly state and much less solve.

Since the range of interaction is small, the matrix f, considered as a function of its first argument, will be substantially constant up to wave numbers of the order of (range)$^{-1}$. On the other hand, the wave functions ϕ_0, describing molecular binding, extend to wave numbers of about 10^9 to 10^{10} and drop off exponentially afterwards. Hence, one can replace the first argument of f by its value on the energy shell, i.e., such that the absolute value of the two arguments is equal. We do not have to consider angular dependence, since only S scattering is of importance here. If we consider the scattering length a as a function of the relative momentum κ, Eq. (42) can be written

$$\psi_l \sim -\frac{\exp(ik_l r)}{r}(2\pi)^{-\frac{3}{2}}\sum_i \frac{m}{\mu_i}\int \varphi_l^*(\mathbf{p})a_i\left(\frac{m_i\mathbf{k}-m\mathbf{p}_i}{m+m_i}\right) \times\delta(\mathbf{k}+\mathbf{p}_i-\mathbf{k}_0-\mathbf{p}_i')\varphi_0(\mathbf{p}_i'\mathbf{p}_n)d\mathbf{p}d\mathbf{p}_i'. \quad (43)$$

Equation (43) determines the influence of molecular binding on resonance scattering of slow neutrons. One can verify that in the range of the $1/v$-law where the "free" scattering cross section is a constant, molecular motion has no influence on the cross section, which is a well-known result of more intuitive analysis. In the resonance region itself an influence of molecular motion exists, but because of the usually small ratio m/m_i it is very small.

In the more general case where the wavelength is comparable with the range of the interaction force, the replacement of f by its value on the energy shell, i.e., the R matrix, is not, in general, justifiable.

Taking this step leads to a formula which is equivalent to the "impulse approximation" proposed by Chew[7] on more intuitive grounds.

It appears that this formula is the result of three independent approximative steps: (1) the use of the first approximation to Eq. (24), (2) the replacement of α by f, and (3) the replacement of the first argument of f by the value corresponding to the energy shell, i.e., replacement of f by the R matrix.

IV. DISCUSSION OF THE HIGHER APPROXIMATIONS

In order to test the merits of diverse approximation methods for short-range forces we consider their convergence properties for the limiting case of point scatterers.

It is well known that the second Born approximation for fixed or free point scatterers is infinite. It is perhaps not as well known that the same infinity occurs for a bound scatterer. According to well-known results, the second approximation is, for a delta-function potential,[8] the solution of the differential equation

$$(\nabla^2+k_m^2)\psi_m(\mathbf{r})=(\hbar^2/2m)\varphi_m^*(\mathbf{r})\psi^{(1)}(\mathbf{r},\mathbf{r}), \quad (44)$$

where

$$\psi^{(1)}(\mathbf{r},\mathbf{r})=\frac{m}{(2\pi)^{5/2}\hbar^2}\left(\sum_n+\int\right)\varphi_n(\mathbf{r})\int\frac{\exp(ik_n|\mathbf{r}-\mathbf{r}'|)}{|\mathbf{r}-\mathbf{r}'|} \times\exp(i\mathbf{k}_0\cdot\mathbf{r})\varphi_n^*(\mathbf{r}')\varphi_0(\mathbf{r}')d\mathbf{r}'. \quad (45)$$

To investigate the convergence of the sum, we need only consider the asymptotic forms of wave functions and energies, since any finite number of terms gives a finite result. Most wave functions of systems of physical significance tend towards plane waves in the high energy limit, and the energies become asymptotically equal to the kinetic energy. Hence, we set

$$\varphi_p\rightarrow(2\pi)^{-\frac{3}{2}}\exp(i\mathbf{p}\cdot\mathbf{r}), \quad (46)$$

and

$$k_p=\hbar[(E-E_p)/2m]^{\frac{1}{2}}\rightarrow ip, \quad (47)$$

and the sum to be evaluated becomes

$$S=\int_{p_0}^{\infty}d\mathbf{p}\exp(i\mathbf{p}\cdot\mathbf{r})\int\frac{\exp(-p|\mathbf{r}-\mathbf{r}'|)}{|\mathbf{r}-\mathbf{r}'|} \times\exp[i(\mathbf{k}_0-\mathbf{p})\cdot\mathbf{r}']\varphi_0(\mathbf{r}')d\mathbf{r}', \quad (48)$$

where p_0 is some large number beyond which the eigenfunctions may be identified with plane waves.

The integration with respect to the angular variables in $\mathbf{p}$ can be carried out first with the result

$$S=4\pi\int_{p_0}^{\infty}pdp\int d\mathbf{r}'\exp[-pr'+i\mathbf{k}_0\cdot(\mathbf{r}+\mathbf{r}')] \times\frac{\sin pr'}{r'^2}\varphi_0(\mathbf{r}'+\mathbf{r}). \quad (49)$$

Since only large values of p matter, only the neighborhood of $r'=0$ will contribute to the second integral. Hence,

$$S=(4\pi)^2\varphi_0(\mathbf{r})\exp(i\mathbf{k}_0\cdot\mathbf{r}) \times\int_{p_0}^{\infty}pdp\int_0^{\infty}\exp(-pr')\sin pr'dr' \quad (50)$$

$$=(4\pi)^2\varphi_0(\mathbf{r})\exp(i\mathbf{k}_0\cdot\mathbf{r})\int_{p_0}^{\infty}\tfrac{1}{2}dp,$$

and the result is infinite. One can conclude that, more generally, Born's approximation is unsuitable for short-range interaction forces.

An alternative approximation method for small scatterers has been proposed by Lippmann and Schwinger.[9]

[7] G. F. Chew, Phys. Rev. **80**, 196 (1950).

[8] N. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions* (Clarendon Press, Oxford, Oxford, 1949). Formulas corrected for normalized incident wave.

[9] B. A. Lippmann and Julian Schwinger, Phys. Rev. **79**, 469 (1950).

Except for constant factors their second approximation differs from Born's second approximation by the addition of a constant term $(-M/2\mu)$ to the exponential in the integrand of Eq. (45). We discuss this corrective term. Instead of Eq. (49) we obtain

$$S'=\frac{-4\pi M}{2\mu}\exp(i\mathbf{k}_0\cdot\mathbf{r})\int_{p_0}^{\infty}pdp\int d\mathbf{r}'\exp(i\mathbf{k}_0\cdot\mathbf{r}')\times\frac{\sin pr'}{r'^2}\varphi_0(\mathbf{r}'+\mathbf{r})d\mathbf{r}'. \quad (51)$$

If the second integral is expanded by integration by parts in descending powers of p, we get

$$\int d\Omega\varphi_0(\mathbf{r})/p=4\pi\varphi_0(\mathbf{r})/p,$$

so that the leading term of the sum $S+S'$ is

$$S+S'=(4\pi)^2\varphi_0(\mathbf{r})\exp(i\mathbf{k}_0\cdot\mathbf{r})\int_{p_0}^{\infty}pdp\left(\frac{1}{2p}-\frac{M}{2\mu p}\right), \quad (52)$$

which converges only for the special case $2\mu/M=2$.[10] The same objection does not necessarily apply to Breit's theory,[11] because a special limiting process is used there. However, this theory concerns only point scatterers.

We now discuss the second approximation to Eq. (24) for the case of point scatterers, when α becomes constant. We obtain from Eq. (19a)

$$(\mathbf{k}|\bar{\gamma}_{lm}|\mathbf{k}')=-\alpha\int\varphi_l^*(\mathbf{p}'+\mathbf{k}'-\mathbf{k})\varphi_m(\mathbf{p}')\times\frac{W(p')-E_m}{W(k')+W(p')-E}d\mathbf{p}', \quad (53)$$

and the second approximation becomes

$$F_l^{(2)}=-\alpha^2\int d\mathbf{k}'\left(\sum_m+\int\right)\frac{1}{W(k')+E_m-E}\times\int\varphi_l^*(\mathbf{p}'+\mathbf{k}'-\mathbf{k})\varphi_m(\mathbf{p}')\frac{W(p')-E_m}{W(k')+W(p')-E}d\mathbf{p}'\times\int\varphi_m^*(\mathbf{p}+\mathbf{k}_0-\mathbf{k}')\varphi_0(\mathbf{p})d\mathbf{p}. \quad (54)$$

Again, asymptotically, the wave functions can be described by plane waves, and the energy can be set equal to the kinetic energy. The contribution of the high energy spectrum is

$$S=-\alpha^2\int d\mathbf{k}'\int_{p_0}^{\infty}\frac{d\mathbf{p}''}{W(k')+W(p'')-E}\times\int\varphi_l^*(\mathbf{p}'+\mathbf{k}'-\mathbf{k})\delta(\mathbf{p}'-\mathbf{p}'')\frac{W(p')-W(p'')}{W(k')+W(p')-E}d\mathbf{p}'\times\int\delta(\mathbf{p}+\mathbf{k}_0-\mathbf{k}'-\mathbf{p}'')\varphi_0(\mathbf{p})d\mathbf{p}. \quad (55)$$

The integral with respect to $\mathbf{p}'$ vanishes, so that the contribution of the high energy spectrum is zero. The difference between Eq. (55) and Born's second approximation for point scatterers is the absence of the ratio

$$[W(p')-E_m]/[W(k')+W(p')-E],$$

in the latter. Without it Eq. (55) would give an infinite result in agreement with the previous calculation in coordinate representation, as one can easily verify.

It appears that the high energy part of the spectrum is, in effect, cut off from the higher approximations to Eq. (24). This is not surprising if one recalls the original motivation of Fermi's calculation, of which the present transformation is merely the rigorous complement.

Equations of the type (5) or (7) are unsuited for the purpose of iteration when U is nearly constant, because in the language of perturbation calculus the intermediate states have too much importance. Hence, a transformation is made which takes many of the intermediate states into account at the outset. From the discussion of the first approximation it is also clear that these are just the high energy states where the bound particle can be considered free. Indeed, we found that the first approximation describes a set of elementary processes in which the scatterer particle scatters as though it were free.

The first approximation to Eq. (24) can be interpreted by the simple rule: Substitute a pseudopotential γ for U and proceed as in perturbation calculus. A more general heuristic rule can now be given for the higher terms: Substitute the pseudopotential γ and proceed by Born's approximation method, cutting off all sums (or integrals) over intermediate states at an energy $E_{\max}$ such that

$$E_{\max}\approx\text{kinetic energy of the state.}$$

This rule is quite similar to one formulated previously in connection with fixed scattering centers.

V. EXPRESSION OF THE MATRIX α IN TERMS OF ORDINARY COLLISION PARAMETERS

If the particles involved in the many-body scattering process are elementary particles and their interaction can be described by two-body interaction operators, the determination of α can be carried out directly with no more difficulty than the determination of the ordinary

[10] Whether the finite result found by Lippmann is due to the special choice of wave functions, which do not belong to the class considered here, or to the limiting process used in the evaluation of the integral, remains undecided.

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

scattering amplitudes. However, the main interest of the present approach lies in the correlation of many-body scattering when the latter is really an interaction between more complex systems. In this case α can often not be calculated, but the solutions of the ordinary scattering problem can be, more or less, inferred from experimental data. Therefore, it is necessary to express α in terms of these solutions.

In the center-of-mass system of the two complex particles the scattering is described by the matrix[4]

$$(k|f|k')=\sum(k|U|k'')(k''|\Phi|k'), \tag{56}$$

where $(k|U|k'')$ is the interaction Hamiltonian in a representation which diagonalizes the energies of the separated systems and the relative momentum of their centers of mass. $(k''|\Phi|k')$ is that wave function which corresponds to the eigenvalue $E(k')$. The matrix f satisfies the integral equation

$$(k|f|k')+\sum\frac{(k|U|k'')(k''|f|k')}{E(k'')-E(k')}=(k|U|k'), \tag{57}$$

and is connected to the asymptotic scattering amplitude by Eq. (21) with f substituted for F.

The connection between the wave function Φ and the matrix f is given by

$$(k|\Phi|k')=\delta(k-k')-\frac{(k|f|k')}{E(k)-E(k')}, \tag{58}$$

the meaning of the denominator being defined by the convention stated in Section I.

Generalizing Eq. (28) we define the matrix α as the solution of the integral equation

$$(k|\alpha|k')+\sum\frac{(k|U|k'')(k''|\alpha|k')}{E(k'')-E_0}=(k|U|k'). \tag{59}$$

Since α depends on the value of E_0, it should be written

$$(k|\alpha|k';E_0),$$

but the third argument will be omitted. Clearly, f is a special case of α

$$(k|\alpha|k';E(k'))=(k|f|k'). \tag{60}$$

We will now express α in terms of f. The similarity between Eqs. (59) and (57) suggests that in analogy with Eq. (56) we set

$$(k|\alpha|k')=\sum(k|U|k'')(k''|q|k'), \tag{61}$$

so that by Eq. (59)

$$\sum(k|U|k'')\left[(k''|q|k')+\frac{(k|\alpha|k')}{E(k'')-E_0}-\delta(k''-k')\right]=0. \tag{62}$$

The matrix q is an auxiliary quantity without direct significance.

If U has an inverse, which we shall assume, the bracket vanishes. Multiplication by $E(k'')-E_0$ gives

$$[E(k)-E_0](k|q|k')+\sum(k|U|k'')(k''|q|k')=[E(k)-E_0]\delta(k-k'). \tag{63}$$

The matrix q is now expanded in terms of eigenfunctions $(k|\Phi|k')$ in which we must for completeness include possible bound-state eigenfunctions u_n with energies ϵ_n.

$$(k|q|k')=\int(k|\Phi|k'')(k''|a|k')+\sum_n u_n(k)a_n(k'). \tag{64}$$

One obtains then in the usual manner

$$(k''|a|k')=\frac{E(k')-E_0}{E(k'')-E_0}(k'|\Phi|k'')^*, \tag{65}$$

and

$$a_n(k')=\frac{E(k')-E_0}{\epsilon_n-E_0}u_n^*(k'). \tag{66}$$

By Eqs. (61) and (64) we obtain

$$(k|\alpha|k')=\sum(k|U|k'')\times\left[\int\frac{(k''|\Phi|k''')(k'|\Phi|k''')^*\{E(k')-E_0\}}{E(k''')-E_0}+\sum_n\frac{E(k')-E_0}{\epsilon_n-E_0}u_n(k'')u_n^*(k')\right]. \tag{67}$$

By Eqs. (56) and (58) and the Schrödinger equation for u_n this can be written

$$(k|\alpha|k')=\int(k|f|k'')(k'|\Phi|k'')^*\frac{E(k')-E_0}{E(k'')-E_0}+\sum_n\frac{[\epsilon_n-E(k)][E(k')-E_0]}{\epsilon_n-E_0}u_n(k)u_n^*(k'), \tag{68}$$

or

$$(k|\alpha|k')=(k|f|k')-\int(k|f|k'')\left[\frac{(k'|f|k'')}{E(k')-E(k'')}\right]^*\frac{E(k')-E_0}{E(k'')-E_0}+\sum_n\frac{[\epsilon_n-E(k)][E(k')-E_0]}{\epsilon_n-E_0}u_n(k)u_n^*(k'). \tag{69}$$

For small scattering cross sections we may expect the bilinear terms to be small and set

$$(k|\alpha|k')\approx(k|f|k'), \tag{70}$$

a result to be expected from Eq. (59). One can see, however, that a large difference between $E(k')$ and E_0 will make the corrective terms large.

The third term in Eq. (69) will become important if E_0 is negative and close to one of the energies ϵ_n. It appears that this term, when introduced into Eq. (18), describes a rearrangement process, real or virtual, in which a bound state between the incident and one of the bound particles is formed. We do not enter upon this subject here.

It has been pointed out previously[12] that in using the α for complex systems in the equations describing multiple scattering, the elastic submatrix $(n_0k|\alpha|n_0k')$ is to be employed which describes only interaction processes which do not change the internal coordinates of the two particles involved (except for spin coordinates which can be taken into account explicitly).

This is a basic limitation of the method used here. If, for instance, the collision of a neutron with a nucleus gives rise to γ-ray emission, then the γ-ray is not considered explicitly in this formulation, although the "γ-ray width" of the neutron scattering cross section is included.

VI. REFRACTION AND DIFFRACTION OF SLOW NEUTRONS BY CRYSTALS, INCLUDING ZERO-POINT MOTION AND ELECTROSTATIC INTERACTION WITH ELECTRONS

As an application of the method the dynamical theory of refraction and diffraction of slow neutrons by large crystals will be presented in a revised form by including the zero-point motion of the nuclei and the electrostatic interaction with electrons.

The theory as developed by Goldberger and Seitz[13] shows a somewhat paradoxical feature in that the nuclei are considered as rigidly fixed, whereas their scattering length is that of loosely bound nuclei, i.e.,

$$a_{\text{eff}}=(m/\mu)a_{\text{free}}\neq a_{\text{fixed}},$$

where a_{free} is the scattering length observed in a free two-body collision[14] and a_{eff} is the scattering length characterizing a nucleus in the lattice. But a_{eff} is, in general, quite different from the scattering length a_{fixed}, which one would observe if the nucleus were rigidly fixed.

To see this we compare the equations describing scattering in the two cases, fixed and free target nucleus, respectively.

$$[-(\hbar^2/2m)\nabla^2+u-E]\psi=0, \tag{71}$$

$$[-(\hbar^2/2\mu)\nabla^2+u-E]\psi=0, \tag{72}$$

for the simplest type of potential interaction, a square well. The two equations differ essentially by an effective coupling constant of ratio m/μ. Considering only the S wave and the low energy limit, the cross section is an erratically varying function of the coupling constant.[15] Hence, a_{free} and a_{fixed} may differ by factors substantially different from m/μ, and it becomes necessary to justify the procedure by considering the motion of the nuclei.

Another reason for this revision is the gain in simplicity. When the zero-point motion is taken into account, the wave function does not have any singularities, even if one idealizes the nuclei as point scatterers, and one can hence use simpler mathematical methods.

We consider an infinite crystal in the ground state and disregard all excited states. In this case the division into incident and scattered wave has no meaning, and we omit the inhomogeneous term in Eq. (18), so that ψ is now the entire wave function. Equation (18) takes the form

$$(W_c+E_0-E)\psi_{i,0}(k)-\sum_{j\neq i}\int(k|\gamma_{i,00}|k')\psi_{j,0}(k')dk'$$

$$-\int(k|\bar{\gamma}_{i,00}|k')\psi_{i,0}(k')dk'=0. \tag{73}$$

The energy E is now an unknown eigenvalue and not given beforehand.

It has been pointed out elsewhere[12] that this procedure of going to the limit of an infinitely extended scatterer is not quite rigorous, but the necessary correction for radiation damping is very small in most practical cases.

It will appear in the following that for the relevant range of wave numbers $\mathbf{k}$

$$E\approx E_0+W_c(k), \tag{74}$$

so that $\gamma_{i,00}$ and $\bar{\gamma}_{i,00}$ become identical by Eqs. (19) and (20). Omitting the unnecessary subscripts 0, we can write for Eq. (73) in view of Eq. (6)

$$(W_c+E_0-E)\psi_i(k)-\int(k|\gamma_i|k')\psi(k')dk'=0, \tag{75}$$

and by summation with respect to i

$$(W_c+E_0-E)\psi(k)-\int(k|\gamma|k')\psi(k')dk'=0, \tag{76}$$

with

$$\gamma=\sum\gamma_i. \tag{77}$$

Further, by Eqs. (19a) and (39) we have for scalar interaction

$$(\mathbf{k}|\gamma|\mathbf{k}')=\frac{-\hbar^2}{(2\pi)^2}\sum_i\frac{a_i}{\mu_i}\int\varphi_0^*(\mathbf{p})\delta(\mathbf{k}+\mathbf{p}_i-\mathbf{k}'-\mathbf{p}_i')$$

$$\times\varphi_0(\mathbf{p}_i'\mathbf{p}_n)d\mathbf{p}_i'd\mathbf{p}, \tag{78}$$

where a_i and μ_i are the "free" scattering length and the reduced mass of the ith nucleus. In coordinate

[12] H. Ekstein (to be published).
[13] M. L. Goldberger and F. Seitz, Phys. Rev. **71**, 294 (1947).
[14] E. Fermi and L. Marshall, Phys. Rev. **71**, 666 (1947).
[15] See reference 6, p. 30, Fig. 4.

representation Eq. (78) can be written

$$(\mathbf{k}|\gamma|\mathbf{k}')=\frac{-\hbar^2}{(2\pi)^2}\sum_i\frac{a_i}{\mu_i}\int|\varphi_0(\mathbf{r})|^2\exp[i\mathbf{r}_i\cdot(\mathbf{k}-\mathbf{k}')]d\mathbf{r}. \quad (79)$$

The integral is the Fourier transform of the probability for finding the ith nucleus at the point $\mathbf{r}_i$.

If Eq. (76) is now written in coordinate representation, one obtains

$$\left(\frac{-\hbar^2}{2m}\nabla^2+U_{\text{eff}}+E_0-E\right)\psi=0, \quad (80)$$

with

$$U_{\text{eff}}=2\pi\hbar^2\textstyle\sum_i(a_i/\mu^i)\displaystyle\int|\varphi_0(\mathbf{r}')|^2\delta(\mathbf{r}-\mathbf{r}_i')d\mathbf{r}'. \quad (81)$$

If there are n different kinds of nuclei with scattering lengths a_j and reduced masses μ_j, we obtain

$$U_{\text{eff}}(\mathbf{r})=2\pi\hbar^2\sum_j^n\frac{a_j}{\mu_j}\sum_i\int|\varphi_0(\mathbf{r}')|^2\delta(\mathbf{r}-\mathbf{r}_i')d\mathbf{r}', \quad (82)$$

where the second summation extends over all nuclei of type j. The sum with respect to i represents evidently the probability for finding any one nucleus of type j at the point $\mathbf{r}$, i.e., the expectation value of the density of nuclei j, viz., ρ_j. Hence, Eq. (82) may be written

$$U_{\text{eff}}(\mathbf{r})=2\pi\hbar^2\sum_j^n\frac{a_j}{\mu_j}\rho_j(\mathbf{r}). \quad (83)$$

This result was to be expected; the effective potential to be used is the Fermi pseudopotential of all nuclei, averaged with respect to the ground state of the crystal.

Since the potential is now a smooth function, the wave function has no singularities, and one can proceed legitimately in the manner of Laue's dynamical theory without the complications of Ewald's lattice sums. We do not enter into the details, since the results are well known. It is a well-known feature of this theory that the strong waves have wave numbers very close to the vacuum wave number corresponding to the given energy, which justifies Eq. (74). One finds, rather obviously, agreement with the formulas given by Goldberger and Seitz for wavelengths which are large in comparison to the spread of the nuclear wave functions. A decrease of intensities is found only when the neutron wavelength becomes comparable to the zero-point motion's amplitude, which is usually of the order of one percent of the interatomic distance. Such wavelengths are never used in diffraction experiments, so that we find agreement with Goldberger and Seitz for all practical purposes. A deviation could only be expected in such extreme cases as solid hydrogen or rather (since spin alignment is impracticable) solid deuterium.

We next turn to the electrostatic interaction between neutrons and electrons. It is only necessary to include the electrons in the γ_i's in Eq. (78), and all other calculations remain correct if the term corresponding to the electron interaction is added.

We obtain then a total effective potential to be introduced into the Schrödinger equation of the neutron

$$U_{\text{eff}}(\mathbf{r})=2\pi\hbar^2\left[\sum_j^n\frac{a_j}{\mu_j}\rho_j(\mathbf{r})+\frac{a_e}{\mu_e}\rho_e(\mathbf{r})\right], \quad (84)$$

where a_e is the scattering length in a free neutron-electron collision and μ_e the reduced mass of the electron, which is practically equal to the electronic mass itself.

According to well-known results of the dynamical theory of x-rays, the integrated intensity of a beam diffracted by a large, perfect crystal is proportional to the appropriate Fourier coefficient of the potential (84).

In addition to the first term which is practically constant, a second term is obtained from Eq. (84), which decreases with the increasing Miller index of the reflecting plane. This decrease, according to experimental results obtained from gases and liquids, is of the order of a few percent in the practical range.[16–18]

The question arises whether the use of diffraction by large crystals would provide a more precise determination of a_e. Offhand, this would seem to be desirable because the well-defined state of the crystal eliminates a number of uncertainties connected with the liquid state. However, the deviations from rigorous periodicity in an actual crystal, even at low temperatures, will substantially affect the result. In particular, isotope and spin effects will tend to decrease intensities while mosaic structure increases them. The latter effect is particularly difficult to estimate, so that the method probably has no advantage over those used previously.

[16] Havens, Rabi, and Rainwater, Phys. Rev. **72**, 634 (1947).
[17] E. Fermi and L. Marshall, Phys. Rev. **72**, 1139 (1947).
[18] Havens, Rainwater, and Rabi, Phys. Rev. **82**, 345 (1951).