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MASTER

MULTIPLE SCATTERING OF THERMAL NEUTRONS

J. P. Plummer

RELEASED FOR ANNOUNCEMENT
IN NUCLEAR SCIENCE ABSTRACTS

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MULTIPLE SCATTERING OF THERMAL NEUTRONS

by

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ABSTRACT

This report examines the quantum mechanical treatment of multiple scattering developed by Watson and co-workers and applies it to thermal neutron scattering in the static approximation. It is shown that recent efforts along similar lines appearing in the literature have been oversimplified approaches to a very complex problem.

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MULTIPLE SCATTERING OF THERMAL NEUTRONS

INTRODUCTION

Recently the problem of multiple scattering has become one of importance in thermal neutron scattering experiments. The only attempts to treat the situation quantitatively are by transport theory codes, without any real justification for the validity of such an approach. Indeed, there are clearly some cases where this type of approach just won't work. Two recent papers^(1,2) have attacked the problem quantum mechanically. Each solves for the leading (see later comments) multiple scattering correction term to the cross section. Their approach is general (Reference (1) assumes the static approximation) in that they get expressions involving two and three-particle correlation functions, which are characteristic of the particular scattering medium in question. If one takes the results of Reference (1) and applies it to an ideal gas model, one gets strange results (more about this later). Furthermore, there is a strong indication that the term calculated is not the leading multiple scattering term at all. Reference (2) does look at the heavy ideal gas model. After some questionable steps, they get an expression which has the multiple scattering correction 10^{11} times the single scattering cross section and negative, for low-incident neutron energy. This correction term is then doctored by a device which seems to be no more than borrowing some of the forward scattering contribution so that the cross section is always positive.

There is a great body of work on the quantum mechanical theory of multiple scattering in general by Watson (and occasional co-workers) appearing in The Physical Review during the years 1953 through 1959.

In my doctoral thesis⁽³⁾, I applied the Watson method, in a crude fashion, to the particular problem of thermal neutron scattering in the static approximation, and then applied the results to an ideal gas model. The treatment, however, was incomplete and left many questions unanswered. Besides Watson's work, Goldberger and Seitz⁽⁴⁾ deal with the problem of neutron scattering (including multiple scattering) in crystals from a different point of view.

This report will commence by carefully reviewing one of the Watson papers⁽⁵⁾. This paper appears to be a thorough and correct (and as nearly rigorous as possible) approach to the problem of explaining multiple scattering mechanically. I shall try to explain Watson's method with more elaboration than he does in those areas in which he is a bit brief (particular attention will be paid to all approximations made), but will leave out much detail that he covers or that is straightforward. In other words, the careful reader of this report should read Reference (5) also, preferably first.

I shall add an innovation of our^{*} own to the Watson method and specialize the approach to the case of thermal neutron scattering in the static approximation. The results will be applied to an ideal gas scattering system. Finally, I will make some observations concerning future work along this line.

FORMAL DEVELOPMENT OF THE MULTIPLE SCATTERING PROBLEM

The scattering medium consists of a large number N of equivalent particles. Its states will be represented by

* G. C. Summerfield, University of Michigan, has been my constant advisor and co-worker.

$$g_{\gamma,M}(\xi) \quad (1)$$

where ξ is some appropriate set of many body coordinates. (We will use Watson's notation throughout this report.) The index γ will refer to the spatial part of the state and M to the spin part. If H_N is the Hamiltonian for the medium, then

$$H_N g_{\gamma,M} = W_{\gamma} g_{\gamma,M} \quad (2)$$

where W_{γ} is the energy of the medium when it is in the state (γ, M) .

The incident particle is described by a complete set of plane wave functions λ_q where $q = (\vec{q}, \nu)$ and $\vec{q}$ is its momentum and ν its spin orientation. Then

$$h \lambda_q = \epsilon_q \lambda_q \quad (3)$$

Here, h is the kinetic energy operator for this particle. The interaction potential of the incident particle and the medium is a sum of two-body interactions

$$V = \sum_{\alpha=1}^N V_{\alpha} \quad (4)$$

where V_{α} is its interaction with the α th particle of the medium.

Defining

$$H_O = H_N + h \quad (5)$$

The Schrodinger equation which describes the scattering is

$$(H_O + V) \psi_a = E_a \psi_a \quad (6)$$

which has the boundary condition that for large distances from the scattering system

$$\psi_a \rightarrow g_{\gamma_O, M_O} \lambda_{q_O} = |a\rangle \quad (7)$$

because the interaction is short range, i.e., $V(|\vec{r}-\vec{r}_\alpha|) \rightarrow 0$ as $|\vec{r}-\vec{r}_\alpha| \rightarrow \infty$. Here (γ_0, M_0) represents the initial state of the scattering system.

The problem will be approached from the standpoint of the formal theory of scattering. The Moller wave matrix Ω is defined such that

$$\psi_a = \Omega g_{\gamma_0 M_0} \lambda_{q_0} = \Omega |a\rangle. \quad (8)$$

Contrast this with the definition of the T matrix

$$V\psi_a = T|a\rangle \quad (9)$$

and it is clear that

$$T = V\Omega. \quad (10)$$

The Schrodinger equation (6) for ψ_a is equivalent to the integral equation for Ω .

$$\Omega = 1 + a^{-1}V\Omega \quad (11)$$

where

$$a = E_a + i\eta - H_0. \quad (12)$$

Here, η is the usual positive, infinitesimal parameter introduced to define integrals involving a^{-1} .

We wish to define an operator F which will separate the scattered wave into parts "coherent" and "incoherent" with respect to the incident wave. The "coherent" wave is that part of the scattered wave which leaves the state of the scattering system unchanged, i.e., remains $|a\rangle$. Thus, we write

$$\Omega = F\Omega_c \quad (13)$$

where F and Ω_c are defined to be the solutions to the equations

$$F = 1 + \frac{1}{a-\theta}(V-\theta)F, \quad \Omega_c = 1 + a^{-1}\theta\Omega_c. \quad (14)$$

The matrix θ is yet to be determined, except that we will stipulate that Ω_c , and therefore θ , must be diagonal in the states $|\gamma\rangle$ describing the spatial state of the scattering system:

$$\langle \gamma'M' | \theta | \gamma M \rangle = \delta_{\gamma\gamma'} \langle \gamma M' | \theta | \gamma M \rangle \quad (15)$$

$$\langle \gamma'M' | \Omega_c | \gamma M \rangle = \delta_{\gamma\gamma'} \langle \gamma M' | \Omega_c | \gamma M \rangle.$$

Clearly Ω_c must be diagonal if $\Omega_c|a\rangle$ is to be the coherent scattered wave. That it is the correct diagonal matrix, i.e., the diagonal part of Ω , will depend on F being selected properly. This will be checked later. It can be shown that (13) and (14) provide a solution to (11).

Actually, as Ω_c is defined by (15), $\Omega_c|a\rangle$ is the "forward" (including spin-flip) scattered wave rather than the "coherent" wave, because a change in one of the indices M destroys complete coherence. Watson assumes for convenience that none of the states $|\gamma M\rangle$ are degenerate, so in the absence of a magnetic field there is no distinction between "coherent" and "forward" in his case. With this understanding, we will continue to use the word "coherent" much of the time.*

It is quite important that we be able to separate the forward-scattered wave from the non-forward scattered wave, because then we can

* The reason we don't require Ω_c to be diagonal in the states $|\gamma M\rangle$ has to do with the fact that experiments don't usually measure final spin states or deal with polarized incident beams.

put the proper attenuation of the incident beam into the problem. (The coherent wave by itself must not conserve particles.) Failure to include the shadow effect, i.e., failure to treat the coherent wave properly, leads to breakdowns in the result for the incoherent wave such as failure of the cross section to obey the optical theorem and, of course, failure of the incoherent wave to show any effects of attenuation. Furthermore, a specific consequence of ignoring beam attenuation for an ideal gas scattering system in the static approximation is that the double-scattering contribution to the cross section is about 10^4 times larger than single scattering for cases for which multiple scattering is known to be of the order of a few percent. The reason I stress this point is that the last two papers in the literature on multiple scattering of thermal neutrons (References (1) and (2)) approach the problem from a simplified point of view that will yield the undesirable consequences described above.

Now let us require that F satisfy

$$F = 1 + \frac{1}{a-\theta} PVF \quad (16)$$

where P is an "operator" acting on VF yet to be specified. If (16) is to be equivalent to (14), then we must require

$$(1-P)V\Omega_c|a\rangle = \theta\Omega_c|a\rangle. \quad (17)$$

Equation (16) is in a convenient form for introducing a "multiple scattering" solution:

$$F = 1 + d^{-1} \sum_{\alpha=1}^N P t_{\alpha} F_{\alpha},$$

$$F_{\alpha} = 1 + d^{-1} \sum_{\beta \neq \alpha}^N P t_{\beta} F_{\beta} , \quad (18)$$

$$t_{\alpha} = V_{\alpha} + V_{\alpha} d^{-1} P t_{\alpha} ,$$

where

$$d = a - \theta .$$

It can be shown that Eq. (18) satisfies Eq. (16). Notice that iterating (18) gives

$$F = 1 + d^{-1} \sum_{\alpha=1}^N P t_{\alpha} + d^{-1} \sum_{\substack{\alpha, \beta=1 \\ \beta \neq \alpha}}^N P t_{\alpha} d^{-1} P t_{\beta} + \dots \quad (19)$$

which in conjunction with Eqs. (13) and (8) provides pretty much the type of wave function one would want in order to describe multiple scattering. The coherent wave, the single scattered incoherent wave, the double scattered incoherent wave, etc., all appear as separate terms. The particle propagates between scatterings (each t_{α} corresponds to a scattering event) according to the propagator d^{-1} . Thus d describes the medium and t_{α} the details of each scattering event. The restriction on the sums—that no two adjacent indices can be equal—also has a physical interpretation: a particle cannot scatter twice in succession off the same nucleus.

There are three things one might question about Eq. (19). One is the fact that the propagator appearing in (19) is d rather than a . The inclusion of θ in the description of the medium is necessary in order to exhibit the previously discussed attenuation of the incident beam.

The presence of the P's in (19) insures, for example, that the double scattering term is actually composed of two incoherent scatters (if it were one incoherent and one forward scatter, it would be, for all practical purposes, a single scattering event). Finally, there is the fact that t_α as given by (18) is not quite the two body scattering operator because of the P and the presence of d instead of a.

The objective now is to choose a P, using the criterion that θ , as determined by Eq. (17), has to be diagonal in the γ -states. Watson's first choice for P is $P = P_{ND}$ where the effect of P_{ND} is best illustrated by

$$\langle \gamma_e | P_{ND} t_\alpha | \gamma_m \rangle = \langle \gamma_e | t_\alpha | \gamma_m \rangle (1 - \delta_{em}) \quad (20)$$

From Eq. (17),

$$\langle \gamma | (1 - P_{ND}) V F \Omega_c | \gamma_o \rangle = \langle \gamma | \theta F \Omega_c | \gamma_o \rangle$$

Using the general relation, which can be proved,

$$V F = \sum_{\alpha} t_{\alpha} F_{\alpha} \quad (21)$$

and the property of P_{ND} (and of $1 - P_{ND}$) Watson shows

$$\langle \gamma' | \theta | \gamma \rangle \approx \delta_{\gamma\gamma'} \langle \gamma | \sum_{\alpha} t_{\alpha} | \gamma \rangle \quad (22)$$

after some manipulation and approximation. (We are suppressing indices other than γ .) The approximation, according to Watson, is better the more uncorrelated the position of the scattering nuclei are. His reasoning escapes me. It appears that the approximation is simply a case of neglecting one part in N (where N is the number of scatterers) of "something", and hence is uniformly good for any type of scattering material.

Another possibility for P which insures that θ is diagonal is to extend the powers of P_{ND} to include control over virtual states. This is called $P = P_0$ and its effect is best shown by the example

$$\langle \gamma_1 | P_0 t_{\alpha 1} | \gamma_2 \rangle \langle \gamma_2 | t_{\alpha 2} | \gamma_3 \rangle \langle \gamma_3 | \cdot \cdot \cdot \cdot | \gamma_n \rangle$$

which means that the expression vanishes if any of the states $\gamma_2, \gamma_3, \dots, \gamma_n = \gamma_0$. If γ_1 is not repeated, $P_0 = 1$. If there were a P_0 paired with each t_α in the expression, then all the states $\gamma_1, \gamma_2, \dots, \gamma_n$ must be distinct or the expression vanishes. In other words, a P_0 operates back on the γ - state preceding it and says it cannot be repeated. Thus, $(1-P_0)$ requires that the γ - state preceding it must be repeated at least once or the whole expression vanishes. Note that both P_0 and P_{ND} affect only the γ index (not M, q or v) of a given state of the entire system.

By a process similar to that used for the case of $P = P_{ND}$, Watson concludes that $P = P_0$ satisfies (17) for

$$\begin{aligned} \langle \gamma' M' q' | \theta | \gamma M q \rangle &\approx \delta_{\gamma \gamma'} \langle \gamma' M' q' | \sum_{\alpha} t_{\alpha} F_{\alpha} | \gamma M q \rangle \\ &\equiv \mathcal{V}_c \end{aligned} \quad (23)$$

where the approximation is essentially the same as before, according to Watson, and my previous comment also applies again—that I don't see that the approximation has anything to do with the structure of the scattering sample.

This latter θ is called the optical model potential. We have just seen that Watson chose to calculate $\langle \gamma | \theta | \gamma \rangle$ where γ is any possible spatial state of the scattering system. The analysis is much simpler, for $P = P_0$, if one tries to calculate $\langle \gamma_0 | \theta | \gamma_0 \rangle$ where $|\gamma_0\rangle$ is a

special γ - state—the initial state of the system. By (17),

$$\begin{aligned}\langle \gamma_0 | (1-P_0)VF | \gamma_0 \rangle &= \langle \gamma_0 | \theta F | \gamma_0 \rangle \\ &= \sum_{\gamma_e} \langle \gamma_0 | \theta | \gamma_e \rangle \langle \gamma_e | F | \gamma_0 \rangle \\ &= \langle \gamma_0 | \theta | \gamma_0 \rangle \langle \gamma_0 | F | \gamma_0 \rangle\end{aligned}$$

because θ is diagonal in the γ - states. The left hand side already satisfies the requirement of $(1-P_0)$ — $\langle \gamma_0 |$ is repeated at least once—so we have

$$\begin{aligned}\langle \gamma_0 | VF | \gamma_0 \rangle &= \langle \gamma_0 | \theta | \gamma_0 \rangle \langle \gamma_0 | F | \gamma_0 \rangle \\ \langle \gamma_0 | \sum_{\alpha} t_{\alpha}^F | \gamma_0 \rangle &= \langle \gamma_0 | \theta | \gamma_0 \rangle \langle \gamma_0 | F | \gamma_0 \rangle\end{aligned}$$

by Eq. (21). Now examine $\langle \gamma_0 | F | \gamma_0 \rangle$ for $P = P_0$.

$$\begin{aligned}\langle \gamma_0 | F | \gamma_0 \rangle &= \langle \gamma_0 | 1+d^{-1} \sum_{\alpha_1} P_0 t_{\alpha_1} + d^{-1} \sum_{\substack{\alpha_1, \alpha_2 \\ \alpha_2 \neq \alpha_1}} P_0 t_{\alpha_1} d^{-1} P_0 t_{\alpha_2} + \dots | \gamma_0 \rangle \\ &= \langle \gamma_0 | 1 | \gamma_0 \rangle + 0 \\ &= 1\end{aligned}$$

All the terms except the first in the expansion for F vanish because of P_0 and the fact that the initial and final states are the same.

Thus, with no approximating,

$$\langle \gamma_0 | \theta | \gamma_0 \rangle = \langle \gamma_0 | \sum_{\alpha} t_{\alpha}^F | \gamma_0 \rangle \quad (24)$$

There is no conflict between this result and Eq. (23). For $\gamma = \gamma_0$,

Watson's approach would yield exactly Eq. (24) instead of (23), although this fact obviously is buried in the approximation he made to get (23). One might think that (24) would be valid for any γ -state, since at first glance the special property of γ_0 being the initial state does not seem to be a factor. But it is. F operates only on Ω_c which is defined to operate only on the initial state $|a\rangle \equiv |\gamma_0 M_0 q_0\rangle$. So the question is, do you really need to know all the matrix elements of the diagonal (in γ -states) matrix, or will $\langle \gamma_0 | \theta | \gamma_0 \rangle$ suffice? We will comment on this each time the need arises to know something about the optical potential.

Let us summarize the possibilities for P and θ .

TABLE I

P	$\langle \gamma \theta \gamma \rangle$
1	0
P_{ND}	$\approx \langle \gamma \sum_{\alpha} t_{\alpha} \gamma \rangle$
P_0	$\approx \langle \gamma \sum_{\alpha} t_{\alpha}^F \gamma \rangle$ $= \langle \gamma \sum_{\alpha 1} t_{\alpha 1} \gamma \rangle + \langle \gamma \sum_{\substack{\alpha 1, \alpha 2 \\ \alpha 1 \neq \alpha 2}} t_{\alpha 1} d^{-1} P_0 t_{\alpha 2} \gamma \rangle + \dots$
P_0	$\langle \gamma_0 \theta \gamma_0 \rangle = \langle \gamma_0 \sum_{\alpha} t_{\alpha}^F \gamma_0 \rangle$

Notice that the θ corresponding to $P = P_{ND}$ is the first term in the expansion of the θ corresponding to $P = P_O$ (the optical potential). Notice further that the second term involves double scattering events in which the incident particle scatters twice incoherently (the presence of the single P_O is enough to insure this) only to return the system to its initial γ -state—surely a highly unlikely type of event except for a scattering system with a high degree of correlation, like a crystal. Even in this extreme case, it is not clear that neglecting these higher order terms (i.e., selecting P_{ND} and $\langle \gamma | \theta | \gamma \rangle = \langle \gamma | \sum_{\alpha} t_{\alpha} | \gamma \rangle$ instead of the full blown optical model) is so bad an approximation. Actually, one can physically interpret what is being neglected. It is pretty clear that one is ignoring the augmenting of the coherent beam arising from the system's returning to its original state after n incoherent scatters. In other words, if one settles for $P = P_{ND}$ and $\langle \gamma | \theta | \gamma \rangle = \langle \gamma | \sum_{\alpha} t_{\alpha} | \gamma \rangle$, one is counting all incident particles suffering at least one incoherent scatter as lost from the coherent (incident) beam. This ignores the possibility that such a neutron can scatter back into the coherent beam and hence augment it. In effect, one is treating multiple incoherent scattering by ignoring multiple scattering in the coherent beam.

Support for this interpretation arises when we check, as we said we would, to see if Ω_c is the right diagonal matrix—i.e., the diagonal part of Ω . From (13)

$$\Omega = F\Omega_c$$

$$\langle \gamma | \Omega | \gamma \rangle = \langle \gamma | F\Omega_c | \gamma \rangle$$

$$\begin{aligned}
&= \sum_{\gamma_e} \langle \gamma | F | \gamma_e \rangle \langle \gamma_e | \Omega_c | \gamma \rangle \\
&= \langle \gamma | F | \gamma \rangle \langle \gamma | \Omega_c | \gamma \rangle
\end{aligned}$$

because Ω_c is diagonal. We have already shown that $\langle \gamma_o | F | \gamma_o \rangle = 1$ for $P = P_o$. The proof holds for any γ -state. The proof does not hold for $P = P_{ND}$ as can quite quickly be shown. Thus, only for $P = P_o$ does F effect the desired separation of the scattered wave into coherent and incoherent parts.

There would seem to be no more sophisticated choice of P than $P = P_o$. It accomplishes perfectly the job it is supposed to do—isolate the coherent beam. At this point it might be worth commenting on the fact that P_o , as an operator, is certainly strange. At the least it must be non-linear. However, P_o should not be regarded as an actual operator but as a counting or bookkeeping aid. What type of scattering events one chooses to categorize by the word "coherent", one does not wish also to include in the "incoherent" contribution. P_o reminds us what we must do at every stage of the game in order to achieve this consistency.

Thus, certainly for cases where the scatterer positions are weakly correlated, one can approximate the optical model by $P = P_{ND}$ and $\langle \gamma | \theta | \gamma \rangle = \langle \gamma | \sum_{\alpha} t_{\alpha} | \gamma \rangle$. The other choice shown in Table I is the trivial choice of $P = 1$, corresponding to $\theta = 0$. Since θ provides the attenuation of the incident beam (as we shall see), this choice is not desirable. This selection incidentally is the unconscious choice of References (1) and (2) as well as applying to part of the results in Reference (3).

A little more, mostly speculation, will be said later concerning the choice of P and θ . For now, notice one more thing. For an ideal gas scattering system, one can quickly convince oneself that $P = P_{ND}$ is quite a good choice (as, of course, we thought it should be). Because of the ideal gas model, it is impossible to return the scattering system to its initial state in fewer than four successive scatterings by the incident particle. Thus the first multiple scattering term in the expansion for the optical potential that does not vanish exactly is the quadruple scattering term; therefore, $\langle \gamma | \theta | \gamma \rangle = \langle \gamma | \sum_{\alpha} t_{\alpha} | \gamma \rangle$ should be quite a good approximation for the ideal gas. As far as the choice of which P to use is concerned, if one calculates only double scattering or triple scattering corrections to the cross section, one should get exactly the same results for $P = P_{ND}$ as for $P = P_0$. The author essentially verified this in Reference (3) by arbitrarily inserting P 's in the multiple scattering expansion. Of course, the attenuation effect did not show because θ was still zero.

Now let's get a clearer idea of the role played by θ . As we mentioned previously, its appearance in the propagator d^{-1} suggests it augments the description of the medium in which the incident particle travels between scatters. Let's make this more explicit. Define

$$\psi_{ca} \equiv \Omega_c |a\rangle \quad (25)$$

Since $|\gamma_0\rangle$ is an eigenstate of Ω_c , it seems likely that $|\gamma_0\rangle \equiv g_{\gamma_0}$ appears as a simple factor in ψ_{ca} . Thus define Φ_{ca} by

$$\psi_{ca} = \Phi_{ca} g_{\gamma_0} \quad (26)$$

or

$$\Phi_{ca} = \langle g_{\gamma_0} | \psi_{ca} \rangle \quad (27)$$

Now, from Eq. (14), Ω_c satisfies

$$\Omega_c = 1 + a^{-1} \theta \Omega_c$$

$$\therefore \Omega_c |a\rangle = |a\rangle + a^{-1} \theta \Omega_c |a\rangle$$

$$\therefore \psi_{ca} = |a\rangle + a^{-1} \theta \psi_{ca}$$

$$\langle g_{\gamma_0} | \psi_{ca} \rangle = \langle g_{\gamma_0} | a \rangle + \sum_{\gamma_e \gamma_m} \underbrace{\langle \gamma_0 | a^{-1} | \gamma_e \rangle \langle \gamma_e | \theta | \gamma_m \rangle}_{\text{(both diagonal)}} \langle \gamma_m | \psi_{ca} \rangle$$

$$\therefore \Phi_{ca} = |M_o \lambda_{q_o} \nu_o\rangle + \frac{1}{\epsilon_{q_o} - h + i\eta} v_c \Phi_{ca}$$

where v_c is defined by

$$v_c = \langle \gamma_o | \theta | \gamma_o \rangle \quad (28)$$

as opposed to the definition of v_c in Eq. (23). Note that we define v_c with respect to a particular γ -state, $\gamma = \gamma_o$.

Continuing,

$$(\epsilon_{q_o} - h) \Phi_{ca} = \underbrace{(\epsilon_{q_o} - h) |M_o \lambda_{q_o} \nu_o\rangle}_{=0} + v_c \Phi_{ca}$$

Thus,

$$(h + v_c) \Phi_{ca} = \epsilon_{q_o} \Phi_{ca} \quad (29)$$

This equation depends on the spatial coordinates of only the incident particle. By its definition, Φ_{ca} is related to the coherent beam of incident particles. Thus, Eq. (29) is an effective reduction of the problem of the interaction of the coherent beam with the medium to that of a particle in a force field.

For a large uniform scattering medium, one can consider v_c to be some function of the momentum operator for the incident particle, i.e., it is diagonal, to a good approximation, with respect to the spatial states (plane waves) of the incident particle. Thus, Eq. (29) has a solution of the form

$$\Phi_{ca} = (2\pi)^{-3/2} e^{i\mathbf{k}_0 \cdot \mathbf{r}} \quad (30)$$

which, when substituted into (29) yields the following equation which $\mathbf{k}_0$ must satisfy:

$$\frac{\hbar^2 \mathbf{k}_0^2}{2m} + v_c(\mathbf{k}_0) = \epsilon_{q_0} \quad (31)$$

For the case of slab geometry, with the incident beam perpendicular to the face of the slab, $\mathbf{k}_0$ is in the direction of $\mathbf{q}_0$, the actual incident particle wave vector.

We take v_c to be complex. Thus, by Eq. (31), $\mathbf{k}_0$ is complex. Since the wave described by Φ_{ca} propagates as $e^{i\mathbf{k}_0 \cdot \mathbf{r}}$ in the medium, a positive imaginary part for $\mathbf{k}_0$ gives the long-sought attenuation of the incident beam. As Watson is careful to point out, $\mathbf{k}_0$ is not an actual particle momentum because Eq. (29) is not the actual Schrodinger equation for the coherent beam of incident particles. It is a reduction of a many-body problem to a related two-body problem. Thus, we are not claiming to have complex momenta!

IDEAL GAS IN THE STATIC APPROXIMATION

The scattered wave function is

$$\psi_a = \Omega |a\rangle = F\Omega_c |a\rangle$$

$$= [1 + d^{-1} \sum_{\alpha 1} P t_{\alpha 1} + d^{-1} \sum_{\substack{\alpha 1, \alpha 2 \\ \alpha 1 \neq \alpha 2}} P t_{\alpha 1} d^{-1} P t_{\alpha 2} + \dots] \phi_{ca} g_{\gamma_0} \quad (32)$$

and it exhibits the desired separation of the various orders of multiple scattering. The first term is the coherent wave, the second the single-scattered incoherent wave, the third the double-scattered incoherent wave, etc.

Now let us specialize to a particular scattering system and assume that the incident particles are thermal neutrons of momentum $\hbar \underline{q}_0$. Consider an ideal gas of heavy atoms (neglect possible spin interactions) so that the static approximation applies. We shall approximate θ by the diagonal part of $\sum_{\alpha} t_{\alpha}$. As we have indicated previously, this should be an excellent approximation for the ideal gas. We can now approximately determine both the real and the imaginary parts of k_0 . We shall later show that $v_c(k_0) \ll \epsilon_{q_0}$ so that the real part of k_0 is much greater than the imaginary part

$$k_0 = k_{0R} + i k_{0I} \quad (33)$$

$$k_{0R} \gg k_{0I}$$

and approximately equal to q_0 .

$$k_{0R} \approx q_0 \quad (34)$$

To estimate k_{0I} , we use the optical theorem:

$$\text{Im} \{f(o)\} = \frac{q_0}{4\pi} \sigma_{\text{tot}} \quad (35)$$

First we make some calculations. From Eq. (31) $v_c(k_o)$ is defined to be

$$\begin{aligned}
 v_c(k_o) &= \langle \underline{k}_o | v_c(\vec{q}_{op}) | \underline{k}_o \rangle ; | \underline{k}_o \rangle = e^{i \underline{k}_o \cdot \underline{r}} \\
 &= \langle \gamma_{o-o} \underline{k}_o | \theta | \gamma_{o-o} \underline{k}_o \rangle \\
 &\approx \langle \gamma_{o-o} \underline{k}_o | \sum_{\alpha} t_{\alpha} | \gamma_{o-o} \underline{k}_o \rangle \\
 &\approx N \langle \gamma_{o-o} \underline{k}_o | t | \gamma_{o-o} \underline{k}_o \rangle
 \end{aligned} \tag{36}$$

We have further made the approximation

$$\langle \gamma_{o-o} \underline{k}_o | \sum_{\alpha=1}^N t_{\alpha} | \gamma_{o-o} \underline{k}_o \rangle \approx N \langle \gamma_{o-o} \underline{k}_o | t | \gamma_{o-o} \underline{k}_o \rangle \tag{37}$$

where t is the two-body scattering operator. Now substitute $k_o = q_o + i k_{oI}$ into Eq. (31); one obtains

$$\frac{\hbar^2 q_o^2}{2m} + 2i\hbar^2 \frac{q_o k_{oI}}{2m} + v_c(k_o) = \epsilon_{q_o}$$

We neglect the square of the small quantity k_{oI} . The imaginary part of this complex equation says

$$\frac{\hbar^2}{m} q_o k_{oI} + \text{Im} \{ v_c(k_o) \} = 0$$

and by (36) have

$$\frac{\hbar^2}{m} q_o k_{oI} + N \text{Im} \langle \gamma_{o-o} \underline{k}_o | t | \gamma_{o-o} \underline{k}_o \rangle = 0$$

We can approximate $\langle \gamma_{o-o} \underline{k}_o | t | \gamma_{o-o} \underline{k}_o \rangle$ by $\langle \gamma_{o-o} \underline{q}_o | t | \gamma_{o-o} \underline{q}_o \rangle$, and then use the optical theorem, since

$$f(o) = \frac{-m}{2\pi\hbar^2} \langle \gamma_{o-o} \underline{q}_o | t | \gamma_{o-o} \underline{q}_o \rangle \tag{38}$$

to get

$$\begin{aligned} \frac{\hbar^2}{m} q_o k_{oI} - \frac{2\pi\hbar^2}{m} N \frac{q_o}{4\pi} \sigma_{tot} &= 0 \\ k_{oI} &= \frac{N\sigma_{tot}}{2} = \frac{\Sigma}{2} = \frac{1}{2\lambda} \\ k_{oI} &= \frac{1}{2\lambda} \end{aligned} \quad (39)$$

where, if there is no absorption present, λ is the scattering mean free path.

Now we can quickly verify that $q_o \gg k_{oI}$. If λ_{deB} is the deBroglie wavelength of the incident particles, then

$$q_o = \frac{1}{\lambda_{deB}}$$

so

$$q_o \gg k_{oI} \quad \text{if} \quad \lambda_{deB} \ll \lambda$$

which is a very good approximation.

Notice that we have had to say something explicit about the optical potential θ to deduce that $k_{oI} = \frac{1}{2\lambda}$, namely

$$\langle \gamma_o | \theta | \gamma_o \rangle \approx \langle \gamma_o | \sum_{\alpha} t_{\alpha} | \gamma_o \rangle \approx N \langle \gamma_o | t | \gamma_o \rangle$$

The point is, we had to know the expectation value of θ just for the initial γ -state, not for any possible γ -state.

Now let's calculate the single scattering term in the scattered wave function of Eq. (32) for this problem. The expression is

$$(2\pi)^{-3/2} \sum_{\alpha} d^{-1} t_{\alpha} e^{i\mathbf{k}_o \cdot \mathbf{r}} g_{\gamma_o} \quad (40)$$

Introduce a complete set of intermediate neutron and nuclear states

$$= (2\pi)^{-9/2} \sum_{\alpha} d^{-1} \sum_{\gamma} \int d^3q | \gamma e^{i\mathbf{q} \cdot \mathbf{r}} \rangle \langle e^{i\mathbf{q} \cdot \mathbf{r}} | P t_{\alpha} | e^{i\mathbf{k}_0 \cdot \mathbf{r}} \rangle g_{\gamma_0}$$

Note: the q 's are real.

Consider

$$\langle e^{i\mathbf{q} \cdot \mathbf{r}} | P t_{\alpha} | e^{i\mathbf{k}_0 \cdot \mathbf{r}} \rangle$$

$$t_{\alpha} = (1 - V_{\alpha} d^{-1} P)^{-1} V_{\alpha}$$

The only approximation known for evaluating the matrix elements of a scattering operator between thermal neutron states is the Lippmann-Schwinger approximation

$$\langle e^{i\mathbf{q}_0 \cdot \mathbf{r}} | t_{\alpha}^{(0)} | e^{i\mathbf{k}_0 \cdot \mathbf{r}} \rangle = \frac{2\pi\hbar^2}{m} a_b e^{i(\mathbf{k}_0 - \mathbf{q}) \cdot \mathbf{r}_{\alpha}} \quad (41)$$

where

$$t_{\alpha}^{(0)} = (1 - V_{\alpha} G_0)^{-1} V_{\alpha}$$

and

$$G_0 = \left[-\frac{\vec{P}_n^2}{2\mu} + i\eta \right]^{-1}$$

and " a_b " is the bound atom scattering length, $\vec{P}_n$ is the momentum operator for the neutron, and μ is the reduced mass of the neutron and nucleus.

Our job is cut out for us. We have to approximate t_{α} by $t_{\alpha}^{(0)}$ which means approximating d^{-1} by G_0 ; i.e., we require

$$W_{\gamma_0} + \epsilon_{q_0} - H_N - h - \theta + i\eta \rightarrow -h + i\eta \quad (42)$$

(Since we assume the nuclei are heavy, $\mu \approx m$, the neutron mass.) The static approximation enables us to ignore W_{γ_0} and H_N .

Now consider from Eq. (36)

$$v_c(k_0) \approx N \langle \gamma_{00}^{k_0} | t | \gamma_{00}^{k_0} \rangle$$

$$\approx -N \frac{2\pi\hbar^2}{m} f(0)$$

We can make an order-of-magnitude comparison of this with

$$\epsilon_{q_0} = \frac{\hbar^2 q_0^2}{2m}$$

and thereby get some idea whether we can neglect θ compared with $\hbar$ in Eq. (42). Assuming $N \sim 10^{23}$, $f(0) \sim 10^{-12}$ cm, and $q_0 \sim 10^8$ cm⁻¹,

$$\frac{v_c(k_0)}{\epsilon_{q_0}} \approx \frac{10^{23} \cdot 10^{-12} \cdot 10}{10^{16}} = \frac{1}{10^4}$$

This should not be interpreted as meaning we can just forget about the optical potential completely. The important thing about the optical potential is that it is complex and even a small amount of damping is significant if the neutron travels far enough in the medium.

Thus, we can see our way clear to approximating d^{-1} by G_0 . In evaluating

$$d^{-1} | \gamma e^{iq \cdot r} \rangle$$

we use only the static approximation (this time) on d so that

$$d \rightarrow d_0 = \left[\epsilon_{q_0} - \hbar - \theta + i\eta \right]^{-1} \quad (43)$$

and thus have

$$d^{-1} | \gamma e^{iq \cdot r} \rangle = \left[\epsilon_{q_0} - \frac{\hbar^2 q^2}{2m} - v_c^{(\gamma)}(q) + i\eta \right]^{-1} | \gamma e^{iq \cdot r} \rangle$$

where

$$v_c^{(\gamma)}(q) \equiv \langle e^{iq \cdot r} | \theta | \gamma e^{iq \cdot r} \rangle$$

as opposed to $v_c(q)$, defined just for $\gamma = \gamma_0$. So here we need all the diagonal elements of θ with respect to the γ - states. Eq. (40) can now be written

$$(2\pi)^{-7/2} \frac{\hbar^2}{m} a_b \sum_{\alpha} \sum_{\gamma} |\gamma\rangle \langle \gamma | e^{ik_0 \cdot r_{\alpha}} \int d^3q \frac{e^{iq \cdot (r - r_{\alpha})}}{\epsilon_{q_0} - \frac{\hbar^2 q^2}{2m} - v_c^{(\gamma)}(q) + i\eta} |\gamma_0\rangle \quad (44)$$

The integral

$$\int \frac{d^3q e^{iq \cdot (r - r_{\alpha})}}{\frac{\hbar^2 q_0^2}{2m} - \frac{\hbar^2 q^2}{2m} - v_c^{(\gamma)}(q) + i\eta} \quad (45)$$

can be evaluated by contour integration to yield

$$\frac{2m}{\hbar^2} \frac{(-2\pi^2)}{|r - r_{\alpha}|} e^{iq' \cdot |r - r_{\alpha}|} \quad (46)$$

where q' is the root of

$$\frac{\hbar^2}{2m}(q_0^2 - q'^2) - v_c^{(\gamma)}(q') = 0$$

In order to get anywhere at this point, one has to (and Watson does)

approximate $v_c^{(\gamma)}$ by $v_c^{(\gamma_0)} \equiv v_c$ so that, by Eq. (31),

$$q' = k_0$$

So, once more, all one needs is $\langle \gamma_0 | \theta | \gamma_0 \rangle$.

Eq. (44) for the single scattered wave becomes finally

$$-(2\pi)^{-3/2} a_b \sum_{\alpha} \frac{e^{ik_0 \cdot |r - r_{\alpha}|}}{|r - r_{\alpha}|} e^{ik_0 \cdot r_{\alpha}} |\gamma_0\rangle \quad (47)$$

which is essentially Watson's result. In going from Eq. (44) to Eq. (47),

we have had to set $P = 1$ so that we could invoke the closure property of the complete set of γ -states. Since we certainly do not want to take $\theta = 0$, this seems to involve approximating P and θ to different orders, according to Table 1. There is nothing inherently wrong in this provided the combination gives a sufficiently good degree of approximation for the ideal gas in the static approximation. Watson apparently feels that it does. I have my doubts and will say more about this later. The effect on the result (47) of choosing $P = P_{ND}$ would be to subtract from (45) a correction term equal to (44) evaluated for $\gamma = \gamma_0$. For single scattering, however, the question isn't important because such a correction term would involve a delta function of the momentum transfer and be identifiable therefore as forward scattering—purely and simply part of the coherent beam.

A similar treatment for the double scattered term in Eq. (32) yields

$$\sum_{\substack{\alpha_1, \alpha_2=1 \\ \alpha_1 \neq \alpha_2}}^N (2\pi)^{-11/2} \left(\frac{\hbar^2}{m}\right)^2 a_b^2 \sum_{\gamma, \gamma_e} \int d^3 q \frac{e^{i\mathbf{q} \cdot \mathbf{r}}}{d(q)} \int d^3 q_e \frac{1}{d(q_e)} |\gamma\rangle$$

$$(x) \langle \gamma | P e^{i(\mathbf{q}_e - \mathbf{q}) \cdot \mathbf{r}_{\alpha 1}} | \gamma_e \rangle \langle \gamma_e | P e^{i(\mathbf{k}_0 - \mathbf{q}_e) \cdot \mathbf{r}_{\alpha 2}} | \gamma_0 \rangle \quad (48)$$

where

$$d(q) = -\frac{\hbar^2 q^2}{2m} + \frac{\hbar^2 q_0^2}{2m} - v_c^{(\gamma)}(q) + i\eta$$

and for $P = 1$, Eq. (48) reduces to

$$(2\pi)^{-3/2} a_b^2 \sum_{\substack{\alpha_1, \alpha_2=1 \\ \alpha_1 \neq \alpha_2}}^N \frac{e^{i\mathbf{k}_0 \cdot (\mathbf{r} - \mathbf{r}_{\alpha 1})}}{|\mathbf{r} - \mathbf{r}_{\alpha 1}|} \frac{e^{i\mathbf{k}_0 \cdot (\mathbf{r}_{\alpha 1} - \mathbf{r}_{\alpha 2})}}{|\mathbf{r}_{\alpha 1} - \mathbf{r}_{\alpha 2}|} e^{i\mathbf{k}_0 \cdot \mathbf{r}_{\alpha 2}} \quad (49)$$

which is essentially Watson's result. The corrections to Eq. (49) stemming from $P = P_{ND}$ are simply the negative of Eq. (48) evaluated for $\gamma_e = \gamma$ (all γ) and for $\gamma_e = \gamma_0$ (all γ). Concerning these correction terms, the author examined the case $P = P_{ND}$ but $\theta = 0$ in Reference (3) (as was mentioned before) and found that the effect on the cross section of these terms was enormous, and not just in the forward direction. Whether such a contribution was a spurious effect due to the absence of attenuation in the model is hard to say. We shall see why it is hard to say when we try to get an analytical result for the cross section.

Our expressions (47) and (49) clearly are not valid for large $\underline{r}$. Eq. (49), for example, shows the neutron plane wave propagating with attenuation from the point at which it enters the slab medium ($\underline{r} = 0$) to the α_2 'nd nucleus, located at $\underline{r}_{\alpha_2}$. A spherical wave propagates with attenuation from this first collision point to the second collision, with the nucleus labeled α_1 . Finally another spherical wave propagates with attenuation from this second collision point arbitrarily far into space.

To get the neutron "out of the scattering medium," we must go back to Eq. (45) and note that $v_c^{(\gamma)}(q) = 0$ outside the scattering medium and thus $q' = k_0$ for $\underline{r}$ inside the scattering system but $q' = q_0$ for $\underline{r}$ outside the scattering system. Matching wave functions at the sample boundary gives for the single scattered wave function outside the scattering sample

$$= (2\pi)^{-3/2} a_b \alpha \ e^{\frac{1}{2} \underline{k}_0 \cdot \underline{r} - \alpha} e^{-\frac{1}{2\lambda} \rho(\underline{r}_{\alpha})} \frac{e^{iq_0 |\underline{r} - \underline{r}_{\alpha}|}}{|\underline{r} - \underline{r}_{\alpha}|} \quad (50)$$

where $\rho(r_\alpha)$ is the distance from the α 'th nucleus to the boundary of the scattering system in the direction $(\underline{r}-\underline{r}_\alpha)$. Eq. (49) can be similarly adjusted after the last scattering. Making the conventional "large r " approximations

$$e^{iq_0|\underline{r}-\underline{r}_\alpha|} \approx e^{iq_0 r} e^{-iq_f \cdot \underline{r}_\alpha}; \quad |\underline{r}-\underline{r}_\alpha| \approx r \quad (51)$$

where $\underline{q}_f = \underline{q}_0 \hat{r}$ because of the static approximation. Eq. (50) becomes

$$-(2\pi)^{-3/2} a_b \sum_{\alpha=1}^N e^{i(\underline{k}_0 - \underline{q}_f) \cdot \underline{r}_\alpha} e^{-\frac{1}{2\lambda} \rho(r_\alpha)} \frac{e^{iq_0 r}}{r}$$

or, since $\underline{k}_0 \approx \underline{q}_0 + \frac{1}{2\lambda}$,

$$= - (2\pi)^{-3/2} a_b \sum_{\alpha=1}^N \left\{ e^{i\underline{k} \cdot \underline{r}_\alpha} e^{-\frac{1}{2\lambda} [x_\alpha + \rho(r_\alpha)]} \right\} \frac{e^{iq_0 r}}{r} \quad (52)$$

where $x_\alpha = \frac{\underline{q}_0}{q_0} \cdot \underline{r}_\alpha$ and $\underline{\kappa} \equiv \underline{q}_0 - \underline{q}_f$.

Similarly, Eq. (49) for the double scattered wave becomes for large r :

$$(2\pi)^{-3/2} a_b^2 \left\{ \sum_{\alpha_1 \neq \alpha_2} e^{i\underline{k}_0 \cdot \underline{r}_{\alpha_2}} \frac{e^{iq_0|\underline{r}_{\alpha_1}-\underline{r}_{\alpha_2}|}}{|\underline{r}_{\alpha_1}-\underline{r}_{\alpha_2}|} e^{-\frac{1}{2\lambda} \rho(r_{\alpha_1})} e^{-iq_f \cdot \underline{r}_{\alpha_1}} \right\} \frac{e^{iq_0 r}}{r} \quad (53)$$

We can evaluate $\rho(r_\alpha)$ approximately (in the sense that the expression holds for $\underline{r}_\alpha$ almost everywhere in the scattering sample) for small angle scattering and for nearly-right-angle scattering.

Small Angle Scattering

$$\cos \theta = \frac{x_0 - x_\alpha}{\rho}$$

$$\rho(\underline{r}_\alpha) = \frac{x_0 - x_\alpha}{\cos \theta} \quad (54)$$

Nearly-Right-Angle Scattering

$$\sin \theta = \frac{y_0 - y_\alpha}{\rho}$$

$$\rho(\underline{r}_\alpha) = \frac{y_0 - y_\alpha}{\sin \theta} \quad (55)$$

In each case, θ is the scattering angle, and $\underline{r}_\alpha = (x_\alpha, y_\alpha, z_\alpha)$.

Before going on to the cross section, let me comment on the inevitable "I could have written that down right off the bat" cries concerning Eqs. (52) and (53). Certainly. Better yet, people have.⁽⁶⁾ If Eqs. (52) and (53) didn't look pretty much the way intuition says they should, then is the time to raise a real outcry. The surprise package in the Watson treatment (of course, it is the closest thing to a rigorous derivation, and worth doing for that alone) is the presence of P . Unless it can be shown that $P = 1$ is a good approximation for cases of interest, intuition gets a little jolt here.

THE CROSS SECTION

Write Eq. (32) for the scattered wave

$$\psi_a(\underline{r}) = [A(r) + B(r) + C(r) + \dots] |\gamma_o\rangle \quad (56)$$

where

$$A = (2\pi)^{-3/2} e^{-\frac{x_o}{2\lambda}} e^{i\underline{q}_o \cdot \underline{r}} \quad (57)$$

for a slab scattering system of thickness x_o . B is given by the expression (52) and C by (53).

The cross section is related to the expectation value in the state ψ_a of the quantum mechanical neutron current operator $\underline{J}$, thermal averaged over all possible scattering system initial states γ_o . Denote this vector quantity by $\langle \underline{j}_{sc} \rangle$.

$$\langle \underline{j}_{sc} \rangle = \frac{\sum_{\gamma_o} e^{-\beta w} \gamma_o \langle \psi_a | \underline{J} | \psi_a \rangle}{\sum_{\gamma_o} e^{-\beta w} \gamma_o} \quad (58)$$

The current operator is usually taken to be

$$\underline{J} = 1/2 [\delta(\underline{r}-\underline{R}), \underline{v}_{op}]_+ \quad (59)$$

where $\underline{r}$ is the neutron position vector, $\underline{R}$ is the evaluation point (for our purposes, the location of the detector), $\underline{v}_{op}$ is the neutron velocity operator

$$\underline{v}_{op} = \frac{\hbar}{mi} \nabla_{\underline{r}}$$

and $[\]_+$ denotes the anti-commutator.

One can show, using A and B for example, that

$$\langle A(\underline{r}) | \underline{J} | B(\underline{r}) \rangle = \frac{\hbar}{2mi} [A^* \text{grad } B - B \text{grad } A^*]_{\underline{r}=\underline{R}} \quad (60)$$

$$= \langle B | \underline{J} | A \rangle^*$$

and therefore,

$$\langle A(\underline{r}) | \underline{J} | A(\underline{r}) \rangle = \frac{\hbar}{m} \text{Im} \left\{ A^* \text{grad } A \right\}_{\underline{r}=\underline{R}} \quad (61)$$

Using these relationships and a little manipulation, Eq. (58) becomes

$$\begin{aligned} \underline{j}_{sc} = Z^{-1} \sum_{\gamma} e^{-\beta w_{\gamma}} & \left\langle \gamma \left| \frac{\hbar}{m} \text{Im} \left\{ A^* \text{grad } A + B^* \text{grad } B + C^* \text{grad } C \right. \right. \right. \\ & + A^* \text{grad } B - B \text{grad } A^* + A^* \text{grad } C - C \text{grad } A^* \\ & \left. \left. + B^* \text{grad } C - C \text{grad } B^* \right\}_{\underline{r}=\underline{R}} \right| \gamma \rangle \end{aligned} \quad (62)$$

where

$$Z = \sum_{\gamma} e^{-\beta w_{\gamma}} ; \beta = \frac{1}{kT} \quad (63)$$

From Eq. (57), it is obvious that

$$\text{grad } A = (2\pi)^{-3/2} e^{-\frac{x_0}{2\lambda}} i e^{i \underline{q}_0 \cdot \underline{r}} \underline{q}_0 \quad (64)$$

so that terms involving grad A contribute to the scattered current only in the forward direction and may be ignored. Since

$$\left. \text{grad}_{\underline{r}} \frac{e^{i \underline{q}_0 \cdot \underline{r}}}{r} \right|_{\underline{r}=\underline{R}} = (i \underline{q}_0 - \frac{1}{R}) \frac{e^{i \underline{q}_0 \cdot \underline{R}}}{R} \hat{\underline{R}} \quad (65)$$

(where $\hat{R}$ is the unit vector $\underline{R}/R$)

the other terms are all vectors in the direction $\hat{R}$.

The differential scattering cross section, $\frac{d\sigma}{d\Omega}$ is obtained by multiplying the magnitude of $\langle \underline{j}_{sc} \rangle$ (for $\underline{R}$ in the direction of $\underline{\Omega}$) by R^2 divided by the average incoming current ($\frac{\hbar q_0}{m}$):

$$\frac{d\sigma}{d\Omega} = \frac{R^2}{q_0} \left\langle \text{Im} \left\{ B^* |\text{grad}_{\underline{R}} B| + C^* |\text{grad}_{\underline{R}} C| + B^* |\text{grad}_{\underline{R}} C| - C |\text{grad}_{\underline{R}} B^*| + \right. \right. \\ \left. \left. A^* |\text{grad}_{\underline{R}} B| - B |\text{grad}_{\underline{R}} A^*| + A^* |\text{grad}_{\underline{R}} C| - C |\text{grad}_{\underline{R}} A^*| \right\}_{\underline{R}=\underline{R}} \right\rangle_T \quad (66)$$

$$\text{where } \left\langle \right\rangle_T \equiv Z^{-1} \sum_{\gamma} e^{-\beta w_{\gamma}} \langle \gamma | \theta | \gamma \rangle ; \quad Z = \sum_{\gamma} e^{-\beta w_{\gamma}} \quad (67)$$

is called the thermal average over initial nuclear states.

The terms in Eq. (66) in order represent single scattering, double scattering, interference between single and double scattering, and the last four terms represent the interference between the coherent beam and the incoherent beam. We have neglected multiple scattering of order higher than double scattering.

One can show that the cross section for single scattering for small scattering angles θ is approximately

$$(2\pi)^{-3} |a_b|^2 N \frac{\lambda}{x_0} \frac{e^{-\frac{x_0}{\lambda} \sec \theta}}{\sec \theta - 1} \left[e^{-\frac{x_0}{\lambda}} [1 - \sec \theta] + 1 \right] \quad (68)$$

where x_0 is the thickness of the slab scattering sample. I don't propose to push this any further. Note that the exponential attenuation factors make it impossible to get anywhere analytically except for

single scattering—and then one can get only approximate results for certain scattering angles. This is for the simplest possible model—the ideal gas in the static approximation.

DISCUSSION

If there is any future to attacking multiple scattering quantum mechanically, it must involve numerical integration. Once on the computer, a model involving particle correlations should not be much more difficult than the ideal gas. However, it would be interesting to clear up the ideal gas problem first because it would shed some light on the regions of validity of the various approximations for θ and P mentioned in this report.

As I have stated, I did the ideal gas case in my thesis for $\theta = P$, $P = P_{ND}$ (or P_0 since there is no difference in the ideal gas model through triple scattering). I also did the problem for $\theta = 0$ and $P = 1$, but the results were absurd, with weird oscillating dependence on the dimensions of the scattering sample, double scattering being approximately 10^4 times single scattering, etc. Setting $P = P_{ND}$ went a long way toward clearing up the difficulties. All the interference terms between the various orders of scattering vanished identically (as intuition says they should). The single scattering contribution (per atom) to $\frac{d\sigma}{d\Omega}$ was simply $|a_b|^2$ and the double scattering contribution was $4\pi\rho|a_b|^4 R_0$ where R_0 was the radius of the spherical scattering sample. It should be pointed out that these results are on shaky ground because of an approximation made upon transforming variables of integration—namely that for a large scattering sample, the limits of integration could be held fixed. However, this should probably not

affect the most interesting point—that even for an ideal gas, one apparently cannot use $P = 1$. I say "apparently" because it is still possible that the spurious results were more a result of setting $\theta = 0$ than $P = 1$. A calculation of the interference term between single and double scattering in Eq. (66) would help settle this point.

As for ultimate application to a scattering system of interest—like a crystal—what choice of P and θ one would need to get an accurate approximation is pure speculation. However, it is comforting to know that

$$\langle \gamma_0 | \theta | \gamma_0 \rangle = \langle \gamma_0 | \sum_{\alpha} t_{\alpha}^F | \gamma_0 \rangle \quad (69)$$

is not an approximation based on weak correlations, but applies to anything, including crystals. So if one is convinced that all he needs to know about θ is $\langle \gamma_0 | \theta | \gamma_0 \rangle$, rather than $\langle \gamma | \theta | \gamma \rangle$ for general γ , then at least he has a solid starting point at which he knows where he stands. (As I have pointed out, Watson's paper indicates that (69) is itself an approximation based on weak correlations.) From there, one can make approximations—i.e., terminate the series $\sum_{\alpha=1}^N t_{\alpha}^F$ after one or two terms—with some hope of examining their validity. This is why I stressed the contention throughout this report that Watson really uses only $\langle \gamma_0 | \theta | \gamma_0 \rangle$ in the end.

Going further, it seems possible that approximating $\langle \gamma_0 | \theta | \gamma_0 \rangle$ by the first term in its series $\langle \gamma_0 | \sum_{\alpha} t_{\alpha} | \gamma_0 \rangle$, might not be a bad approximation even for a crystal. That about which it is really difficult even to speculate is the choice of P . Presumably, since each choice of P leads to a corresponding value for $\langle \gamma_0 | \theta | \gamma_0 \rangle$ (see Table 1), going from $P = P_0$ through $P = P_{ND}$ to $P = 1$ involves a

relaxing of inter-atom correlations because it is obvious this is the case for the θ 's. Yet it is a point well worth checking because it would be a considerable simplification if one could get by with $P = 1$. As for θ , I have no idea how one could proceed if he found it necessary to take the first two terms in the expansion for the right hand side of Eq. (69).

It would be interesting to determine whether, for a scattering system with interactions, the leading multiple scattering correction to the cross section is the cross term between single and double scattering (as implied by References (1) and (2)) or the purely double scattering term (as my $P = P_{ND}$, $\theta = 0$ calculation indicates for an ideal gas). This would determine which term (if not both) would have to be calculated for all the various models of interest.

Perhaps the most serious limitation of this whole model of multiple scattering is the apparently unavoidable use of the static approximation. How one would do the problem for the case of energy transfer is not clear at all.

If it turns out that one cannot get by with simple choices of θ and P , it might well be that the primary value of a quantum mechanical approach to multiple scattering would be to justify the transport theory approach and perhaps define its regions of validity. Watson touches on this point in another paper. (7)

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