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To cite this version:

D. Boose, Jean-Yves Fortin, J.M. M Luck. Quantum scattering by a disordered target - The mean cross section. 2021. hal-02413552v2

HAL Id: hal-02413552
https://univ-tours.hal.science/hal-02413552v2
Preprint submitted on 5 Nov 2021
Quantum scattering by a disordered target — The mean cross section

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Abstract.
We study the variation of the mean cross section with the density of the samples in the quantum scattering of a particle by a disordered target. The target consists of a set of pointlike scatterers, each having an equal probability of being anywhere inside a sphere whose radius may be modified. We first prove that scattering by a pointlike scatterer is characterized by a single phase shift \(\delta\) which takes on its values in \(]0, \pi[\) and that the scattering by \(N\) pointlike scatterers is described by a system of only \(N\) equations. We then show with the help of numerical calculations that there are two stages in the variation of the mean cross section as the density of the samples (the radius of the target) increases (decreases). Depending on the value of \(\delta\), the mean cross section first either increases or decreases, each one of the two behaviours being originated by double scattering; it decreases uniformly for any value of \(\delta\) as the density increases further on, a behaviour which results from multiple scattering and which follows that of the cross section for diffusion by a hard sphere potential of decreasing radius. The expression of the mean cross section is derived in the particular case of an unlimited number of contributions of successive scatterings.

Keywords: disordered systems, multiple scattering
1. Introduction

Many works (see, e.g., [1], [2], [3], [4], [5]) have been done concerning the description of the quantum scattering of a particle in disordered systems (one usually prefers to speak of "transport" rather than "scattering" if the system is infinite or semi-infinite), but all of them fail to preserve unitarity. The lack of unitarity has two different origins:

→ the most evident origin lies in the fact that not all sequences of multiple scattering are taken into account, but usually only those in which the particle is only scattered once by each particular scatterer

→ another origin for the lack of unitarity lies in the fact that the operator which describes the scattering by a single scatterer is always replaced by its first-order Born approximation.

The paper has two purposes, which are:

• to develop a formalism in which unitarity is preserved, which means 1) to use the full operator describing the scattering by a single scatterer and 2) to take into account all sequences of multiple scattering

• to study scattering "by" (instead of "in") disordered systems 1) of finite size (which is still largely a new topic, see however [6]), and 2) consisting of individual scatterers, the scattering by which is characterized by phase shifts (disordered systems are usually modelled by a continuous random potential "landscape"), in order to find quantum effects which cannot be seen in disordered systems of infinite size.

These two goals can be simultaneously achieved by modelling disordered systems as a target with a random distribution of pointlike scatterers.

The paper is divided into six sections and has two appendices. Section 2 gives the derivation of the infinite set of equations which describes the quantum scattering of a particle by a target consisting of identical potential wells with spherical symmetry. In Section 3 we prove that scattering by a pointlike scatterer is characterized by a single phase shift which takes on its values in the interval $]0, \pi[$ and that the infinite set of equations reduces to a system of only $N$ equations if the target consists of $N$ pointlike scatterers. In Section 4 we show that the optical theorem holds for any number of pointlike scatterers. In Section 5 we present and discuss the results of a numerical study about the scattering by a disordered target consisting of pointlike scatterers, in which we have examined the variation of the mean cross section with the density of the samples, and so with the radius of the target, for different values of the phase shift. A summary of the main results of the paper is given in Section 6. Each of the appendices is devoted to the derivation of an expression of the mean cross section which has been used in the interpretation of the numerical results, namely that in the approximation of single and double scattering (Appendix A) and that for an unlimited number of contributions of successive scatterings (Appendix B).
2. Formalism

Let us consider the scattering of a quantum particle by a target which consists of a set of \( N \) stationary scatterers. Each scatterer is modelled by a potential well, the potential function being chosen square integrable if the depth is not finite. The scatterers are so arranged that no two neighbouring wells are close enough to overlap. The Hamiltonian operator of the system is given by

\[
\hat{H} = \hat{h}_0 + \sum_{r=1}^{N} \hat{v}_r,
\]  

(2.1)

where \( \hat{h}_0 \) is the kinetic energy operator and \( \hat{v}_r \) is the operator of multiplication by the potential function of the \( r \)th scatterer. The particle, which has mass \( m \), is assumed to move with momentum \( \hbar \vec{k} \) before scattering; it therefore has the energy \( E = \hbar^2 k^2 / 2m \), where \( k \) is the magnitude of the wave vector.

The operators which describe the scattering by a single scatterer and by the whole set of scatterers are respectively given by [7]

\[
\hat{t}_r(E) = \hat{v}_r + \frac{1}{(E + i\epsilon)\hat{I} - \hat{h}_0 - \hat{v}_r} \hat{v}_r
\]  

(2.2)

and

\[
\hat{T}(E) = \left( \sum_{r=1}^{N} \hat{v}_r \right) + \left( \sum_{r=1}^{N} \hat{v}_r \right) \frac{1}{(E + i\epsilon)\hat{I} - \hat{H}} \left( \sum_{s=1}^{N} \hat{v}_s \right).
\]  

(2.3)

These operators are integral operators in the momentum representation; each kernel is bounded and (uniformly) continuous, as the corresponding potential function is square integrable and has bounded support.

It is convenient to write the operator \( \hat{T}(E) \) as

\[
\hat{T}(E) = \sum_{r=1}^{N} \hat{T}_r(E),
\]  

(2.4)

with

\[
\hat{T}_r(E) = \hat{v}_r + \sum_{s=1}^{N} \frac{1}{(E + i\epsilon)\hat{I} - \hat{H}} \hat{v}_s.
\]  

(2.5)

An operator \( \hat{T}_r(E) \) may be considered as the transition operator corresponding to the (hypothetical) scattering process in which the particle is always last scattered by the \( r \)th scatterer. These operators are related by the set of equations [8]

\[
\hat{T}_r(E) = \hat{t}_r(E) + \sum_{s=1}^{N} \frac{1}{(E + i\epsilon)\hat{I} - \hat{h}_0} \hat{T}_s(E)
\]  

with \( \hat{T}_s(E) \) for \( s \neq r \).  

(2.6)

Repeated substitution of each equation into the others shows that the particle can be scattered any number of times by each particular scatterer; scattering by the target may therefore be considered the result of multiple scattering among the scatterers [9].
The probability amplitude $f(\vec{k}' ; \vec{k})$ for the particle to be scattered in the direction of the wave vector $\vec{k}'$ is proportional to the particular value $T(\vec{k}', \vec{k}; E)$ of the kernel of the operator $\hat{T}(E)$ [10]. We have

$$f(\vec{k}' ; \vec{k}) = -(2\pi)^2 \frac{m}{\hbar^2} T(\vec{k}', \vec{k}; E) = -(2\pi)^2 \frac{m}{\hbar^2} \sum_{r=1}^{N} T_r(\vec{k}', \vec{k}; E),$$

(2.7)

where $T_r(\vec{k}', \vec{k}; E)$ is the value of the kernel of the operator $\hat{T}_r(E)$ for the chosen wave vectors. It follows from (2.6) that the kernels of these operators are related by the set of equations

$$T_r(\vec{\eta}, \vec{\xi}; E) = t_r(\vec{\eta}, \vec{\xi}; E) + 2 \frac{m}{\hbar^2} \sum_{s=1}^{N} \delta_{rs} \int d\vec{\kappa} e^{-i(\vec{\kappa} \cdot \vec{R}_r - \vec{\kappa} \cdot \vec{R}_s)} t(\vec{\kappa}, \vec{k}; E) T_s(\vec{R}, \vec{k}; E)$$

$$k^2 - \kappa^2 + i\epsilon$$

(2.8)

where $t_r(\vec{\eta}, \vec{\xi}; E)$ is the kernel of the operator $\hat{t}_r(E)$ and $\kappa$ is the magnitude of the wave vector $\vec{\kappa}$. In particular,

$$T_r(\vec{\kappa}', \vec{\kappa}; E) = t_r(\vec{\kappa}', \vec{\kappa}; E) + 2 \frac{m}{\hbar^2} \sum_{s=1}^{N} \delta_{rs} \int d\vec{\kappa} e^{-i(\vec{\kappa} \cdot \vec{R}_r - \vec{\kappa} \cdot \vec{R}_s)} t(\vec{\kappa}', \vec{k}; E) T_s(\vec{R}, \vec{k}; E)$$

$$k^2 - \kappa^2 + i\epsilon$$

(2.9)

We shall assume that the scatterers are identical and restrict ourselves to potential functions with spherical symmetry. The kernel of an operator $\hat{t}_r(E)$ can then be written in the form

$$t_r(\vec{\eta}, \vec{\xi}; E) = e^{i(\vec{\xi} - \vec{\eta} \cdot \vec{R}_r)} t(\vec{\eta}, \vec{\xi}; E)$$

(2.10)

where $t(\vec{\eta}, \vec{\xi}; E)$ is the function to which any such kernel would reduce if the centre of the corresponding potential well were taken as the origin of coordinates and $\vec{R}_r$ is the vector from the chosen origin to the centre of the $r$th potential well.

Substituting this equation into (2.9) and writing each function $T_r(\vec{\kappa}, \vec{k}; E)$ in the form

$$T_r(\vec{\kappa}, \vec{k}; E) = e^{-i\vec{\kappa} \cdot \vec{R}_r} \sum_{u=1}^{N} e^{i\vec{\kappa} \cdot \vec{R}_u} \mathcal{T}_{ru}(\vec{\kappa}, \vec{k}; E)$$

(2.11)

in (2.7) and (2.9), we obtain

$$f(\vec{k}' ; \vec{k}) = -(2\pi)^2 \frac{m}{\hbar^2} \sum_{r=1}^{N} \sum_{u=1}^{N} e^{-i\vec{k}' \cdot \vec{R}_r} e^{i\vec{k} \cdot \vec{R}_u} \mathcal{T}_{ru}(\vec{k}', \vec{k}; E),$$

(2.12)

with

$$\mathcal{T}_{ru}(\vec{k}', \vec{k}; E) = t(\vec{k}', \vec{k}; E) \delta_{ru}$$

$$+ 2 \frac{m}{\hbar^2} \sum_{s=1}^{N} \int d\vec{\kappa} e^{i(\vec{R}_r - \vec{R}_s) \cdot \vec{\kappa}} t(\vec{k}', \vec{k}; E) \mathcal{T}_{su}(\vec{R}, \vec{k}; E)$$

$$k^2 - \kappa^2 + i\epsilon$$

(2.13)
The new set of equations can be transformed to another with no dependence upon direction. This is done by expanding both sides of each equation in the basis \( \{ Y_{lm} \} \) of the spherical harmonics and comparing the two expansions term by term.

The expansion of the functions \( \mathcal{T}_{ru}(\vec{k}, \vec{k}'; E) \) is given by

\[
\mathcal{T}_{ru}(\vec{k}, \vec{k}'; E) = 4\pi \sum_{l_1=0}^{\infty} \sum_{m_1=-l_1}^{l_1} \sum_{l_2=0}^{\infty} \sum_{m_2=-l_2}^{l_2} \mathcal{T}^{(ru)}_{l_1m_1;l_2m_2}(\vec{k}, \vec{k}'; E) Y_{l_1m_1}(\Omega_{\vec{k}}) Y_{l_2m_2}(\Omega_{\vec{k}})',
\]

\((r, u = 1, \ldots, N), \quad (2.14)\)

where \( \Omega_{\vec{k}} \) and \( \Omega_{\vec{k}'} \) are the directions of the wave vectors. Since the potential function is invariant under rotation, the function \( t(\vec{k}, \vec{k}'; E) \) has the simpler expansion

\[
t(\vec{k}, \vec{k}'; E) = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{l} t_l(k, \kappa; E) Y^*_l(\Omega_{\vec{k}}) Y_l(\Omega_{\vec{k}}),
\]

\((2.15)\)

where \( \Omega_{\vec{k}} \) is the considered direction of scattering. The functions \( e^{i\vec{k}.(\vec{R}_r - \vec{R}_s)} \) must also be expanded to obtain the expanded form of the right-hand side of the equations. One has [11]

\[
e^{i\vec{k}.(\vec{R}_r - \vec{R}_s)} = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{l} j_l(\kappa R_{rs}) Y^*_l(\Omega_{\vec{k}}) Y_l(\Omega_{\vec{R}_{rs}}),
\]

\((r, s = 1, \ldots, N; s \neq r), \quad (2.16)\)

where \( R_{rs} \) and \( \Omega_{\vec{R}_{rs}} \) are the magnitude and direction of the vector \( \vec{R}_{rs} = \vec{R}_r - \vec{R}_s \) from the centre of the \( s \)th to that of the \( r \)th potential well and \( j_l(x) \) is the spherical Bessel function of order \( l \).

Substitution of these expansions into (2.13) and use of the orthonormality relations of the spherical harmonics leads to the infinite set of equations

\[
\mathcal{T}^{(ru)}_{l_1m_1;l_2m_2}(k, k'; E) = t_{l_1}(k, k'; E) \delta_{r_u} \delta_{l_1l_2} \delta_{m_1m_2}
\]

\[+ 8\pi \frac{m}{h^2} \sum_{l_3=0}^{\infty} \sum_{m_3=-l_3}^{l_3} \sum_{l_4=0}^{\infty} \sum_{m_4=-l_4}^{l_4} j_{l_3} j_{l_4} \sum_{r=1}^{N} \sum_{s \neq r} \frac{4\pi(2l_3+1)(2l_4+1)}{2l_1+1} \delta_{l_4m_4}
\]

\[\times \langle l_3 l_4 0 0 | l_1 0 \rangle \langle l_3 l_4 m_3 m_4 | l_1 m_1 \rangle Y_{l_4m_4}(\Omega_{\vec{R}_{rs}}) \int_0^{\infty} \kappa^2 d\kappa \frac{j_{l_4}(\kappa R_{rs}) t_{l_1}(k, \kappa; E) \mathcal{T}^{(su)}_{l_3m_3;l_2m_2}(k, k'; E)}{\kappa^2 - \kappa^2 + i\epsilon},
\]

\((r, u = 1, \ldots, N)
\]

\((l_1, l_2 = 0, 1, \ldots; m_{1(2)} = -l_{1(2)}, \ldots, l_{1(2)}), \quad (2.17)\)

where \( \langle l_3 l_4 0 0 | l_1 0 \rangle \) and \( \langle l_3 l_4 m_3 m_4 | l_1 m_1 \rangle \) are Clebsch-Gordan coefficients [10] coming from the integration over \( \Omega_{\vec{k}} \). Since the coefficient \( \langle l_3 l_4 0 0 | l_1 0 \rangle \) is equal to 0 when the sum \( l_1 + l_3 + l_4 \) is odd, the right-hand side of the equations includes only the terms for which this sum is even.
The integral in (2.17) may be evaluated by contour integration. The result is

$$2 \int_0^\infty \kappa^2 \, d\kappa \, \frac{j_{l_3}(\kappa R_s) t_{l_4}(k, \kappa ; E)}{k^2 - \kappa^2 + i\epsilon} \mathcal{T}_{l_3m_3;l_4m_4}^{(su)}(\kappa, k ; E)$$

$$= \int_{-\infty}^\infty \kappa^2 \, d\kappa \, \frac{h_{l_3}^{(1)}(\kappa R_s) t_{l_4}(k, \kappa ; E)}{k^2 - \kappa^2 + i\epsilon} \mathcal{T}_{l_3m_3;l_4m_4}^{(su)}(\kappa, k ; E)$$

$$= -i \pi k \, h_{l_3}^{(1)}(k R_s) t_{l_4}(k, k ; E) \mathcal{T}_{l_3m_3;l_4m_4}^{(su)}(k, k ; E)$$

$$\quad (r, s, u = 1, \ldots, N ; \ s \neq r)$$

$$\quad (l_1, l_2, l_3, l_4 = 0, 1, \ldots ; m_{2(3)} = -l_{2(3)}, \ldots, l_{2(3)}) \quad (2.18)$$

where $h_{l_3}^{(1)}(x)$ is the spherical Hankel function of the first kind of order $l$. The range of integration could be extended over the whole line by using the relations

$$t_{l_4}(k, -\kappa ; E) = (-1)^{l_4} t_{l_4}(k, \kappa ; E) \quad (2.19)$$

and

$$\mathcal{T}_{l_3m_3;l_4m_4}^{(su)}(-\kappa, k ; E) = (-1)^{l_3} \mathcal{T}_{l_3m_3;l_4m_4}^{(su)}(\kappa, k ; E) \quad (2.20)$$

which follow from the rotational invariance of the potential function, and the fact that the sum $l_1 + l_3 + l_4$ is even. The contribution of the complex part of the contour to the integral is arbitrarily small, as can be shown by using the inequalities

$$|t_{l_4}(k, \text{Re}\{\kappa\} + i \text{Im}\{\kappa\} ; E)| < \Delta_{l_4} e^{+|\text{Im}\{\kappa\}|a} \quad (2.21)$$

and

$$|\mathcal{T}_{l_3m_3;l_4m_4}^{(su)}(\text{Re}\{\kappa\} + i \text{Im}\{\kappa\} , k ; E)| < \Delta_{l_3l_4} e^{+|\text{Im}\{\kappa\}|a}, \quad (2.22)$$

where $a$ is the radius of the potential wells ($\Delta_{l_4}$ and $\Delta_{l_3l_4}$ are constants), and the fact that any distance $R_{rs}$ is greater than $2a$.

Substituting (2.18) into (2.17), we obtain the set of equations which describes the scattering of a particle by a target consisting of identical potential wells with spherical symmetry. It is

$$\mathcal{T}_{l_3m_3;l_4m_4}^{(ru)}(k, k ; E)$$

$$\quad + i \left(2\pi\right)^2 \frac{mk}{\hbar^2} t_{l_4}(k, k ; E) \sum_{l_3=0}^{l_3} \sum_{m_3=-l_3}^{l_3} \sum_{l_4=0}^{l_4} \sum_{m_4=-l_4}^{l_4} \sqrt{\frac{4\pi(2l_3+1)(2l_4+1)}{2l_1+1}}$$

$$\times \langle l_3 l_4 0 0 | l_1 0 \rangle \langle l_3 l_4 m_3 m_4 | l_1 m_1 \rangle$$

$$\times \sum_{s=1}^{N} \sum_{s \neq r} \frac{h_{l_4}^{(1)}(k R_s) Y_{l_4 m_4}(\Omega_{R_s}) \mathcal{T}_{l_3m_3;l_4m_4}^{(su)}(k, k ; E)}{h_{l_4}^{(1)}(k R_s)}$$

$$= t_{l_4}(k, k ; E) \delta_{ru} \delta_{l_4 l_2} \delta_{m_4 m_2}$$

$$\quad (r, u = 1, \ldots, N)$$

$$\quad (l_1, l_2 = 0, 1, \ldots ; m_{1(2)} = -l_{1(2)}, \ldots, l_{1(2)}). \quad (2.23)$$
3. Pointlike scatterers

The set has infinitely many equations because the expansion of the function \( t(\vec{k}, \vec{k}'; E) \) has an unlimited number of terms. However, in the particular case in which \( t(\vec{k}, \vec{k}'; E) \) does not depend on the directions of the wave vectors, which means that

\[
t(\vec{k}, \vec{k}; E) = t_0(k, k; E),
\]

it turns out as a consequence of the invariance of the system under time reversal that only the \( N^2 \) expansion coefficients \( \mathcal{T}_{00:00}^{(ru)}(k, k; E) \) are different from 0 and so the set has only \( N^2 \) equations. The proof is as follows. Substitution of (3.1), which may be written \( t_i(k, k; E) = t_0(k, k; E) \delta_{i0} \), into (2.23) leads to the equality

\[
\mathcal{T}_{t_1m_1:t_2m_2}^{(ru)}(k, k; E) = \mathcal{T}_{00:00}^{(ru)}(k, k; E) \delta_{t0}
\]

\[
(r, u = 1, ..., N)
\]

\[
(l_1, l_2 = 0, 1, ... ; m_1(2) = -l_1(2), ..., l_1(2)).
\]

(3.2)

Time-reversal symmetry implies that

\[
f(\vec{k}; \vec{k}) = f(-\vec{k}; -\vec{k}).
\]

(3.3)

It follows that the functions \( \mathcal{T}_{ru}(\vec{k}, \vec{k}; E) \) satisfy the relation

\[
\mathcal{T}_{ru}(\vec{k}, \vec{k}; E) = \mathcal{T}_{ur}(-\vec{k}, -\vec{k}; E)
\]

(3.4)

and so their expansion coefficients the relation

\[
\mathcal{T}_{l_2m_2;l_1m_1}^{(ru)}(k, k; E) = (-1)^{l_1-m_1+l_2-m_2} \mathcal{T}_{l_1-m_1:l_2-m_2}^{(ur)}(k, k; E)
\]

\[
(r, u = 1, ..., N)
\]

\[
(l_1, l_2 = 0, 1, ... ; m_1(2) = -l_1(2), ..., l_1(2)).
\]

(3.5)

Alternate use of (3.2) and (3.5) then gives

\[
\mathcal{T}_{l_1m_1:l_2m_2}^{(ru)}(k, k; E) = \mathcal{T}_{00:00}^{(ru)}(k, k; E) \delta_{t0}
\]

\[
= (-1)^{l_2-m_2} \mathcal{T}_{l_2-m_2:00}^{(ur)}(k, k; E) \delta_{t0}
\]

\[
= \mathcal{T}_{00:00}(k, k; E) \delta_{t0} \delta_{l0}
\]

\[
= \mathcal{T}_{00:00}(k, k; E) \delta_{t0} \delta_{l0}
\]

(3.6)

\[
(r, u = 1, ..., N)
\]

\[
(l_1, l_2 = 0, 1, ... ; m_1(2) = -l_1(2), ..., l_1(2)).
\]

which completes the proof.

Substituting this equation into (2.23) and using the facts that \( \langle 0000 | 00 \rangle = 1 \), \( Y_{00}(\Omega_{R_{rs}}) = 1/m \pi \), and \( h_{00}^{(1)}(kR_{rs}) = -i e^{ikR_{rs}}/kR_{rs} \), we obtain the set of equations corresponding to the case considered, which is

\[
\sum_{s=1}^{N} \frac{e^{ikR_{rs}}}{kR_{rs}} \mathcal{T}_{00:00}^{(su)}(k, k; E)
\]

\[
= t_0(k, k; E) \delta_{ru}
\]

\[
(r, u = 1, ..., N).
\]

(3.7)
The function \( t(\vec{k}', \vec{k}; E) \) has no angular dependence if the scatterer is pointlike. A pointlike scatterer can be modelled by any potential well of spherical symmetry whose radius \( a \) is arbitrarily small. Scattering by such a scatterer is characterized by the sole phase shift \( \delta_0 = \delta \) because it is only for the wave function corresponding to \( l = 0 \) that the logarithmic derivative at \( r = a \) has a limit when \( a \) tends to 0. The relation for the dependence of \( \delta \) on \( k \) is obtained as follows. Since the wave function outside the well is proportional to \( \sin(\vec{k}r + \delta) \), its logarithmic derivative at \( r = a \) tends to \( k \cos \delta / \sin \delta \) in the limit. Setting this ratio equal to the value \( c \) to which the logarithmic derivative of the wave function inside the well tends in the limit, one finds

\[
\cot \delta = \frac{c}{k}. \tag{3.8}
\]

The expression of the function \( t(\vec{k}', \vec{k}; E) \) for a pointlike scatterer is

\[
t(\vec{k}', \vec{k}; E) = t_0(k, k; E) = -\frac{\hbar^2}{(2\pi)^2 mk} \sin \delta e^{i\delta}. \tag{3.9}
\]

Since this expression remains invariant if one replaces \( \delta \) by \( \delta + \pi \), the interval of variation of the phase shift can be restricted to \([0, \pi]\).

Substituting (3.9) into (3.7), we obtain

\[
\mathcal{T}^{(ru)}_{00,00}(k, k; E) - \sin \delta e^{i\delta} \sum_{s=1}^{N} \left( e^{ikR_{rs}} \right) \mathcal{T}^{(su)}_{00,00}(k, k; E)
\]

\[
= -\frac{\hbar^2}{(2\pi)^2 mk} \sin \delta e^{i\delta} \delta_{ru} \quad (r, u = 1, \ldots, N). \tag{3.10}
\]

This set of \( N^2 \) equations for the variables \( \mathcal{T}^{(ru)}_{00,00}(k, k; E) \) can be reduced to a system of only \( N \) equations for the dimensionless variables \( \Theta_r \) defined by

\[
\Theta_r = -(2\pi)^2 \frac{mk}{\hbar^2} (\cot \delta - i) \sum_{u=1}^{N} e^{i\vec{k} \cdot \vec{R}_{ru}} \mathcal{T}^{(ru)}_{00,00}(k, k; E)
\]

\[
(r = 1, \ldots, N). \tag{3.11}
\]

The proof is as follows. Multiplying each equation by the factor \( e^{i\vec{k} \cdot \vec{R}_{ru}} = e^{i\vec{k} \cdot \vec{R}_{rs}} e^{i\vec{k} \cdot \vec{R}_{su}} \) and then adding the equations with the same value of the index \( r \), we obtain the set of \( N \) equations

\[
\sum_{u=1}^{N} e^{i\vec{k} \cdot \vec{R}_{ru}} \mathcal{T}^{(ru)}_{00,00}(k, k; E)
\]

\[- \sin \delta e^{i\delta} \sum_{s=1}^{N} \left( e^{ikR_{rs}} \right) e^{i\vec{k} \cdot \vec{R}_{rs}} \sum_{u=1}^{N} e^{i\vec{k} \cdot \vec{R}_{su}} \mathcal{T}^{(su)}_{00,00}(k, k; E)
\]

\[
= -\frac{\hbar^2}{(2\pi)^2 mk} \sin \delta e^{i\delta} \quad (r = 1, \ldots, N). \tag{3.12}
\]

Each of these equations can be expressed in terms of the new variables \( \Theta_r \). This leads to the system of equations

\[
\Theta_r - \sin \delta e^{i\delta} \sum_{s=1}^{N} \left( e^{ikR_{rs}} \right) e^{i\vec{k} \cdot \vec{R}_{rs}} \Theta_s = 1
\]
which completes the proof. The reduced set of equations is obviously better suited for calculations than the original one.

Since the functions $T_{ru}(\vec{k}', \vec{k}; E)$ have no angular dependence, the expression of the scattering amplitude is very simple for pointlike scatterers. Substituting $T_{00,00}(k, k; E)$ for $T_{ru}(\vec{k}', \vec{k}; E)$ in (2.12) and using the definition of the variables $\Theta_r$, we find

$$f(\vec{k}; \vec{k}) = \frac{1}{k} \sin \delta e^{i\delta} \sum_{r=1}^{N} e^{-i(\vec{k} - \vec{k}) \cdot \vec{R}_r} \Theta_r.$$  (3.14)

4. Cross section

The cross section $\sigma_{\text{tot}}$ for scattering by the target (the subscript is an abbreviation for "totality of the scatterers") is obtained by integrating $|f(\vec{k}; \vec{k})|^2$ over $\Omega_{\vec{k}}$. We find

$$\sigma_{\text{tot}} = \sigma \left[ \sum_{r=1}^{N} |\Theta_r|^2 + \sum_{r=1}^{N} \sum_{s=1}^{N} \frac{\sin(kR_{rs})}{kR_{rs}} e^{i\vec{k} \cdot \vec{R}_{rs}} \Theta_r^* \Theta_s \right].$$  (4.1)

where $\sigma = (4\pi/k^2) \sin^2\delta$ is the cross section for scattering by an individual scatterer.

The optical theorem [10] is not only verified for a single pointlike scatterer, as one has $(k/4\pi) \sigma = \text{Im}\{1/k \sin \delta e^{i\delta}\}$, but also for a set of any number of them. The proof is as follows. Multiplication of each equation in (3.13) by $\Theta_r^*$ gives

$$|\Theta_r|^2 - \sin \delta e^{i\delta} \sum_{s=1}^{N} \frac{e^{ikR_{rs}}}{kR_{rs}} e^{i\vec{k} \cdot \vec{R}_{rs}} \Theta_r^* \Theta_s = \Theta_r^*$$  (r = 1, ..., N).  (4.2)

Adding all these equations and taking the real and the imaginary part of the resulting equality, we obtain the two equalities

$$\sum_{r=1}^{N} |\Theta_r|^2 - \sin \delta \sum_{r=1}^{N} \sum_{s=1}^{N} \frac{\cos(kR_{rs} + \delta)}{kR_{rs}} e^{i\vec{k} \cdot \vec{R}_{rs}} \Theta_r^* \Theta_s = \sum_{r=1}^{N} \text{Re}\{\Theta_r\}$$  (4.3)

and

$$\sin \delta \sum_{r=1}^{N} \sum_{s=1}^{N} \frac{\sin(kR_{rs} + \delta)}{kR_{rs}} e^{i\vec{k} \cdot \vec{R}_{rs}} \Theta_r^* \Theta_s = \sum_{r=1}^{N} \text{Im}\{\Theta_r\}.$$  (4.4)

Multiplying the first and the second equality by $\sin \delta$ and $\cos \delta$ respectively and adding, we find

$$\sin \delta \sum_{r=1}^{N} |\Theta_r|^2 + \sin \delta \sum_{r=1}^{N} \sum_{s=1}^{N} \frac{\sin(kR_{rs})}{kR_{rs}} e^{i\vec{k} \cdot \vec{R}_{rs}} \Theta_r^* \Theta_s$$

$$= \sin \delta \sum_{r=1}^{N} \text{Re}\{\Theta_r\} + \cos \delta \sum_{r=1}^{N} \text{Im}\{\Theta_r\}.$$  (4.5)
Substitution of this new equality into (4.1) leads to

\[
\frac{k}{4\pi} \sigma_{\text{tot}} = \frac{1}{k} \sin \delta \left[ \sin \delta \sum_{r=1}^{N} \text{Re}\{\Theta_r\} + \cos \delta \sum_{r=1}^{N} \text{Im}\{\Theta_r\} \right]
\]

\[= \text{Im}\{f(\vec{k}; \vec{k})\}, \tag{4.6}\]

which completes the proof.

The cross section can also be written as a sum of terms each of which but the last gives the contribution of an increasing number \(m\) of successive scatterings. This sum is obtained by repeated substitution of the system of equations into (4.6). We find

\[
\sigma_{\text{tot}} = N\sigma + \frac{4\pi}{k^2} \sum_{m=2}^{M} (\sin \delta)^m \text{Im}\left\{ e^{i m \delta} \sum_{r_1=1}^{N} \sum_{r_2=1}^{N} \ldots \sum_{r_m=1}^{N} \frac{e^{i k R_{r_1 r_2} \ldots r_m}}{k R_{r_1 r_2} \ldots r_m} \right\}
\]

\[+ \frac{4\pi}{k^2} (\sin \delta)^{M+1} \text{Im}\left\{ e^{i(M+1) \delta} \sum_{r_1=1}^{N} \sum_{r_2=1}^{N} \ldots \sum_{r_{M+1}=1}^{N} \frac{e^{i k R_{r_1 r_2} \ldots r_{M+1}}}{k R_{r_1 r_2} \ldots r_{M+1}} \right\}, \tag{4.7}\]

where \(M\) is arbitrary. The contribution of a given number \(m\) of scatterings to the cross section consists of the sum of those of \(N(N-1)^{m-1}\) different sequences of scatterings. The first term in the expression provides the contribution of a single scattering, which is given by the sum of the individual cross sections as the particle can be scattered by any of the scatterers. The last term gives the expression of the difference between the exact expression of the cross section and the sum of contributions corresponding to \(M\) substitutions, and so that of the remainder in the approximation of the former by the latter. In the simplest approximation the expression of the cross section reduces to the contribution of a single scattering; this approximation is obviously more accurate the larger the distance between the closest scatterers.

5. Numerical study

The fact that the set of equations to be solved in order to obtain one value of the cross section is finite when the scatterers are pointlike makes this type of scatterer especially suitable for numerical studies in which a large number of such values is needed. In this section we present and discuss the results of a numerical study about the scattering by a disordered target consisting of pointlike scatterers. The target has been modelled by a set of \(N\) scatterers having each an equal probability of being at any position inside a sphere whose radius \(R\) may be modified; samples fitting in the same volume have been assigned the same value of the density \(\rho = 3N/4\pi R^3\). We have studied the variation of the normalized mean cross section \(\langle \sigma_{\text{tot}} \rangle / N\sigma\) with the density \(\rho\) of the samples, and so
with the radius R of the target, for different values of the phase shift. The value of the cross section for a sample at a particular value of the phase shift has been obtained by substituting the solution of (3.13) into (4.6), which gives an expression of $\sigma_{\text{tot}}$ linear in the variables. The value of the mean cross section corresponding to a particular value of the density and of the phase shift has been obtained by calculating the mean of the values of the cross section of 300 different samples with these values of the density and the phase shift. The calculations have been done for $N = 100$ and with $m = k = \bar{h} = 1$. The values of the phase shift have been taken in the particular interval $[\pi/2, \pi]$, the reason being that the features of the mean cross section discussed in this paper do not only exist for any value in this interval but also for any value in $[0, \pi/2]$; for values of the phase shift that belong to $]0, \pi/2[$, the mean cross section has additional features, which will be discussed in a separate paper. The results of the numerical study are shown in the two figures below.

Figures 1 and 2 show the variation of the normalized mean cross section with the density of the samples for two sets of values of the phase shift (the scale on both axes is logarithmic in each figure).

![Figure 1](image1.png)

**Figure 1.** Variation of the normalized mean cross section $\langle \sigma_{\text{tot}} \rangle / N\sigma$ with the density $\rho$ of the samples for a set of values of the phase shift.

The obtained curves have a common feature, namely that the value of the normalized mean cross section is close to 1 when the density is very small, and so the radius very large. This is a consequence of the fact that the distance between the closest scatterers is sufficiently large in a typical arrangement of very low density for the contribution of a single scattering to be the largest one and so for the cross section to be almost equal to $N\sigma$. The figures show also that the mean cross section first either decreases (Fig. 1) or increases (in the two figures) as the density increases; moreover, it always decreases uniformly as the density increases further on. The detailed explanation for each one of
Figure 2. Variation of the normalized mean cross section \( \langle \sigma_{\text{tot}} \rangle / N\sigma \) with the density \( \rho \) of the samples for another set of values of the phase shift. The chosen number of scatterers is shown by an horizontal dashed line.

these two, less expected features of the mean cross section is given in the remainder of the section.

The decrease and the increase are both originated by double scattering; the reason for which the mean cross section can first deviate from \( N\sigma \) in opposite ways is provided by its expression in the approximation of single and double scattering. This expression is derived in Appendix A. The result is

\[
\langle \sigma_{s+d} \rangle = N\sigma + \frac{9N(N-1)}{4(kR)^6} \left[ \sin(2\delta) C(kR) + \cos(2\delta) S(kR) \right] \sigma ,
\]  

(5.1)

(the subscript "tot" has been replaced by "s+d", which is an abbreviation for "s(ingle) and d(ouble scattering)", in order to avoid any confusion with the exact cross section), with

\[
C(kR) = \frac{(kR) \cos(4kR)}{16} - \frac{\sin(4kR)}{64} + \frac{(kR)^3}{3},
\]

(5.2)

and

\[
S(kR) = \frac{(kR) \sin(4kR)}{16} + \frac{\cos(4kR)}{64} + \frac{(kR)^4}{2} - \frac{(kR)^2}{8} - \frac{1}{64}. 
\]

(5.3)

When the radius is large enough, and so the density small enough, the contribution of double scattering is dominated by its term of least power, which is the one in \( 1/(kR)^2 \).

The normalized mean cross section is then well approximated by

\[
\langle \sigma_{\text{tot}} \rangle / N\sigma = 1 + \frac{9}{8} (N-1) \frac{\cos(2\delta)}{(kR)^2} \\
= 1 + \frac{1}{2} (N-1) \cos(2\delta) \left( \frac{9\pi\rho}{2Nk^3} \right)^{\frac{2}{3}}.
\]

(5.4)
This equation shows that if the phase shift takes on its values in \( \pi/4, 3\pi/4 \), the contribution of double scattering is less than 0, which implies that the mean cross section decreases as the density increases (Fig. 1); on the contrary, if the phase shift takes on its values either in \( 0, \pi/4 \) or \( 3\pi/4, \pi \), this contribution is greater than 0, with the consequence that the mean cross section increases as the density increases (in the two figures).

The fact that both the increase and the decrease are caused by double scattering alone is illustrated by the next two figures, in which the variation of \( \langle \sigma_{\text{tot}} \rangle \) is compared to that of \( \langle \sigma_{s+d} \rangle \) for two different values of the phase shift, one belonging to the interval \( \pi/4, 3\pi/4 \) (Fig. 3) and the other to the interval \( 3\pi/4, \pi \) (Fig. 4). One sees that \( \langle \sigma_{\text{tot}} \rangle \) has the same behaviour as \( \langle \sigma_{s+d} \rangle \), deviating from \( N \) by decreasing when \( \delta \) belongs to \( \pi/4, 3\pi/4 \) and increasing when it belongs to \( 3\pi/4, \pi \), in agreement with (5.4). In addition, Fig. 4 shows that the mean cross section is not bounded in the approximation of single and double scattering, which comes from the fact that the ratio \( C(kR)/(kR)^6 \) diverges when the radius becomes arbitrarily small.

![Figure 3. Comparison of the variations of \( \langle \sigma_{\text{tot}} \rangle/N\sigma \) and \( \langle \sigma_{s+d} \rangle/N\sigma \) with the density \( \rho \) of the samples for a value of the phase shift belonging to the interval \( \pi/4, 3\pi/4 \).](image)

The uniform decrease of the mean cross section is caused by an unlimited number of contributions of successive scatterings to the cross section, that is to say, by multiple scattering. The expression of the mean cross section corresponding to an unlimited number of contributions of successive scatterings is derived in detail in Appendix B. We find

\[
\left( \frac{k^2}{4\pi} \right) \left( \frac{N - 1}{N} \right) \langle \sigma_{\text{tot}} \rangle
\]
Figure 4. Comparison of the variations of $\langle \sigma_{\text{tot}} \rangle / N\sigma$ and $\langle \sigma_{s+d} \rangle / N\sigma$ with the density $\rho$ of the samples for a value of the phase shift belonging to the interval $[3\pi/4, \pi]$.

\[
\langle \sigma_{\text{tot}} \rangle = \sum_{l=0}^{\infty} (2l + 1) \text{Im} \left\{ j_l(kR) j_{l+1}(kR) - (kR) j_l(kR) j_{l+1}(kR) \right\},
\]

with

\[
\mathcal{K} = k \sqrt{1 + \frac{3(N - 1) \sin \delta e^{i\delta}}{(kR)^3}}.
\]

In Figures 5 and 6 the mean cross section is compared to the curve obtained from the expression in (5.5), in which the sum has been truncated at $l = 150$, for the values of the phase shift that have been taken in the two previous figures.

Each figure shows that the expression in (5.5) reproduces well the mean cross section except in the uninteresting range of values of the density in which the approximation of single scattering is valid. This discrepancy reflects the fact that the contributions of more and more partial waves have to be taken into account in the sum as the radius increases, and so as the density decreases. One can therefore conclude that the uniform decrease is caused by multiple scattering.

It is interesting to derive the expression to which (5.5) reduces when $R$ tends to 0. We find

\[
\langle \sigma_{\text{tot}} \rangle \approx \frac{4\pi}{k^2} \text{Im} \left\{ j_0(kR) (kR) e^{ikR} \right\} \approx 4\pi R^2.
\]

This means that when the value of the density becomes arbitrarily large, the mean cross section tends towards the cross section for diffusion by a hard sphere whose radius is the same as that of the target, a behaviour which is clearly observed in Figures 5 and 6.
Figure 5. Comparison of the variations of the normalized mean cross section and of the expression of $\langle \sigma_{\text{tot}} \rangle / N \sigma$ given by (5.5), in which the sum has been truncated at $l = 150$ (dashed line), for a value of the phase shift belonging to the interval $[\pi/4, 3\pi/4]$. The full line gives the values of the normalized cross section for diffusion by a hard sphere of radius $R$.

Figure 6. Comparison of the variations of the normalized mean cross section and of the expression of $\langle \sigma_{\text{tot}} \rangle / N \sigma$ given by (5.5), in which the sum has been truncated at $l = 150$ (dashed line), for a value of the phase shift belonging to the interval $[3\pi/4, \pi]$. The full line gives the values of the normalized cross section for diffusion by a hard sphere of radius $R$. 
6. Summary

In this paper, we have developed a formalism which describes the quantum scattering of a particle by a disordered target consisting of pointlike scatterers. The formalism has the important feature of preserving unitary because it takes into account all sequences of multiple scattering. We have used it in a numerical study about the scattering by a disordered target modelled by a set of pointlike scatterers which have each an equal probability of being at any position inside a sphere whose radius may be modified. We have studied the variation of the mean cross section with the density of the samples, and so with the radius of the target, for different values of the phase shift. The study has shown that the mean cross section goes through successive stages as the density increases, and so as the radius decreases. The mean cross section is nearly constant at very low density, which reflects the fact that the particle is only scattered once before leaving the target. Depending on the value of the phase shift, the mean cross section either increases or decreases as the density increases, each one of the two behaviours being originated by double scattering. As the density increases further on, the mean cross section decreases uniformly whatever the value of the phase shift, a behaviour which is caused by multiple scattering and which follows that of the cross section for diffusion by a hard sphere potential of decreasing radius.

Appendix A: Expression of the mean cross section in the approximation of single and double scattering

This appendix is devoted to the derivation of the expression of the mean cross section that includes only the contributions of single and double (m = 2) scattering. It follows from (4.7) that the mean cross section is given in this particular approximation by

\[
\langle \sigma_{s+d} \rangle = N \sigma + \sigma \text{ Im} \left\{ e^{2i\delta} \sum_{r=1}^{N} \sum_{s=1}^{N} \left( e^{ikR_{rs}} / kR_{rs} \right) e^{i\vec{k}.\vec{R}_{rs}} \right\}
\]

(A.1)

(the subscript is for "s(ingle) and d(ouble scattering)"); finding its expression amounts therefore to hardly more than finding that of the mean of \( e^{ikR_{rs}} / kR_{rs} \) \( e^{i\vec{k}.\vec{R}_{rs}} \).

Since each scatterer has an equal probability of being at any position in the target (whose center is taken as the origin of coordinates), we have

\[
\left\langle \left( e^{ikR_{rs}} / kR_{rs} \right) e^{i\vec{k}.\vec{R}_{rs}} \right\rangle = \frac{1}{V^2} \int_{V} d\vec{R}_{r} \int_{V} d\vec{R}_{s} \frac{e^{ikR_{rs}} e^{i\vec{k}.\vec{R}_{rs}}}{kR_{rs}}
\]

\[
= \frac{1}{4\pi} \frac{1}{4\pi} \frac{9}{R^{6}} \int_{V} d\vec{R}_{r} \int_{V} d\vec{R}_{s} \frac{e^{ikR_{rs}} e^{i\vec{k}.\vec{R}_{rs}}}{kR_{rs}}.
\]

(A.2)

where \( V \) and \( R \) are the volume and radius of the target. The integration is most easily done working with the set of angular variables that consists of the azimuthal and polar angles \( \Theta_{rs} \) and \( \Phi_{rs} \) of the vector \( \vec{R}_{rs} \), the angle \( \theta_{rs} \) between the vectors \( \vec{R}_{r} \) and \( \vec{R}_{s} \), and the angle \( \phi_{rs} \) between the planes that are defined by the vectors \( \vec{R}_{r} \) and \( \vec{R}_{s} \) and by the
vectors $\vec{R}_{rs}$ and $\vec{k}$ (which is assumed to determine the direction of the third axis). The expression of the product of volume elements for this choice of angular variables is

$$d\vec{R}_r d\vec{R}_s = R_r^2 dR_r R_s^2 dR_s \sin \Theta_{rs} d\Theta_{rs} d\Phi_{rs} \sin \theta_{rs} d\theta_{rs} d\phi_{rs},$$  \hspace{1cm} (A.3)

where $R_{rs}$ is the magnitude of the vector $\vec{R}_{rs}$.

The expression of the mean of $(e^{ikR_{rs}/kR_{rs}}) e^{i\vec{k}.\vec{R}_{rs}}$ may be obtained by successive averages over pairs of variables; the variables with respect to which the integration has been done will be indicated in a subscript. The average over $\Theta_{rs}$ and $\Phi_{rs}$ gives

$$\left\langle \left( \frac{e^{ikR_{rs}}}{kR_{rs}} \right) e^{i\vec{k}.\vec{R}_{rs}} \right\rangle_{(\Theta_{rs}, \Phi_{rs})}$$

$$= \frac{1}{4\pi} \frac{e^{ikR_{rs}}}{kR_{rs}} \int_0^\pi \sin \Theta_{rs} d\Theta_{rs} \int_0^{2\pi} d\Phi_{rs} e^{iR_{rs} \cos \Theta_{rs}}$$

$$= \sum_{n=0}^\infty \frac{(2i)^n}{(n+1)!} (kR_{rs})^{n-1}. \hspace{1cm} (A.4)$$

It follows that

$$\left\langle \left( \frac{e^{ikR_{rs}}}{kR_{rs}} \right) e^{i\vec{k}.\vec{R}_{rs}} \right\rangle = \sum_{n=0}^\infty \frac{(2i)^n}{(n+1)!} \left\langle (kR_{rs})^{n-1} \right\rangle_{(\theta_{rs}, \phi_{rs}; R_r, R_s)} \hspace{1cm} (A.5)$$

and so we need the expression of the mean of $(kR_{rs})^{n-1}$ for any $n$ to obtain that of the mean of $(e^{ikR_{rs}/kR_{rs}}) e^{i\vec{k}.\vec{R}_{rs}}$.

The average of $(kR_{rs})^{n-1}$ over the angles gives

$$\left\langle (kR_{rs})^{n-1} \right\rangle_{(\theta_{rs}, \phi_{rs})}$$

$$= \frac{k^{n-1}}{4\pi} \int_0^\pi \sin \theta_{rs} d\theta_{rs} \int_0^{2\pi} d\phi_{rs} (R_r^2 + R_s^2 - 2R_r R_s \cos \theta_{rs})^{n-1}$$

$$= \frac{k^{n-1}}{2(n+1)} \left( \frac{(R_r + R_s)^n - |R_r - R_s|^n}{R_r R_s} \right)^{n-1} \hspace{1cm} (n = 0, 1, ...). \hspace{1cm} (A.6)$$

The average of the obtained expression gives that of the mean of $(kR_{rs})^{n-1}$. We find

$$\left\langle (kR_{rs})^{n-1} \right\rangle_{(\theta_{rs}, \phi_{rs}; R_r, R_s)}$$

$$= \left\langle \frac{k^{n-1}}{2(n+1)} \left( \frac{(R_r + R_s)^n - |R_r - R_s|^n}{R_r R_s} \right) \right\rangle_{(R_r, R_s)}$$

$$= \frac{9}{R^6} \frac{k^{n-1}}{2(n+1)} \int_0^R R_r dR_r \int_0^R R_s dR_s [(R_r + R_s)^n - |R_r - R_s|^n]$$

$$= \frac{72 (2kR)^{n-1}}{(n+2)(n+3)(n+5)} \hspace{1cm} (n = 0, 1, ...). \hspace{1cm} (A.7)$$

Substituting the expression of the mean of $(kR_{rs})^{n-1}$ into (A.5), we obtain

$$\left\langle \left( \frac{e^{ikR_{rs}}}{kR_{rs}} \right) e^{i\vec{k}.\vec{R}_{rs}} \right\rangle$$

$$= \frac{72}{2kR} \sum_{n=0}^\infty \frac{(4iR)^n}{(n+1)!(n+2)(n+3)(n+5)}$$
\[ \frac{144}{(4kR)^5} \left[ e^{4ikR} - 1 - 4ikR - \frac{(4ikR)^2}{2} - \frac{(4ikR)^3}{6} \right] \]
\[ + i \frac{144}{(4kR)^6} \left[ e^{4ikR} - 1 - 4ikR - \frac{(4ikR)^2}{2} - \frac{(4ikR)^3}{6} - \frac{(4ikR)^4}{24} \right]. \quad (A.8) \]

Substitution of the expression of the mean of \( (e^{ikR_{rs}/kR_{rs}}) e^{i\vec{k} \cdot \vec{R}_{rs}} \) into (A.1) leads to that of the mean cross section in the approximation of single and double scattering, which is
\[ \langle \sigma_{s+d} \rangle = N\sigma + \frac{9N(N-1)}{4(kR)^6} \left[ \sin(2\delta) C(kR) + \cos(2\delta) S(kR) \right]\sigma, \quad (A.9) \]
with
\[ C(kR) = \frac{(kR) \cos(4kR)}{16} - \frac{\sin(4kR)}{64} + \frac{(kR)^3}{3} \quad (A.10) \]
and
\[ S(kR) = \frac{(kR) \sin(4kR)}{16} + \frac{\cos(4kR)}{64} + \frac{(kR)^4}{2} - \frac{(kR)^2}{8} - \frac{1}{64}. \quad (A.11) \]

The functions \( C(kR) \) and \( S(kR) \) take on only positive values. It is to be noted that the mean cross section is not bounded in the approximation of single and double scattering because the function \( C(kR)/(kR)^6 \) behaves like \( 1/kR \) when \( R \) tends to 0.

**Appendix B: Expression of the mean cross section for an unlimited number of contributions of successive scatterings**

This appendix is devoted to the derivation of the expression of the mean cross section for an unlimited number of contributions of successive scatterings to the cross section. The relevant expression for the cross section is obtained from (4.7) by discarding the remainder term and letting the integer \( M \) become infinitely large. The formula giving the mean cross section is then
\[ \langle \sigma_{tot} \rangle = N\sigma \]
\[ + \frac{4\pi}{k^2} \sum_{m=2}^{M} (\sin\delta)^m \text{Im} \left\{ e^{im\delta} \sum_{r_1=1}^{N} \sum_{r_2=1}^{N} \ldots \sum_{r_m=1}^{N} \left( e^{ikR_{r_1r_2}} \right) \right\} \]
\[ \times \left( e^{ikR_{r_2r_3}} \right) \ldots \left( e^{ikR_{r_{m-1}r_m}} \right) e^{i\vec{k} \cdot \vec{R}_{r_1r_m}} \right\}, \quad (B.1) \]
where \( M \) is as large as desired. Since \( \sigma = (4\pi/k^2) \sin^2\delta \), this formula may be written as
\[ \langle \sigma_{tot} \rangle = \frac{4\pi}{k^2} N \sum_{m=1}^{M} (N-1)^{m-1}(\sin\delta)^m \text{Im} \left\{ e^{im\delta} M_m(kR) \right\}, \quad (B.2) \]
with
\[ M_1(kR) = 1 \quad (B.3) \]
and

\[
M_m(kR) = \frac{1}{N(N-1)^{m-1}} \left[ \sum_{r_1=1}^{N} \sum_{r_2=1}^{N} \cdots \sum_{r_m=1}^{N} \left( \frac{e^{ikRr_1r_2}}{kR_{r_1r_2}} \right) \right] \\
\times \left( \frac{e^{ikRr_2r_3}}{kR_{r_2r_3}} \right) \cdots \left( \frac{e^{ikRr_{m-1}r_m}}{kR_{r_{m-1}r_m}} \right) e^{i\vec{k}.\vec{R}_{r_m}}
\]

(m = 2, 3, ...). \hspace{1em} (B.4)

Since each scatterer has an equal probability of being at any position inside a sphere of volume \(V\) and radius \(R\) (whose center is taken as the origin of coordinates), we have

\[
M_m(kR) = \frac{1}{\sqrt{V}} \int_{V} d\vec{R}_1 \int_{V} d\vec{R}_2 \cdots \int_{V} d\vec{R}_m \left( \frac{e^{ikR_{12}}}{kR_{12}} \right) \\
\times \left( \frac{e^{ikR_{23}}}{kR_{23}} \right) \cdots \left( \frac{e^{ikR_{m-1}m}}{kR_{m-1}m} \right) e^{-i\vec{k}.\vec{R}_1} e^{i\vec{k}.\vec{R}_m}
\]

(m = 2, 3, ...). \hspace{1em} (B.5)

Introducing the reduced vectors

\[
\vec{u}_i = \vec{R}_i/R \quad (i = 1, 2, ...), \hspace{1em} (B.6)
\]

we may also write the expression of \(M_m(kR)\) as

\[
M_m(kR) = \frac{3^m}{(4\pi)^m} \int d\vec{u}_1 \int d\vec{u}_2 \cdots \int d\vec{u}_m \left( \frac{e^{ikR|\vec{u}_2 - \vec{u}_1|}}{kR|\vec{u}_2 - \vec{u}_1|} \right) \\
\times \left( \frac{e^{ikR|\vec{u}_3 - \vec{u}_2|}}{kR|\vec{u}_3 - \vec{u}_2|} \right) \cdots \left( \frac{e^{ikR|\vec{u}_m - \vec{u}_{m-1}|}}{kR|\vec{u}_m - \vec{u}_{m-1}|} \right) e^{-i\vec{k}.\vec{u}_1} e^{i\vec{k}.\vec{u}_m}
\]

(m = 2, 3, ...), \hspace{1em} (B.7)

where each integration is over all points inside a sphere of radius 1. The mean of the contribution of any number of successive scatterings may be written in the form

\[
M_{n+1}(kR) = \int_{0}^{1} du \mathcal{P}_n(u, kR) \quad (n = 0, 1, ...)
\]

with

\[
\mathcal{P}_0(u, kR) = 3 u^2, \hspace{1em} (B.9)
\]

\[
\mathcal{P}_1(u, kR) = 3u^2 \frac{3}{(4\pi)^2} \int d\Omega_{\vec{u}} e^{i\vec{k}.\vec{u}} \int d\vec{r}_1 e^{-i\vec{k}.\vec{u}_1} \left( \frac{e^{ikR|\vec{u} - \vec{u}_1|}}{kR|\vec{u} - \vec{u}_1|} \right), \hspace{1em} (B.10)
\]

and

\[
\mathcal{P}_n(u, kR) = 3u^2 \frac{3^n}{(4\pi)^{n+1}} \int d\Omega_{\vec{u}} \int d\vec{u}_1 \int d\vec{u}_2 \cdots \int d\vec{u}_n \left( \frac{e^{ikR|\vec{u}_2 - \vec{u}_1|}}{kR|\vec{u}_2 - \vec{u}_1|} \right) \\
\times \left( \frac{e^{ikR|\vec{u}_3 - \vec{u}_2|}}{kR|\vec{u}_3 - \vec{u}_2|} \right) \cdots \left( \frac{e^{ikR|\vec{u}_n - \vec{u}_{n-1}|}}{kR|\vec{u}_n - \vec{u}_{n-1}|} \right) e^{-i\vec{k}.\vec{u}_1}
\]
\[
\times \left( \frac{e^{ikR|\vec{u}-\vec{u}_n|}}{kR|\vec{u} - \vec{u}_n|} \right) e^{iR\vec{k}\cdot\vec{u}}
\]

\( (n = 2, 3, \ldots). \)  \( \text{(B.11)} \)

The recursion formula for the quantities \( P_n(u, kR) \) is then obtained by substituting the expansions \([11]\)

\[
e^{ikR|\vec{u}_s-\vec{u}_r|}
\]

\[
= 4\pi i \sum_{l=0}^{\infty} \sum_{m=-l}^{l} j_l(kR \text{Min}(u_r, u_s)) h_l^{(1)}(kR \text{Max}(u_r, u_s)) Y_{lm}^*(\Omega_{\vec{u}_r}) Y_{lm}^{*\prime}(\Omega_{\vec{u}_s})
\]

\( (s \neq r), \)  \( \text{(B.13)} \)

where \( u_{r(s)} \) and \( \Omega_{\vec{u}_{r(s)}} \) are the magnitude and direction of the vector \( \vec{u}_{r(s)} \) and where \( \text{Min}(u_r, u_s) \) is the smaller and \( \text{Max}(u_r, u_s) \) the larger of \( u_r \) and \( u_s \), into (B.11). Using the notations \( \Omega_{\vec{u}_r} = \Omega_r \) \( (r = 1, \ldots, n) \), we obtain

\[
P_n(u, kR) = 3u^2(4\pi)^{i^n} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} j_l(kR) Y_{lm}^*(\Omega_{\vec{k}})
\]

\[
\sum_{l'=0}^{\infty} \sum_{m'=0}^{m'} (-i)^{l'} Y_{l'm'}^*(\Omega_{\vec{k}}) \sum_{l_1=0}^{l} \sum_{m_1=-l_1}^{l_1} \sum_{l_2=0}^{l_2} \sum_{m_2=-l_2}^{l_2} \cdots \sum_{l_n=0}^{l_n} \sum_{m_n=-l_n}^{l_n} \cdots \sum_{l_0=0}^{l_0} \sum_{m_0=-l_0}^{l_0} \cdots
\]

\[
\times \int_0^1 3u_1^2 du_1 \int_0^1 3u_2^2 du_2 \cdots \int_0^1 3u_n^2 du_n j_{l_1}(kR \text{Min}(u_1, u_2))
\]

\[
\times h_{l_1}^{(1)}(kR \text{Max}(u_1, u_2)) j_{l_2}(kR \text{Min}(u_2, u_3))
\]

\[
\times h_{l_2}^{(1)}(kR \text{Max}(u_2, u_3)) \cdots j_{l_{n-1}}(kR \text{Min}(u_{n-1}, u_n))
\]

\[
\times h_{l_{n-1}}^{(1)}(kR \text{Max}(u_{n-1}, u_n)) j_{l_n}(kR \text{Min}(u_n, kr))
\]

\[
\times h_{l_n}^{(1)}(kR \text{Max}(u_n, kr)) j_{l'}(kRU) \int d\Omega_{\vec{k}} \int d\Omega_1
\]

\[
\times \int d\Omega_2 \cdots \int d\Omega_n Y_{l'm_1}^*(\Omega_1) Y_{l_1m_1}(\Omega_2)
\]

\[
\times Y_{l_2m_2}^*(\Omega_2) Y_{l_2m_2}(\Omega_3) \cdots Y_{l_{n-1}m_{n-1}}^*(\Omega_{n-1}) Y_{l_{n-1}m_{n-1}}(\Omega_n)
\]

\[
\times Y_{l_nm_n}^*(\Omega_n) Y_{l_nm_n}(\Omega_{kr}) Y_{l'n'}(\Omega_1).
\]

\( \text{(B.14)} \)

Use of the orthogonality relation for the spherical harmonics and of the identity \([11]\)

\[
\sum_{m=-l}^{l} Y_{lm}^*(\Omega_{\vec{k}}) Y_{lm}(\Omega_{\vec{k}}) = \frac{2l+1}{4\pi}
\]

\( \text{(B.15)} \)

then leads to

\[
P_n(u, kR) = 3u^2i^n \sum_{l=0}^{\infty} (2l+1) j_l(kRu)
\]
We obtain
\[
\times \int_0^1 3 u_1^2 du_1 \int_0^1 3 u_2^2 du_2 \ldots \int_0^1 3 u_n^2 du_n \frac{j_l(kR\text{Min}(u_1, u_2))}{j_l(kR\text{Max}(u_1, u_2))} \times \frac{1}{j_l(kR\text{Min}(u_2, u_3))} \times \frac{1}{j_l(kR\text{Min}(u_3, u_n))} \times \frac{1}{j_l(kR\text{Min}(u_n, u))} \times \frac{1}{j_l(kR\text{Min}(u, u))} j_l(kR\text{Min}(u, u)) j_l(kR\text{Min}(u, u)) j_l(kR\text{Min}(u, u)) j_l(kR\text{Min}(u, u)) j_l(kR\text{Min}(u, u)) \quad (n = 2, 3, \ldots) \quad (B.16)
\]

and
\[
P_1(u, kR) = 3 u^2 i \sum_{l=0}^\infty (2l + 1) j_l(kR) j_l(kR\text{Min}(u, u)) j_l(kR\text{Min}(u, u)) j_l(kR\text{Min}(u, u)) j_l(kR\text{Min}(u, u)) j_l(kR\text{Min}(u, u)) \quad (n = 1, 2, \ldots) \quad (B.17)
\]

We then decompose \(P_n(u, kR)\) as
\[
P_n(u, kR) = u \sum_{l=0}^\infty (2l + 1) j_l(kR) P_l^{(n)}(u, kR) \quad (n = 1, 2, \ldots) \quad (B.18)
\]

We obtain
\[
P_l^{(n)}(u, kR) = 3 u^2 i^n \int_0^1 3 u_1^2 du_1 \int_0^1 3 u_2^2 du_2 \ldots \int_0^1 3 u_n^2 du_n \frac{j_l(kR\text{Min}(u_1, u_2))}{j_l(kR\text{Max}(u_1, u_2))} \times \frac{1}{j_l(kR\text{Min}(u_2, u_3))} \times \frac{1}{j_l(kR\text{Min}(u_3, u_n))} \times \frac{1}{j_l(kR\text{Min}(u_n, u))} j_l(kR\text{Min}(u_n, u)) j_l(kR\text{Min}(u_n, u)) j_l(kR\text{Min}(u_n, u)) j_l(kR\text{Min}(u_n, u)) j_l(kR\text{Min}(u_n, u)) \quad (n = 2, 3, \ldots)
\]
\[= 3i u h^{(1)}_l(kRu) \int_0^u ds s j_l(kRs) P_{n-1}^{(l)}(s, kR)\]
\[+ 3i u j_l(kRu) \int_u^1 ds s h_l^{(1)}(kRs) P_{n-1}^{(l)}(s, kR)\]
\[(n = 2, 3, \ldots) \quad (B.19)\]

and
\[P_1^{(l)}(u, kR) = 3i u \int_0^1 3 u^2 du j_l(kRu) j_l(kR \min(u_1, u))\]
\[\times h_l^{(1)}(kR \max(u_1, u))\]
\[= 3i u h_l^{(1)}(kRu) \int_0^u 3 s^2 ds j_l(kRs) j_l(s)\]
\[+ 3i u j_l(kRu) \int_u^1 3 s^2 ds h_l^{(1)}(kRs) j_l(s)\]
\[= 3i u h_l^{(1)}(kRu) \int_0^u ds s j_l(kRs) P_0^{(l)}(s, kR)\]
\[+ 3i u j_l(kRu) \int_u^1 ds s h_l^{(1)}(kRs) P_0^{(l)}(s, kR),\]
\[(B.20)\]

with
\[P_0^{(l)}(s, kR) = 3 s j_l(kRs s). \quad (B.21)\]

This definition of \(P_0^{(l)}(u, kR)\) is compatible with that of \(P_0(u, kR)\) as given in (B.9) because of the identity
\[\sum_{l=0}^{\infty} (2l + 1) j_l^2(u) = 1. \quad (B.22)\]

Each function \(P_n^{(l)}(u, kR)\) satisfies a differential equation which is obtained by deriving the recursion relation twice with respect to the variable \(u\). Using the facts that [11]
\[j_l(z) \frac{d}{dz} h_l^{(1)}(z) - h_l^{(1)}(z) \frac{d}{dz} j_l(z) = \frac{1}{z^2} \quad (l = 0, 1, \ldots) \quad (B.23)\]

and
\[\frac{d^2}{dz^2} f_l(z) + 2 \frac{d}{dz} f_l(z) + \left(1 - \frac{l(l + 1)}{z^2}\right)f_l(z) = 0 \quad (l = 0, 1, \ldots) \quad (B.24)\]

for both \(j_l(z)\) and \(h_l^{(1)}(z)\), we obtain
\[\frac{d^2}{du^2} P_n^{(l)}(u, kR) = -\frac{3}{kR} P_{n-1}^{(l)}(u, kR) - \left((kR)^2 - \frac{l(l + 1)}{u^2}\right) P_n^{(l)}(u, kR)\]
\[(n \neq 0) \quad (l = 0, 1, \ldots) \quad (B.25)\]

and
\[\frac{d^2}{du^2} P_0^{(l)}(u, kR) = -\left((kR)^2 - \frac{l(l + 1)}{u^2}\right) P_0^{(l)}(u, kR)\]
\[(l = 0, 1, \ldots). \quad (B.26)\]

Comparison between these last two equations shows that
\[P_{-1}^{(l)}(u, kR) = 0 \quad (l = 0, 1, \ldots). \quad (B.27)\]
We now introduce the generating function

\[ G^{(l)}(x, u, kR) = \sum_{n=0}^{\infty} x^n \mathcal{P}_n^{(l)}(u, kR) \]  

(B.28)

It follows from (B.25) and (B.26) that the generating function satisfies the equation

\[ \frac{\partial^2}{\partial u^2} G^{(l)}(x, u, kR) = -\left((kR)^2 + \frac{3x}{kR} - \frac{l(l+1)}{u^2}\right) G^{(l)}(x, u, kR) \]

\[ (l = 0, 1, \ldots). \]  

(B.29)

The mean cross section can be calculated with the help of the generating function. Substituting (B.18) into (B.8) and then (B.8) into (B.2), we obtain

\[ \langle \sigma_{\text{tot}} \rangle = \frac{4\pi}{k^2} N \sum_{l=0}^{\infty} (2l + 1) \langle \sigma_{\text{tot}} \rangle^{(l)}, \]  

(B.30)

with

\[ \langle \sigma_{\text{tot}} \rangle^{(l)} = \text{Im}\left\{ \sin \delta e^{i\delta} \int_0^1 du \ u j_l(kR u) \sum_{n=0}^{\infty} (N - 1) \sin \delta e^{i\delta} \mathcal{P}_n^{(l)}(u, kR) \right\}. \]

(B.31)

Taking \( M \) to be infinitely large and using (B.28), we find

\[ \langle \sigma_{\text{tot}} \rangle^{(l)} = \text{Im}\left\{ \sin \delta e^{i\delta} \int_0^1 du \ u j_l(kR u) G^{(l)}(x = (N - 1) \sin \delta e^{i\delta}, ukR) \right\}. \]

(B.32)

The regular solution of (B.29) is

\[ G^{(l)}(x, u, kR) = A_l(x) u j_l(kR u) \left(\sqrt{(kR)^2 + \frac{3x}{kR}} u\right) \]  

\[ (l = 0, 1, \ldots). \]  

(B.33)

The function \( A_l(x) \) is found as follows. It follows from (B.19) that

\[ \mathcal{P}_n^{(l)}(u = 1, kR) = 3i h_l^{(1)}(kR) \int_0^1 ds s j_l(kRs) \mathcal{P}_{n-1}^{(l)}(s, kR), \]

\[ (l = 0, 1, \ldots). \]  

(B.34)

This implies that

\[ \sum_{n=1}^{\infty} x^n \mathcal{P}_n^{(l)}(u = 1, kR) = 3i h_l^{(1)}(kR) \int_0^1 ds s j_l(kRs) \sum_{n=1}^{\infty} x^n \mathcal{P}_{n-1}^{(l)}(s, kR), \]

\[ (l = 0, 1, \ldots). \]  

(B.35)

and so

\[ G^{(l)}(x, u = 1, kR) - \mathcal{P}_0^{(l)}(u = 1, kR) = 3i x h_l^{(1)}(kR) \int_0^1 ds s j_l(kRs) G^{(l)}(x, s, kR). \]

\[ (l = 0, 1, \ldots). \]  

(B.36)
Substituting (B.33) in the case \(u = 1\) as well as in the general case and (B.21) in the case \(s = 1\) into this equation, we obtain

\[ A_l(x) j_l \left( \sqrt{(kR)^2 + \frac{3x}{kR}} \right) - 3j_l(kR) \]

\[ = 3i x h_l^{(1)}(kR) A_l(x) \int_0^1 ds \, s^2 j_l(kR s) j_l \left( \sqrt{(kR)^2 + \frac{3x}{kR}} s \right). \]

\[ (l = 0, 1, \ldots). \tag{B.37} \]

Using the fact that

\[ I_l(x, kR) = \int_0^1 ds \, s^2 j_l(kR s) j_l \left( \sqrt{(kR)^2 + \frac{3x}{kR}} s \right) \]

\[ = \frac{kR}{3x} \left[ \sqrt{(kR)^2 + \frac{3x}{kR}} \, j_l(kR) \, j_{l+1} \left( \sqrt{(kR)^2 + \frac{3x}{kR}} \right) \right. \]

\[ \left. - (kR) \, j_l \left( \sqrt{(kR)^2 + \frac{3x}{kR}} \right) \, j_{l+1}(kR) \right] \]

\[ (l = 0, 1, \ldots), \tag{B.38} \]

we obtain

\[ A_l(x) = \frac{3 \, j_l(kR)}{j_l(kR) - 3i x h_l^{(1)}(kR) I_l(x, kR)} \]

\[ (l = 0, 1, \ldots), \tag{B.39} \]

where we have used the notation \(kR = \sqrt{(kR)^2 + \frac{3x}{kR}}.\) Substituting this equation into (B.33), we obtain the expression of the generating function, which is

\[ G^{(l)}(x, u, kR) = \frac{3u \, j_l(kR)}{j_l(kR) - 3i x h_l^{(1)}(kR) I_l(x, kR)} \]

\[ (l = 0, 1, \ldots). \tag{B.40} \]

Substituting this equation into (B.32), we find

\[ \langle \sigma_{\text{tot}} \rangle^{(l)} = \text{Im} \left\{ \frac{3 \sin \delta \, e^{i\delta} \, j_l(kR) \, I_l(x = (N - 1) \sin \delta e^{i\delta}, kR)}{j_l(kR) - 3i (N - 1) \sin \delta e^{i\delta} \, h_l^{(1)}(kR) \, I_l(x = (N - 1) \sin \delta e^{i\delta}, kR)} \right\}. \tag{B.41} \]

Using (B.38) in this equation and then using (B.30), we obtain the expression of the mean cross section for an unlimited number of contributions of successive scatterings. We find

\[ \left( \frac{k^2}{4\pi} \right) \left( \frac{N - 1}{N} \right) \langle \sigma_{\text{tot}} \rangle \]

\[ = \sum_{l=0}^{\infty} (2l + 1) \text{Im} \left\{ i \left[ \frac{(kR) \, j_l(kR) \, j_{l+1}(kR) - (kR) \, j_l(kR) \, j_{l+1}(kR)}{(kR) \, h_l^{(1)}(kR) \, j_{l+1}(kR) - (kR) \, j_l(kR) \, h_{l+1}^{(1)}(kR)} \right] \right\}, \tag{B.42} \]
with

$$\mathcal{K} = k \sqrt{1 + \frac{3(N - 1) \sin \delta e^{i \delta}}{(kR)^3}}. \quad (B.43)$$
References