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Multiple scattering and the Rehr–Albers–Fritzsche formula for the propagator matrix

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Abstract. The propagator matrix is one ingredient in exact theories of multiple scattering. It occurs in the addition theorem (or translation formula) for expanding a spherical outgoing multipole, singular at one point, in terms of regular spherical solutions about another point. It also occurs in the two-centre expansion of the free-space Green's function (or free-particle propagator). Many methods have been devised for computing the propagator matrix, but one of the most efficient, numerically, is based on a formula obtained in 1990 by Rehr and Albers and by Fritzsche. A clear derivation of this formula is given. The formula is also simplified, leading to an expansion in inverse powers of kb, where k is the wavenumber and b is the spacing. This leads to consistent approximations, which are asymptotic as $kb \to \infty$.

1. Introduction

'Multiple scattering' means different things to different scientists, but a general definition might be 'the interaction of fields with two or more obstacles'. For example, a typical multiple-scattering problem in classical physics is the scattering of sound waves by two rigid spheres. Further examples, such as the scattering of spherical electron waves by a cluster of atoms, can be found in condensed-matter physics [9, 20].

The problem of acoustic scattering by two spheres can be solved exactly by a method that goes back to Lord Rayleigh. Suppose that the spheres are centred at O_1 and O_2. Write the scattered field u as a superposition of outgoing multipoles ψ_n^m (separated solutions of the Helmholtz equation in spherical polar coordinates), one set singular at O_1 and the other set singular at O_2:

$$u = \sum_{n,m} (a_n^m \psi_n^m(\boldsymbol{r}_1) + b_n^m \psi_n^m(\boldsymbol{r}_2)).$$

(Precise definitions will be given later.) Then, determine the coefficients a_n^m and b_n^m by applying the boundary condition on each sphere in turn: this requires the expansion of $\psi_n^m(\boldsymbol{r}_2)$ in terms of regular spherical solutions centred on O_1, $\hat{\psi}_n^m(\boldsymbol{r}_1)$. Thus, we need the *addition theorem*

$$\psi_n^m(\boldsymbol{r}_2) = \sum_{\nu,\mu} S_{n\nu}^{m\mu}(\boldsymbol{b}) \hat{\psi}_\nu^\mu(\boldsymbol{r}_1)$$

which is valid for $r_1 < b$, where $r_1 = |\boldsymbol{r}_1|$, $b = |\boldsymbol{b}|$ and $\boldsymbol{r}_2 = \boldsymbol{r}_1 + \boldsymbol{b}$.

The matrix $\boldsymbol{S} = (S_{n\nu}^{m\mu})$ is called the *separation matrix* or the *translation matrix* or the *propagator matrix*. It also appears in the *two-centre expansion* of the fundamental solution (or 'free-particle propagator'). Thus, with $\boldsymbol{R} = \boldsymbol{a} + \boldsymbol{b} + \boldsymbol{c}$, we have [9, p 494]

$$\frac{\mathrm{e}^{\mathrm{i}kR}}{kR} = 4\pi \mathrm{i} \sum_{n,m} \sum_{\nu,\mu} (-1)^n S_{n\nu}^{m\mu}(\boldsymbol{b}) \overline{\hat{\psi}_n^m(\boldsymbol{a})} \hat{\psi}_\nu^\mu(\boldsymbol{c}) \tag{1.1}$$

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where $R = |\boldsymbol{R}|$ and the overbar denotes complex conjugation; this formula is certainly valid if $a + c < b$.

Exact expressions for $\boldsymbol{S}$ have been known for over 40 years; see, for example [4, 1]. The standard expression involves a sum of $\min(n, \nu)$ terms, each of which contains a multipole $\psi_q^s(\boldsymbol{b})$ and a Gaunt coefficient. (Gaunt coefficients can be written as the product of two Clebsch–Gordan coefficients or as the product to two Wigner 3-j symbols, apart from trivial factors.)

However, in numerical applications, one often wants to compute $S_{n\nu}^{m\mu}$ for many values of n and ν; the standard expression is inefficient for this purpose. Consequently, many authors have developed various algorithms for computing $\boldsymbol{S}$. Some of these provide efficient ways of evaluating the standard expression, perhaps by recursive techniques; see, for example, the papers by Chew [2], Kim [11] and Xu [19]. However, it is known that some recurrence relations are numerically unstable in certain circumstances [13].

Some authors begin by obtaining new expressions for $\boldsymbol{S}$, or good approximations to $\boldsymbol{S}$. Two such approaches are worthy of note. First, there are methods based on *diagonalization*. These were developed for use in *fast multipole methods*, which provide efficient numerical methods for solving the boundary integral equations of acoustic-scattering theory. See, for example, papers by Coifman *et al* [3], Rokhlin [17], Epton and Dembart [6] and Rahola [15] for more information.

Second, there are methods based on *separation*. These use a formula of the form

$$S_{n\nu}^{m\mu}(\boldsymbol{b}) = \frac{\mathrm{e}^{\mathrm{i}kb}}{\mathrm{i}kb} \sum_{N,M} \mathcal{S}_{nN}^{mM}(\boldsymbol{b}) \tilde{\mathcal{S}}_{\nu N}^{\mu M}(\boldsymbol{b}) \tag{1.2}$$

where the dependence on (n, m) and (ν, μ) is separated. Such a formula was obtained by Rehr and Albers [16] and by Fritzsche [7], and is the focus of this paper.

It is known that many published approximations to $\boldsymbol{S}$ can be obtained by truncating the series in (1.2); see [7, 16]. Numerically, one often retains only a few terms, but this can lead to serious errors, especially if kb is not large [8]. Nevertheless, it has been demonstrated by Sébilleau [18] that, when properly truncated, (1.2) gives a very efficient and accurate algorithm for computing $\boldsymbol{S}$. Moreover, he has also derived recursion relations for calculating the terms in (1.2).

With this as background, we have re-examined (1.2) and its derivation. First, we show in section 3 that one of the summations in (1.2) can be evaluated analytically. This leads to an explicit formula for $\boldsymbol{S}$ in inverse powers of kb: consistent asymptotic approximations of $\boldsymbol{S}$ can then be obtained by truncating this expansion.

Second, in section 4, we give a clear derivation of (1.2). We do this mainly because the existing derivations are defective or sketchy. Given the efficacy of (1.2), and its widespread use in condensed-matter physics, it seems worthwhile to give such a derivation. Moreover, we hope to bring the method to the attention of those working on related multiple-scattering problems in other branches of physics.

2. The Rehr–Albers–Fritzsche formula

Let (r, θ, ϕ) be spherical polar coordinates at O_2. Suppose, for simplicity, that $\boldsymbol{b} = b\hat{\boldsymbol{z}}$, where $\boldsymbol{b}$ is the position vector of O_1 with respect to O_2 and $\hat{\boldsymbol{z}}$ is a unit vector along the z-axis (so that O_1 is at $r = b$, $\theta = 0$). (The general situation, in which O_1 is not on the z-axis can be handled by introducing rotation matrices; this was done by Danos and

Maximon [4].) It follows that

$$S_{n\nu}^{m\mu}(b\hat{\boldsymbol{z}}) = (-1)^n S_{n\nu}^{m}(kb)\,\delta_{m\mu} \tag{2.1}$$

where δ_{ij} is the Kronecker delta; the coefficients $S_{n\nu}^{m}(b)$ are called *z-axis propagators*. The introduction of the factor $(-1)^n$ on the right-hand side ensures that we have the symmetry property,

$$S_{n\nu}^{m}(kb) = S_{\nu n}^{m}(kb).$$

Moreover, the coefficients $S_{n\nu}^{m}$ do not depend on the sign of m, so that, henceforth, we can assume that $m \geqslant 0$.

Before giving an explicit formula for $S_{n\nu}^{m}(kb)$, let us fix our notation and normalizations. We define normalized spherical harmonics by

$$Y_n^m(\hat{\boldsymbol{r}}) = Y_n^m(\theta,\phi) = (4\pi)^{-1/2} A_n^m P_n^m(\cos\theta)\mathrm{e}^{\mathrm{i}m\phi}$$

for $n = 0, 1, 2, \ldots$ and $m = 0, \pm1, \pm2, \ldots, \pm n$, where A_n^m is a normalization factor, defined by

$$A_n^m = (-1)^m\sqrt{2n+1}\sqrt{\frac{(n-m)!}{(n+m)!}} \tag{2.2}$$

and P_n^m is an associated Legendre function, defined by

$$P_n^m(t) = \frac{(1-t^2)^{m/2}}{2^n n!}\frac{\mathrm{d}^{m+n}}{\mathrm{d}t^{m+n}}(t^2-1)^n.$$

Then, we define the outgoing spherical wavefunctions by

$$\psi_n^m(\boldsymbol{r}) = h_n^{(1)}(kr)Y_n^m(\hat{\boldsymbol{r}})$$

where $h_n^{(1)}$ is a spherical Hankel function, and the regular spherical wavefunctions by

$$\hat{\psi}_n^m(\boldsymbol{r}) = j_n(kr)Y_n^m(\hat{\boldsymbol{r}})$$

where j_n is a spherical Bessel function.

We can now state the formula published in 1990 by Rehr and Albers [16] and by Fritzsche [7]. It is

$$S_{n\nu}^{m}(kb) = (-1)^m\mathrm{i}^{n+\nu}A_n^m A_\nu^{-m}\frac{\mathrm{e}^{\mathrm{i}kb}}{\mathrm{i}kb}\sum_\ell \frac{w^{2\ell+m}}{\ell!(\ell+m)!}d_\nu^\ell(w)d_n^{\ell+m}(w) \tag{2.3}$$

for $m \geqslant 0$, where

$$w = \frac{\mathrm{i}}{2kb}$$

and

$$d_n^\ell(w) = \sum_s \frac{(n+s)!w^{s-\ell}}{(n-s)!(s-\ell)!}. \tag{2.4}$$

Let us make some preliminary comments on (2.3). First of all, it is exact. Second, all summations are finite; to be precise, the summation in (2.3) is from $\ell = 0$ to $\ell = \min(\nu, n-m)$ whereas the summation in (2.4) is from $s = \ell$ to $s = n$. Thus, to evaluate (2.3), a single sum must be calculated wherein each term consists of the product of two sums. In fact, we will show (see (3.1) below) that part of this calculation can be carried out analytically, leaving a double sum. Nevertheless, the most important property of (2.3), numerically, is that the dependence on n and ν is separated. Finally, (2.3) gives an expression for $S_{n\nu}^{m}$ as an exponential multiplied by terms involving inverse powers of kb; this leads naturally to various approximations if $kb \gg 1$.

3. Reduction to a double sum

Consider the summation in (2.3). Explicitly, we have

$$\sum_{\ell} \frac{w^{2\ell+m} d_\nu^\ell d_n^{\ell+m}}{\ell!(\ell+m)!} = \sum_{\ell,s,t} \frac{w^{s+t}}{\ell!(\ell+m)!} \frac{(\nu+s)!}{(\nu-s)!(s-\ell)!} \frac{(n+t)!}{(n-t)!(t-\ell-m)!}$$

where, in accordance with Pauli's 'law of sloppiness' [14, p 126], we do not worry unduly about the summation limits. Introducing a new summation variable $j = s+t$, the right-hand side becomes

$$\sum_j w^j \sum_s \frac{(\nu+s)!}{(\nu-s)!} \frac{(n+j-s)!}{(n-j+s)!} \sum_\ell \frac{1}{\ell!(s-\ell)!(\ell+m)!(j-s-m-\ell)!}$$

wherein the ℓ-sum can be written in terms of binomial coefficients as

$$\frac{1}{s!(j-s)!} \sum_\ell \binom{s}{\ell} \binom{j-s}{j-s-m-\ell} = \frac{1}{s!(j-s)!} \binom{j}{j-s-m}.$$

Hence,

$$\sum_{\ell} \frac{w^{2\ell+m} d_\nu^\ell d_n^{\ell+m}}{\ell!(\ell+m)!} = \sum_j w^j j! \sum_s \frac{(\nu+s)!}{(m+s)!s!(\nu-s)!} \frac{(n+j-s)!}{(j-s-m)!(j-s)!(n-j+s)!}.$$

Thus, apart from the summation limits (which will be obtained later), we have the following result.

Theorem 1.

$$S_{n\nu}^m(kb) = (-1)^m \mathrm{i}^{n+\nu} \frac{\mathrm{e}^{\mathrm{i}kb}}{\mathrm{i}kb} \sum_{j=|m|}^{n+\nu} j! \left(\frac{\mathrm{i}}{2kb}\right)^j \sum_{s=s_0}^{s_1} \mathcal{A}_s(\nu, |m|) \mathcal{A}_{j-s}(n, -|m|) \tag{3.1}$$

for all $kb > 0$, where $s_0 = \max(0, j-n)$, $s_1 = \min(\nu, j-|m|)$ and

$$\begin{aligned} \mathcal{A}_s(\nu, m) &= (-1)^m A_\nu^{-m} \frac{(\nu+s)!}{(m+s)!s!(\nu-s)!} \\ &= \sqrt{2\nu+1} \sqrt{\frac{(\nu+m)!}{(\nu-m)!}} \frac{(\nu+s)!}{(m+s)!s!(\nu-s)!}. \end{aligned} \tag{3.2}$$

It is interesting to compare (3.1) with the Rehr–Albers–Fritzsche formula (2.3). Thus, the dependence on n and ν is separated in both, but (2.3) involves the *functions* $d_n^\ell(w)$ whereas (3.1) involves the *coefficients* $\mathcal{A}_s(n, m)$. Formula (3.1) can also be used to obtain *consistent* approximations for large kb. Thus, for the leading-order approximation ($j = 0$), we must take $m = 0$ whence $s_0 = s_1 = 0$ giving

$$S_{n\nu}^m(kb) \sim \delta_{m0} \frac{\mathrm{e}^{\mathrm{i}kb}}{\mathrm{i}kb} \mathrm{i}^{n+\nu} \sqrt{2n+1} \sqrt{2\nu+1} \qquad \text{as } kb \to \infty \tag{3.3}$$

which is known as the *plane-wave approximation* [12]. If we include terms of $\mathrm{O}((kb)^{-2})$, we obtain

$$S_{n\nu}^m(kb) \sim \delta_{m0} S_{n\nu}^{\mathrm{PWA}} \{1 + w[n(n+1) + \nu(\nu+1)]\} - w\delta_{|m|1} S_{n\nu}^{\mathrm{PWA}} \sqrt{n(n+1)} \sqrt{\nu(\nu+1)}$$

as $kb \to \infty$, where $\delta_{m0} S_{n\nu}^{\mathrm{PWA}}$ is the right-hand side of (3.3) and $w = \mathrm{i}/(2kb)$.

4. The Rehr–Albers–Fritzsche formula: a proof

The published derivations of (2.3) are unsatisfactory for several reasons, as discussed below in section 4.1. As (2.3) is so useful, both for numerical work and for generating asymptotic approximations, it seems worthwhile to give a more transparent derivation. We begin with an integral representation for $\mathrm{e}^{\mathrm{i}kR}/R$.

Theorem 2.

$$\frac{\mathrm{e}^{\mathrm{i}kR}}{R} = \frac{1}{4\pi^2}\int_{\mathcal{C}} \frac{\xi^2}{\xi^2 - k^2}\int_{\Omega} \exp(\mathrm{i}\xi\hat{\boldsymbol{r}}\cdot\boldsymbol{R})\,\mathrm{d}\Omega(\hat{\boldsymbol{r}})\,\mathrm{d}\xi \tag{4.1}$$

where $R = |\boldsymbol{R}| > 0$ and $\hat{\boldsymbol{r}} \in \Omega$, the unit sphere. The contour $\mathcal{C}$ goes from $\xi = -\infty$ to $\xi = +\infty$, passing above the simple pole at $\xi = -k$ and below the simple pole at $\xi = +k$.

Proof. Direct calculation shows that the inner integral is $4\pi j_0(\xi R)$, whence the right-hand side of (4.1) is

$$\frac{1}{2\pi\,\mathrm{i}R}\int_{\mathcal{C}} \frac{\xi}{\xi^2 - k^2}(\mathrm{e}^{\mathrm{i}\xi R} - \mathrm{e}^{-\mathrm{i}\xi R})\,\mathrm{d}\xi = \mathcal{I}_+ - \mathcal{I}_-$$

say, where

$$\mathcal{I}_\pm = \frac{1}{2\pi\,\mathrm{i}R}\int_{\mathcal{C}} \frac{\xi}{\xi^2 - k^2}\mathrm{e}^{\pm\mathrm{i}\xi R}\,\mathrm{d}\xi.$$

These integrals can be evaluated using Cauchy's residue theorem. Thus, for $\mathcal{I}_+$, close the contour using a large semicircle in the upper half of the complex ξ-plane. There is no contribution from this semicircle as it recedes to infinity, by Jordan's lemma. The contour encloses the simple pole at $\xi = +k$ (but not the pole at $\xi = -k$). Hence, evaluating the residue, we see that

$$\mathcal{I}_+ = \tfrac{1}{2}\mathrm{e}^{\mathrm{i}kR}/R.$$

Similarly, for $\mathcal{I}_-$, close the contour in the lower half of the complex ξ-plane. Taking account of the direction of traversal around the contour, and evaluating the residue of the pole at $\xi = -k$, we find that $\mathcal{I}_- = -\mathcal{I}_+$, and the result follows. □

In the above proof, we split the ξ-integral into two, $\mathcal{I}_+$ and $\mathcal{I}_-$, and then evaluated each separately, one by closing the contour in the upper half-plane and one by closing the contour in the lower half-plane. This is a standard technique. However, care is needed to ensure that $\mathcal{I}_+$ and $\mathcal{I}_-$ exist separately: the splitting is not unique, and some splittings may introduce additional singularities at $\xi = 0$. For example, a common mistake is to split using

$$2j_n(\xi R) = h_n^{(1)}(\xi R) + h_n^{(2)}(\xi R); \tag{4.2}$$

each of the spherical Hankel functions is $\mathrm{O}(\xi^{-n-1})$ as $\xi \to 0$.

The representation (4.1) is a variant of well known formulae using volume integrals; for example, DeSanto [5, p 64] shows that

$$\frac{\mathrm{e}^{\mathrm{i}kR}}{R} = \frac{1}{2\pi^2}\lim_{\varepsilon\to 0+}\iiint \frac{\exp(\mathrm{i}\boldsymbol{\xi}\cdot\boldsymbol{R})}{|\boldsymbol{\xi}|^2 - (k + \mathrm{i}\varepsilon)^2}\,\mathrm{d}\boldsymbol{\xi}. \tag{4.3}$$

However, (4.1) is preferable for at least two reasons: it does not involve adding a small imaginary part to the wavenumber; and it uses an integration along the entire real ξ-axis, so that contour-integral methods are readily available.

Note that, in (4.1) (and (4.3)), one cannot interchange the order of integration: the resulting ξ-integral diverges.

We are going to combine theorem 2 with the two-centre expansion of $\mathrm{e}^{\mathrm{i}kR}/R$, (1.1), so as to obtain an alternative expression for $S_{n\nu}^{m\mu}(b\hat{\boldsymbol{z}})$. Thus, write $\boldsymbol{R} = \boldsymbol{a} + \boldsymbol{b} + \boldsymbol{c}$, and then use the standard expansion of a plane wave [9, p 373] twice, once in the form

$$\exp(\mathrm{i}\xi\hat{\boldsymbol{r}}\cdot\boldsymbol{a}) = 4\pi\sum_{n,m}\mathrm{i}^n j_n(\xi a)\overline{Y_n^m(\hat{\boldsymbol{a}})}Y_n^m(\hat{\boldsymbol{r}})$$

and once in the form

$$\exp(\mathrm{i}\xi\hat{\boldsymbol{r}}\cdot\boldsymbol{c}) = 4\pi\sum_{\nu,\mu}\mathrm{i}^\nu j_\nu(\xi c)Y_\nu^\mu(\hat{\boldsymbol{c}})\overline{Y_\nu^\mu(\hat{\boldsymbol{r}})}$$

where

$$\sum_{n,m} \equiv \sum_{n=-\infty}^{\infty}\sum_{m=-n}^{n}.$$

Substituting in (4.1), the inner integral becomes

$$(4\pi)^2\sum_{n,m}\sum_{\nu,\mu}\mathrm{i}^{n+\nu}j_n(\xi a)j_\nu(\xi c)\overline{Y_n^m(\hat{\boldsymbol{a}})}Y_\nu^\mu(\hat{\boldsymbol{c}})\mathcal{I} \tag{4.4}$$

where

$$\mathcal{I} = \int_\Omega \exp(\mathrm{i}\xi\hat{\boldsymbol{r}}\cdot\boldsymbol{b})Y_n^m(\hat{\boldsymbol{r}})\overline{Y_\nu^\mu(\hat{\boldsymbol{r}})}\,\mathrm{d}\Omega(\hat{\boldsymbol{r}}).$$

Now, assume that $\boldsymbol{b} = b\hat{\boldsymbol{z}}$, whence $\hat{\boldsymbol{r}}\cdot\boldsymbol{b} = b\cos\theta$ and

$$\begin{aligned}\mathcal{I} &= 2\pi\delta_{m\mu}\int_0^\pi \mathrm{e}^{\mathrm{i}\xi b\cos\theta}Y_n^m(\hat{\boldsymbol{r}})\overline{Y_\nu^m(\hat{\boldsymbol{r}})}\sin\theta\,\mathrm{d}\theta \\ &= \tfrac{1}{2}\delta_{m\mu}\int_{-1}^1 \mathrm{e}^{\mathrm{i}\xi bt}G_m(t;n,\nu)\,\mathrm{d}t \end{aligned}\tag{4.5}$$

where

$$G_m(t;n,\nu) = A_n^m A_\nu^m P_n^m(t)P_\nu^m(t) \tag{4.6}$$

and A_n^m is defined by (2.2). G_m has the following properties:

$$G_m(t;n,\nu) \text{ is a polynomial of degree } n+\nu \tag{4.7}$$

$$G_{-m}(t;n,\nu) = G_m(t;n,\nu) \tag{4.8}$$

$$G_m(-t;n,\nu) = (-1)^{n+\nu}G_m(t;n,\nu) \tag{4.9}$$

$$G_m(t;n,\nu) \equiv 0 \qquad \text{for } |m| > \min(n,\nu).$$

The first of these implies that

$$G_m^{(j)}(t;n,\nu) \equiv 0 \qquad \text{for } j > n+\nu$$

where $G_m^{(j)} = (\mathrm{d}^j/\mathrm{d}t^j)G_m$. Hence, repeated integration by parts gives

$$\int_{-1}^1 \mathrm{e}^{\mathrm{i}Xt}G_m(t)\,\mathrm{d}t = \sum_{j=0}^{n+\nu}\left[\frac{\mathrm{e}^{\mathrm{i}Xt}}{\mathrm{i}X}\left(\frac{-1}{\mathrm{i}X}\right)^j G_m^{(j)}(t)\right]_{-1}^1$$

where we have written $G_m(t)$ for $G_m(t;n,\nu)$. But, from (4.9),

$$G_m^{(j)}(-t;n,\nu) = (-1)^{n+\nu+j}G_m^{(j)}(t;n,\nu)$$

whence

$$\int_{-1}^{1} \mathrm{e}^{\mathrm{i}Xt} G_m(t)\,\mathrm{d}t = \sum_{j=0}^{n+\nu} G_m^{(j)}(1) \frac{(-1)^j}{(\mathrm{i}X)^{j+1}} \{\mathrm{e}^{\mathrm{i}X} - (-1)^{n+\nu+j}\mathrm{e}^{-\mathrm{i}X}\}. \tag{4.10}$$

We will evaluate $G_m^{(j)}(1)$ later (lemma 4); it turns out that $G_m^{(j)}(1) = 0$ for $j < |m|$, so that the lower limit in (4.10) can be replaced by $j = |m|$.

Having evaluated $\mathcal{I}$, we next consider the outer integral; it is of the form

$$\int_{\mathcal{C}} \frac{\xi^2}{\xi^2 - k^2} j_n(\xi a) j_\nu(\xi c) \int_{-1}^{1} \mathrm{e}^{\mathrm{i}\xi bt} G_m(t; n, \nu)\,\mathrm{d}t\,\mathrm{d}\xi = \mathcal{L} \tag{4.11}$$

say. From (4.10), we see that the inner integral is $\mathrm{O}(\xi^{-n-\nu})$ as $\xi \to 0$. However, $j_n(\xi a) j_\nu(\xi c) = \mathrm{O}(\xi^{n+\nu})$ as $\xi \to 0$, whence the integrand in the outer integral is analytic at $\xi = 0$. So,

$$\mathcal{L} = \sum_{j=|m|}^{n+\nu} G_m^{(j)}(1) \frac{(-1)^j}{(\mathrm{i}b)^{j+1}} \{\mathcal{L}_+ - (-1)^{n+\nu+j}\mathcal{L}_-\}$$

where

$$\mathcal{L}_\pm = \int_{\mathcal{C}} \frac{\xi^{-j+1}}{\xi^2 - k^2} j_n(\xi a) j_\nu(\xi c) \mathrm{e}^{\pm \mathrm{i}\xi b}\,\mathrm{d}\xi.$$

Assuming that $b > (a + c)$, we can close the contour for $\mathcal{L}_\pm$ as for $\mathcal{I}_\pm$ in the proof of theorem 2, giving

$$\mathcal{L}_+ = \pi \mathrm{i} k^{-j} j_n(ka) j_\nu(kc) \mathrm{e}^{\mathrm{i}kb}$$

and $\mathcal{L}_- = (-1)^{n+\nu+j+1}\mathcal{L}_+$, whence

$$\mathcal{L} = 2\pi \mathrm{i} k \mathrm{e}^{\mathrm{i}kb} j_n(ka) j_\nu(kc) \sum_{j=|m|}^{n+\nu} G_m^{(j)}(1) \frac{(-1)^j}{(\mathrm{i}kb)^{j+1}}.$$

Combining this formula with (4.1), (4.4) and (4.5), we obtain

$$\frac{\mathrm{e}^{\mathrm{i}kR}}{kR} = 4\pi \mathrm{i} \mathrm{e}^{\mathrm{i}kb} \sum_{n,m,\nu} \mathrm{i}^{n+\nu} \overline{\hat{\psi}_n^m(\boldsymbol{a})} \hat{\psi}_\nu^m(\boldsymbol{c}) \sum_{j=|m|}^{n+\nu} G_m^{(j)}(1) \frac{(-1)^j}{(\mathrm{i}kb)^{j+1}}$$

for $b > (a + c)$. Finally, comparison with the two-centre expansion (1.1) and the definition (2.1) gives the following result.

Theorem 3.

$$S_{n\nu}^m(kb) = \frac{\mathrm{e}^{\mathrm{i}kb}}{\mathrm{i}kb} \mathrm{i}^{n+\nu} \sum_{j=|m|}^{n+\nu} G_m^{(j)}(1; n, \nu) \left(\frac{\mathrm{i}}{kb}\right)^j$$

for all $kb > 0$, where $G_m(t; n, \nu)$ is defined by (4.6).

Note that although the argument above gives the result for $b > (a + c)$, $S_{n\nu}^m(kb)$ itself does not depend on a and c, and so analytic continuation shows that the result must hold for all $b > 0$.

The coefficients $G_m^{(j)}(1; n, \nu)$ in theorem 3 are given by the next lemma.

Lemma 4. For $0 \leqslant |m| \leqslant \min(n, \nu)$ and $|m| \leqslant j \leqslant n + \nu$,

$$G_m^{(j)}(1; n, \nu) = (-1)^m \frac{j!}{2^j} \sum_{k=k_0}^{k_1} \mathcal{A}_k(\nu, |m|) \mathcal{A}_{j-k}(n, -|m|) \tag{4.12}$$

where $k_0 = \max(0, j - n)$, $k_1 = \min(\nu, j - |m|)$ and $\mathcal{A}_k(\nu, m)$ is defined by (3.2). For all other values of j, m, n and ν, $G_m^{(j)}(1; n, \nu) = 0$.

Proof. From (4.8), it is enough to take $m \geqslant 0$. From [10, equation 8.751(1)], we have

$$P_n^m(t) = \frac{(n+m)!}{(n-m)!}\frac{(1-t^2)^{m/2}}{2^m m!}F(m-n, m+n+1; m+1; \tfrac{1}{2}(1-t))$$

where F is a hypergeometric function. Hence,

$$G_m(t) = A_n^{-m}A_\nu^{-m}(2^m m!)^{-2}(1-t^2)^m F_n F_\nu$$

where

$$F_n \equiv F(m-n, m+n+1; m+1; \tfrac{1}{2}(1-t))$$

and we have used

$$[(n+m)!/(n-m)!]A_n^m = A_n^{-m}.$$

(This expression for $G_m(t)$ can be used to show (4.7).) Now, put $z = \frac{1}{2}(1-t)$ whence $1-t^2 = 4z(1-z)$. Then, use [10, equation 9.131(1)]

$$(1-z)^{\alpha+\beta-\gamma}F(\alpha, \beta; \gamma; z) = F(\gamma-\alpha, \gamma-\beta; \gamma; z)$$

with $\alpha = m-\nu$, $\beta = m+\nu+1$ and $\gamma = m+1$ to give

$$(1-z)^m F_\nu = F(-\nu, \nu+1; m+1; z).$$

Explicitly, we have

$$F(-\nu, \nu+1; m+1; z) = \sum_{k=0}^{\nu} a_k(\nu, m)z^k$$

and

$$F(m-n, m+n+1; m+1; z) = \sum_{k=0}^{n-m} b_k(n, m)z^k$$

where

$$a_k(\nu, m) = \frac{(-1)^k m!(\nu+k)!}{(m+k)!k!(\nu-k)!}$$

and

$$b_k(n, m) = \frac{(-1)^k m!(n+m+k)!(n-m)!}{(m+k)!k!(n-m-k)!(n+m)!}.$$

Hence, after rearranging the double summation, we find that

$$G_m(t; n, \nu) = z^m \sum_{s=0}^{n+\nu-m} C_s z^s \tag{4.13}$$

where

$$C_s = A_n^{-m}A_\nu^{-m}\sum_{k=0}^{s}\frac{a_k(\nu, m)}{m!}\frac{b_{s-k}(n, m)}{m!} \qquad \text{for } 0 \leqslant s \leqslant n+\nu-m.$$

In fact, as $a_k = 0$ for $k > \nu$ and $b_k = 0$ for $k > n-m$, the summation is actually from $k = \max(0, s-n+m)$ to $k = \min(s, \nu)$. Simplifying further gives

$$C_s = (-1)^s \sum_k \mathcal{A}_k(\nu, m)\mathcal{A}_{s+m-k}(n, -m)$$

where $\mathcal{A}_k(\nu, m)$ is defined by (3.2).

Finally, let us compare the expansion (4.13) with the Taylor series for $G_m(t)$ about $t = 1$, which is

$$G_m(t) = \sum_{j=0}^{n+\nu} \frac{(-2)^j}{j!} G_m^{(j)}(1) z^j.$$

This shows that $G_m^{(j)}(1) = 0$ for $j < m$, and gives the desired formula (4.12). □

When theorem 3 is combined with lemma 4, theorem 1 is obtained, and this latter result is equivalent to the formula of Rehr, Albers and Fritzsche.

4.1. Remarks

Here, we make some remarks concerning the papers [7, 16]. Both Fritzsche [7, equation (6)] and Rehr and Albers [16, equation (7)] begin with a volume-integral representation for $S_{n\nu}^{m\mu}$. The derivation of this formula by Fritzsche [7] is flawed because of the use of (4.2).

Fritzsche proceeds by obtaining a formula for $S_{n\nu}^{m}(kb)$ (his equation (10)), involving the integral $\mathcal{I}$, defined by (4.5). He states that $\mathcal{I}$ 'can be calculated straightforwardly' [7, p 1415] but does not give any details.

Rehr and Albers proceed differently. Apart from inessential factors, they arrive at an integral similar to $\mathcal{L}$, defined by (4.11). Next, they interchange the order of integration: the resulting ξ-integral is divergent. Despite this, it is claimed that 'the integral over ξ can be done by contour integration (closing in the upper half-plane for $t > 0$ and in the lower half-plane for $t < 0$)' [16, p 8147]. But, with $t > 0$ for example, this argument would only give the claimed result if $bt > (a + c)$, whereas the remaining t-integral is over $-1 \leqslant t \leqslant 1$. Finally, Rehr and Albers use a very interesting formula for (a variant of) the Laplace transform of the product of two functions [16, appendix B]. Their derivation of this formula is also incomplete, although their final formula can be shown to be correct. However, we have shown above that this formula is not needed in order to obtain theorem 1.

5. Conclusions

The Rehr–Albers–Fritzsche formula can be used as the basis for a very efficient and accurate algorithm for computing the propagator matrix $\boldsymbol{S}$. Here, we have clarified the derivation of this formula, and shown how it can be simplified further. This simplification leads directly to asymptotic approximations for large kb. We hope that these will find application in other areas of science and engineering, where multiple-scattering computations are widespread.

References

[1] Boström A, Kristensson G and Ström S 1991 Transformation properties of plane, spherical and cylindrical scalar and vector wave functions *Field Representations and Introduction to Scattering* ed V V Varadan, A Lakhtakia and V K Varadan (Amsterdam: North-Holland) pp 165–210

[2] Chew W C 1992 Recurrence relations for three-dimensional scalar addition theorem *J. Electromag. Waves Appl.* **6** 133–42

[3] Coifman R, Rokhlin V and Wandzura S 1993 The fast multipole method for the wave equation: a pedestrian prescription *IEEE Ant. Propag. Mag.* **35** (3) 7–12

[4] Danos M and Maximon L C 1965 Multipole matrix elements of the translation operator *J. Math. Phys.* **6** 766–78

[5] DeSanto J A 1992 *Scalar Wave Theory* (Berlin: Springer)

[6] Epton M A and Dembart B 1995 Multipole translation theory for the three-dimensional Laplace and Helmholtz equations *SIAM J. Sci. Comput.* **16** 865–97
[7] Fritzsche V 1990 A new spherical-wave approximation for photoelectron diffraction, EXAFS and MEED *J. Phys.: Condens. Matter* **2** 1413–24
[8] Fritzsche V 1992 Shortcomings of separable representations of the Green function in multiple-scattering theory for photoelectron diffraction and extended x-ray absorption fine structure *J. Electron Spectrosc. Relat. Phenom.* **58** 299–314
[9] Gonis A 1992 *Green Functions for Ordered and Disordered Systems* (Amsterdam: North-Holland)
[10] Gradshteyn I S and Ryzhik I M 1980 *Table of Integrals, Series, and Products* (New York: Academic)
[11] Kim K T 1996 The translation formula for vector multipole fields and the recurrence relations of the translation coefficients of scalar and vector multipole fields *IEEE Trans. Ant. Propag.* **44** 1482–7
[12] Lee P A and Pendry J B 1975 Theory of the extended x-ray absorption fine structure *Phys. Rev.* B **11** 2795–811
[13] Manar F and Brouder Ch 1995 A fast free Green function calculation in multiple-scattering theory *Physica* **208&209B** 79–80
[14] Peierls R 1979 *Surprises in Theoretical Physics* (Princeton, NJ: Princeton University Press)
[15] Rahola J 1996 Diagonal forms of the translation operators in the fast multipole algorithm for scattering problems *BIT* **36** 333–58
[16] Rehr J J and Albers R C 1990 Scattering-matrix formulation of curved-wave multiple-scattering theory: Application to x-ray-absorption fine structure *Phys. Rev.* B **41** 8139–49
[17] Rokhlin V 1993 Diagonal forms of translation operators for the Helmholtz equation in three dimensions *Appl. Comput. Complex Anal.* **1** 82–93
[18] Sébilleau D 1995 New recurrence relations for matrix elements of the propagator *J. Phys.: Condens. Matter* **7** 6211–20
[19] Xu Y -L 1996 Calculation of the addition coefficients in electromagnetic multisphere-scattering theory *J. Comput. Phys.* **127** 285–98 (1997 *J. Comput. Phys.* **134** 200 (erratum))
[20] Zeller R 1992 Band-structure methods *Unoccupied Electronic States (Topics in Applied Physics 69)* ed J C Fuggle and J E Inglesfield (Berlin: Springer) pp 24–49