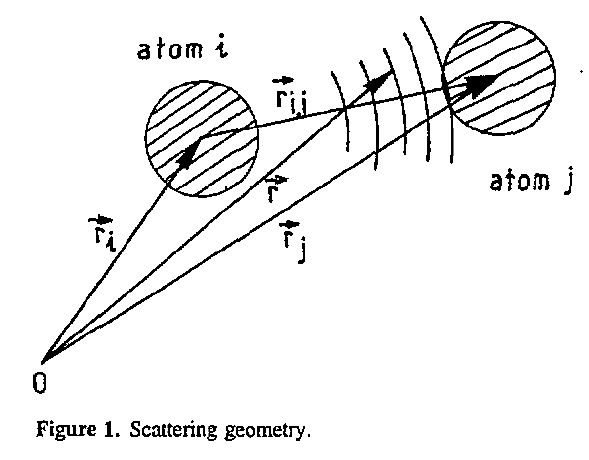
Following D. Sebilleau, J. Phys. Condens. Matter **7**, 6211 (1995).

Let us consider an outgoing spherical wave of angular momentum centered on an atom *i* situated at ***r****i* with respect to the origin, and incoming on an atom *j* located at ***r****j*. From partial wave theory [1], we know that such a wave can be represented by the wave function (to within a constant amplitude factor)

|  |  |
| --- | --- |
|  |  |

With being a spherical Hankel function of the first kind [2], a spherical harmonic and the unit vector in the direction of ***r***.



Such a wave cannot be scattered directly by atom *j* but must first be re-expanded as a linear combination of spherical waves centered on the scatterer:

|  |  |
| --- | --- |
|  |  |

Where as defined in Figure 1.

The coefficients of the linear combination are the matrix elements of the free electron propagator taken between state centered at ***r****j* and state centered at ***r****i* .

Relations such as equation (2) are called addition theorems and have been known for some time now. Here,

|  |  |
| --- | --- |
|  |  |

(NOTE TO SELF – this can be used to check the RA implementation) With

|  |  |
| --- | --- |
|  |  |

is a Gaunt coefficient and is usually expressed in terms of Wigner’s 3j symbols for numerical calculations.

Introducing the Hankel polynomial [2] by

|  |  |
| --- | --- |
|  |  |

i.e., the correction factor to the asymptotic form of the spherical Hankel function, we can write conveniently in terms of its reduced form

|  |  |
| --- | --- |
|  |  |

We can now rotate the bond direction onto the z-axis to take advantage of the fact that z is a quantization axis for the angular momentum. The expression of along the z direction will be therefore much simplified. Introducing the z-axis reduced free-electron propagator matrix elements in an angular momentum representation by

|  |  |
| --- | --- |
|  |  |

And applying rotation matrices [8, Messiah], we can expand this in a magnetic quantum number series:

|  |  |
| --- | --- |
|  |  |

Where are the spherical polar coordinates of .

Writing the Gaunt coefficients in (3) in terms of Wigner’s 3j symbols leads to

|  |  |
| --- | --- |
|  |  |

It is worth noting that this quantity and the corresponding one for do not depend on the sign of **. From now on we will consequently write them as and . Moreover, these two quantities are symmetrical with respect to interchange of l and lprime:

|  |  |
| --- | --- |
| , |  |

These two properties are fundamental as they allow us to reduce the number of values to be computed. Furthermore, the set of values of m can most of the time be limited to the first few without significant loss of accuracy. The reason for this was argued by Barton and Shirley [5] and most recently by Rehr and Albers [9]. We refer the reader to these references for a comprehensive discussion of the matter.

## The Rehr and Albers approach

One elegant way to find a fast procedure to compute the is to use the Rehr and Albers separable representation of the matrix elements of the free-electron propagator. Following their main result, we write

|  |  |
| --- | --- |
|  |  |

Where the contributions from the L incoming partial waves and from the various Lprime outgoing partial waves have been separated. The indices and are my introductions and . The other quantities are given by

|  |  |
| --- | --- |
|  |  |
|  |  |

## Wigner 3j symbols and Gaunt coefficients

|  |  |
| --- | --- |
|  |  |

|  |  |
| --- | --- |
|  |  |

Where the Wigner 3j symbols are defined as

|  |  |
| --- | --- |
|  |  |

There are several schemes for computing these symbols in the literature, reference Sebilleau. The method he recommends is as follows.

|  |  |
| --- | --- |
|  |  |

The computation of the coefficient B can be further simplified by noting that it admits a simple recurrence relation:

|  |  |
| --- | --- |
|  |  |

## Multiple Scattering Theory

|  |  |
| --- | --- |
|  |  |
|  |  |

|  |  |
| --- | --- |
|  |  |
|  |  |

The larger advantage of the separable representation is that it allows “precomputation” of matrices summing over L and converts those sums to matrix multiplications.