The Rehr-Albers Method

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The expansion in spherical waves of the dimensionless outgoing free propagator:

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About the fixed sites R and Rprime:

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Rehr and Albers define the propagator matrix elements as (Ref. Lloyd and Smith, Adv. Phys. 21, 69 (1972)):

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The primary focus of RA’s paper is to define a form of the propagator which separates contributions from L and Lprime:

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# The Dyson Equation

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For the free atom:

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Operating on both sides with the inverse operator:

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Gives (multiplying through the minus sign):

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The complete solution of equation 160 is the particular plus the general solution:

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We know that this is the solution to the free atom case:

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If we define the free space Green’s operator

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Then

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And in the multiple-scattering path formulation,

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Now in the cluster scattering case,

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Let’s define the symbol

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So that

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Expanding out,

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Grouping terms,

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Define the full potential symbol

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Projecting this onto a set of phase shifted spherical waves at the absorber,

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In the absence of the absorber potential, the wave function can be expanded in terms of free spherical waves. Outside of the muffin-tin sphere, the wave function can be expanded in terms of phase-shifted free spherical waves:

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Properties of this basis:

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Proofs:

Since we know

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Inserting the complete set:

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And the identity is proven.

Orthogonality of the basis:

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Insert a complete set of states in coordinate space:

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And the orthogonality is proven.

Relationship to free spherical waves (non-shifted)

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Returning to the MS derivation:

Projecting this onto a set of phase shifted spherical waves at the absorber, the coefficients of the expansion in free spherical waves about the absorber are:

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Definition of T-matrices:

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So that

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Expanding out,

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Decomposition in spherical waves:

1. Expand field in the absence of the absorber potential in free spherical waves (analogous to derivation of Rayleigh relation when field is a plane wave)
2. Compare that to

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To compute the amplitudes beta\_l.

So the coefficients

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Where the alpha\_l are the coefficients of the expansion:

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Which in coordinate space is:

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Comparing to the free wave:

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That’s an important expression, because the atomic wave function is

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And the radial charge density is

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Integrating this charge density over the muffin-tin gives:

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This last equation gives the total charge within the muffin-tin.

Alright, so the problem reduces to finding the betas:

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For both the direct and full-scattering cases, the direct case being:

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Note that when computing the chi-function, the factors of k over 2 pi will drop out, and the I ^l factors will disappear in the amplitude squared. So the only important part is the spherical wave coefficient.

Define the coefficients for direct and full scattering as:

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The chi-function represents the oscillatory part of the signal with respect to *angle of incidence*. In the expression for the total incident charge within the absorber muffin-tin, the only part that varies with angle is the beta:

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HOWEVER, the muffin-tin integral WILL affect how each coefficient is weighted.

For right now, we’ll calculate the betas. THEN we’ll worry about how to handle the core wavefunctions.

One strategy – knowing the amplitudes beta of the free spherical waves, we can match the wave functions at the muffin-tin radius to determine the amplitude of the core wave function. But isn’t this what I tried to do before?

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Should it be?

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And

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Is the scattering t-matrix for the atom located at **R**, where

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## Direct term

Make note that we are assuming that the absorber is at the origin.

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We replace the plane wave with its expansion in spherical waves (Rayleigh’s theorem):

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Since

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And that is the direct term.

Actually, one should note that the betas are a function of L and not just angular momentum.

The integrated charge is:

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Using Unsold’s Theorem:

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Gives

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And the magnetic quantum number does not matter here (as expected).

## Direct Term Not at Origin

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Change variables:

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We replace the plane wave with its expansion in spherical waves (Rayleigh’s theorem):

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## Single-scattering term

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Normalization of GLL: If rho = 0 , I expect GLL = 1, check this.

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The coefficients are:

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Where f is NOT a function of L.

The integrated charge is:

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Which, I’m thinking, is likely NOT independent of m. Then again, it could be. Better to just be explicit about it to be sure.

## Double-scattering term

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Inserting more complete sets, progressing from right to left,

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We define the scattering matrix:

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And substituting:

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We define the introduction matrix:

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And substituting, we achieve the final result:

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# Higher orders of scattering

Are achieved by inserting successive factors of the scattering matrix and corresponding spherical wave factors:

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Summarizing:

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Extension Method:

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Try redefining:

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So that:

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The only place that khat appears is in the Q, so by calculating the series up to Q, we can quickly regenerate for different incident angles (i.e., by working with the RootAmplitude of all paths).

In matrix multiplication format, and for a single path and L:

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! Need to answer the question – for L = (l, m), do the n-values contribute or are they all the same for each m, meaning that the overall sum gains a factor of (2l + 1) and reduces to l-sum?

Try redefining:

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Where the index n is the RA Order (typically 1, 3, or 6), and m is all (l,m) values, dimension:

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So for Lmax = 10, m = 120.

# Calculation Method

Compute the matrices F, P and Gamma-twiddle (M).

Public Class Matrix

Encapsulates the data and rules for mathematical operations of matrices.

Public Class ScatteringMatrixFactory

Methods to return F, P and GammaTwiddle. Encapsulate algorithms to provide computational efficiency (eliminate recalculation of equivalent matrices). Hides a data store for caching results.

Public Class ScatteringPath

1. Start with the calculation of the direct term.
2. Next tabulate all single – scattering amplitudes
   1. Both with and without the termination factor – save the “without” result for future appending.
3. Calculate the amplitude for each tabulated path.
4. For each path
   1. If the amplitude of the path is > some cutoff value, generate new paths by adding a leg

Get the next path in the list

Append a new leg on it

If the amplitude of the new path is > cutoff, save it, otherwise discard it.

For a 3 atom cluster, works like this:

1. 0 (automatic pass)
2. 10 (pass)
   1. 010 (pass)
      1. 1010
      2. 2010
   2. 210 (fail)
3. 20 (pass)
   1. 020
   2. 010

* Implement as a multithreaded work queue – one queue is paths needing calculation, another is paths needing extension. Different worker threads execute the calculations, adding those paths to the extension queue if amplitude is big enough. Another thread works the extension queue, adding nodes and filling the calculate queue with the resulting paths. Iterate until no nodes are left in the calculate queue. Elegant!