DESDCalculation Class

This class performs the actual DESD calculation.

Dependencies:

* Cluster class
* PhaseShift
* MuffinTin

The class implements a multiple scattering algorithm based on the real-space separable propagator method of Rehr and Albers.

# Derivation of the desorption rate equations:

The rate *R* at which atoms or molecules of a particular chemical species leave the surface can be expressed as a simple product of the incident electron flux *I*, the probability that an incident electron will cause an excitation which could potentially lead to desorption, and the total probability *D* that the excitation results in a desorbate escaping the surface.

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In the most general case, there may be multiple types of excitations giving rise to multiple desorption channels, and the total rate is the sum of the rates of the individual channels *j*:

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For any one desorption channel, the time-independent excitation rate is given by Fermi’s Golden Rule:

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Where the labels *i* and *f* denote the initial and final states of the system, respectively (including the incident electron and any outgoing ionization electrons, assuming the desorption is triggered by an ionization event. In general, the final state could include non-ionized excited states such as plasmons or phonons), and is the density of final states.

The transition probability is proportional to the square of the integral of the interaction over all of the space appropriate to the problem:

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Several qualities of this integral make it very challenging to calculate:

* the electron-electron interaction is a long-ranged Coulomb interaction, necessitating integration over a large volume (potentially extending to the entire solid)
* the final state can be complex, with one or more outgoing electrons, holes, and/or quasiparticles, and many possible degenerate channels

These complexities notwithstanding, there are several features of ESD that allow us to make various simplifying approximations. First, approximate the initial state wave function as the simple product of the wave functions of the (ground state) solid and the incident electron moving in the potential of the solid:

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Giving

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Assuming a one-electron interaction:

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The magnitude of the rate difference between two adjacent incident vectors k1 and k2 is:

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In this approximation the initial state is given by the anti-symmetric Slater determinant:

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Within the muffin-tin potential, exchange is approximated by the Slater approximation when solving for Psi1, and includes the exchange interaction with the target electron. So we will ignore the exchange integral contribution.

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The initial-state interaction between the incident electron and the solid will be comprehended in the Hartree-Fock-Slater approximation, in which the incident electron moves in the total field of the other *N* electrons and ion cores, and includes exchange in the Slater approximation.

Assumptions:

* ESD occurs due to a *single* *electron* excitation event predicated by an interaction with the incident electron.

Assuming that the incident flux is constant, and that the probability of desorption is constant (for a given incident electron energy),

We shall make several assumptions to radically simplify the problem, while retaining the essential physics of interest:

We shall ignore the details of the final state (radiative & non-radiative core hole relaxation, Auger decays, etc)

Our experiment is focusing on the dependence of the total ESD rate on the incident electron direction and not energy. The energetic of the interaction is constant, so we care only about those components of the interaction which depend on k-hat.

Let’s assume that the interaction is between two electrons only, both moving in the potential of the solid (and are eigenfunctions of the potential of the solid)

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We assume that the incident electron is described by the wave function and that the “target” electron is in a (negative energy) bound state of the “target” atom .

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Where the interaction Hamiltonian is a screened Coulomb potential with screening length .

If we further assume that anddo not depend on ,(this is not necessarily true, but we rely upon the integration to make the assertion not too false), then the final state integral can be replaced by a constant term:

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The target electron wave function is essentially zero outside of the muffin-tin radius, so the limits of integration become:

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Now we further approximate that the screening length , and the majority of the contribution to the excitation rate

If we replace the Coulomb potential with its multipole expansion:

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The target wavefunction is expressed in terms of spherical harmonics and the radial wave functions:

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Subbing all of these in,

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Since the orthogonality of the spherical harmonics states that

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Then the expression above simplifies to

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To a first approximation, the likelihood of a deep core excitation event is proportional to the amount of incident electron charge in the near vicinity of the core state (i.e, within the muffin-tin radius). While final-state effects dependent on the details of the outgoing electron k-vectors will have some structure effects, these will be treated as higher order corrections.

Strategy – what would the equations be in a time-reversed picture? If I picture waves of pure angular momentum l radiating outwards from the (absorber) atom (analogous to the photoemission process without the optical interaction and the core hole), scattering through the solid and then propagating to the detector, I’d expect to see some amplitude arrive there, corresponding to the amplitude placed into that l-state of the absorber if time is reversed. If I do this for all angular momenta and sum (coherently?), that should be proportional to the total amplitude, and therefore the total charge density.

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The incident electron in the solid satisfies the Schrodinger equation

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The Hamiltonian is given by

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Where

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Is the kinetic energy operator (free space Hamiltonian), and the energy in the solid is adjusted for the inner and optical potentials:

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is the free space energy (the incident electron beam energy).

The wave function of the incident electron within the (spherically symmetric) absorber muffin-tin is given by the expansion in terms of the radial wave functions and the spherical harmonics:

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We will make the assertion that, all other things being equal, the probability of ionization of the target atom (leading to subsequent desorption) is proportional to the total incident electron charge density in the vicinity of the core level, i.e., within the muffin-tin.

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The associated homogenous equation is

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Which has the solution

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Note that, for complex E, the wave vector k is also complex, and the plane wave solutions decay.

For the general solution, we begin by operating on both sides of Eq. 30:

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The full solution of Eq. 30 is the particular solution plus the general solution:

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Since the operator 1 / (E – H0) is divergent, we move the poles onto the imaginary axis by adding a factor of , with the understanding that we will take the limit at the end of it all.

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We define the Green’s operator G as

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Let’s think a bit. What I want to know is the wave function in the vicinity of the absorber atom

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In an r-basis:

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To within, I believe, a normalization factor. CHECK THIS.

I could consider the time-reversed problem and look at spherical outgoing waves from the origin of pure angular momentum, scattering to outgoing plane waves. The sum of all L for the spherical waves would give a set of phased plane waves that would interfere and produce a total outgoing amplitude. I actually kind of like this approach.

Step-model:

1. Incident electron interacts with the ground state solid potential and forms a LEED state.
2. The charge density due to the incident electron interacts with a core or valence electron in the solid to produce a e-2e final state (plus a hole). The e-2e final state also could be e + exciton.
3. For deeper core holes, it can decay via an Auger process to a shake-up or shake-off final state.
4. Valence hole or exciton can migrate and self-trap (via phonon interactions) and produce a dissociative state.
5. Dissociative state decays to produce an outgoing ion or neutral atom + surface vacancy.

Time-reversed problem – consider a spherical wave of pure angular momentum radiating outwards from the target muffin-tin:

Now, the wave function outside of the muffin tin is given by:

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Projecting this function onto the spherical wave basis:

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The inner integral

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Subbing:

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Let’s isolate the integrals over r:

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I’m not absolutely sure of this, but I \*think\* the normalization of the wave functions is such that it is always real (this is what we assume when calculating the phase shifts – the imaginary terms (those involving yn) drop out. If this is the case in general, then we can ignore the contribution to the wave function from the spherical Bessel function of the second kind, and we get:

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And therefore

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Note that if we defined the spherical wave basis set without the factor of i^l, this would give back the exact same thing we started with. Let’s try that:

Going back to the start:

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Orthonormality of the spherical wave basis:

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Works just fine. This also passes the completeness test.

Now, the wave function outside of the muffin tin is given by:

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Note that the spherical Bessel function of the first kind is the real part of the spherical Hankel function. SO – this works, and the outgoing spherical wave is identical to:

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Also note that

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Hmm. This’d be “neater” if it was sin, like in the t-matrix.

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I wonder… does the factor of 2i come from the calculation of the t-matrix in the angular momentum basis?

Going back a few steps:

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Zoom in on the last integral:

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I have a sneaking suspicion that the imaginary part is zero.

## From Rehr & Albers 1990

The cl(rho) are the dimensionless polynomial factors that multiply the asymptotic (meaning, here, the series expansion) form of the spherical Hankel function:

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The series expansion is:

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Hmmm… Interesting. Rehr says he’s adopted throughout the convention of Messiah for spherical Bessel functions, spherical harmonics, Legendre polynomials, and rotation matrices. What does Messiah say about h?

AhHA – Messiah has a different phase convention for spherical Bessel functions than what I’ve been using. WONDERFUL.

## Messiah Convention

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Rehr and Albers give

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Having specific values

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Which matches Rehr.

## Standard Convention

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And the Cl(rho) have the same definition as Messiah, if we keep the imaginary multiplier out front.

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Asymptotic forms of the spherical Bessel functions:

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Asymptotic form of the spherical Hankel function of the first kind:

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# Derivation of the Separable Representation of the Propagator

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Where k is the free particle kinetic energy. Note that rho is dimensionless.

The dimensionless outgoing free propagator is

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We expanding this in terms of spherical waves about the fixed sites **R** and **R**’ by inserting complete sets of states:

We have defined the displaced spherical wave basis such that

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And the unit projection operator is:

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Projecting G onto the r-basis:

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Bleah, this is going wack.

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# Free Atom (Direct Term)

Calculate amplitude for each of the orbitals in the case of an incident plane wave and a single target atom.

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To within a normalization constant.

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# Outgoing Partial Wave Method

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We assume that the outgoing wave function is composed of pure spherical waves.

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The first (direct) term:

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Expand the plane wave in terms of spherical harmonics:

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Total amplitude summing over all L:

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Now that is the *direct* term.

Expanding the spherical harmonic in terms of the associated Legendre polynomial:

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I can see no obvious simplification here, although I’m sure there must be one (spherical symmetry due to sum over m).

Specific values for angular momenta:

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## Multiple-Scattering Terms:

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I believe I need another free-space propagator in there, since the “first” scatterer is the absorber atom (already considered in the phase shift of the outgoing wave)

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Single-scattering:

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Here the sum over neighbors excludes the source atom.

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Now, the wave function outside of the muffin tin is given by:

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And the radial part of the wave function is:

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With derivative w.r.t. r:

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Now at the muffin-tin matching radius R, the logarithmic derivative must match:

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Hmmm. That doesn’t work out right.

# Multiple Scattering Derivation

We wish to find the complete time-independent solution to the Schrodinger equation for the initial state of an electron incoming to an atom which is part of a solid:

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Or

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Where the full Hamiltonian is

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Where it is understood that *H*0 is the free-space kinetic energy operator, *Va* is the potential of the atom which is to interact with the incident electron and the potentials *Vn* are those of the remaining atoms in the solid. The energy *E* is understood to be complex, containing a real, propagating part and a complex attenuating part.

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## Free-space particular solution

The particular solution of Equation 160 is

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Which has plane wave solutions

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And wave number

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In Hartree units

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The general solution is

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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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If we define the free space Green’s operator

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Then

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## Atomic scattering particular solution

The particular solution of Equation 160 is

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Which has solution, expanded in spherical harmonics:

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The radial part of the solution is, in the region outside of the muffin-tin,

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Inside of the muffin-tin, the wave function is the numerical solution.

The normalization constants a are chosen so that

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Substituting:

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The radial wave functions are infinite in extent, so we invoke volume normalization (the radial wave function is normalized such that):

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Reduction of magnetic quantum number:

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Since the integral over the radial wave functions is independent of m, each term contributes (2l+1) times:

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Applying the definition of the normalization of the r-multiplied wave functions:

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Applying the Basel problem, where

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And then applying the principle of detailed balance, it must be true that

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And therefore

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This expression has been verified in Excel, and shows that the amplitude is dominated by the first few terms.

The general solution is

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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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If we define the free space Green’s operator

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Then

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Following Pendry’s discussion of the amplitude of partial waves:

Outside the range of the absorber muffin-tin potential, the total wave function can be decomposed into its partial waves:

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Since the potential is spherically symmetric, the radial wave function cannot depend on the z-component of angular momentum *m*. In the region just outside of the muffin-tin boundary, the radial wave function has the form:

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This form has the equivalent representation <http://galileo.phys.virginia.edu/classes/752.mf1i.spring03/Scattering_II.htm>:

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The minus sign comes from the *standard* convention for Bessel and Neumann functions.

NOTE – there is a minus sign difference between the standard and Messiah conventions for the spherical Neumann function and therefore the spherical Hankel function. Pendry uses standard convention so let’s stick with that.

Now in the no-scattering case (no potential), the phase shift is zero.

We can decompose this expression into scattered and unscattered components:

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Note that both of these are radial wave functions, and gain a spherical harmonic in the full solution.

To find how a plane wave scatters, we decompose the plane wave in terms of spherical waves centered on the muffin-tin:

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Note that there is no potential effect in this expression, so therefore by comparison is:

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And the amplitude of each (direct) partial wave is:

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Since this normalization must hold in the presence of the potential, we can construct the scattered wave as:

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Adding these together and putting in the angular solution (spherical harmonics), the full solution is:

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Checking the normalization of this wavefunction:

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Substituting:

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(Work on the above some more)

Going back a few steps:

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Wait a minute – actually this isn’t correct – the form given for the wave function is NOT regular at the origin – it gets matched to the atomic wave functions inside of the muffin-tin. So therefore there is no expectation that it is normalized.

Connection to atomic wave functions:

We can utilize the amplitudes of the individual partial waves:

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Knowing the charge density inside of the muffin-tin for each of the partial waves, we make the assertion that the total excitation cross-section scales like the (summed) total charge density.

* Take whatever the field is and expand it in partial waves about the origin
* Gives amplitude of each partial wave
* Apply modulus (a star a) to scale charge inside muffin-tin
* Add up and normalize to the direct wave.

1. Demonstrate that we can solve the direct wave case
2. Determine MS formulation for scattered waves, test with direct wave.

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At the muffin-tin matching radius, these forms are equal:

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By the principle of detailed balance,

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OK, so we expand the full result in terms of (free) spherical waves about the absorber, then use that to determine the amplitude of each partial wave.

Returning to our previously-scheduled solution:

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Expanding out to the multiple-scattering series:

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In coordinate representation,

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Successive terms are identified with the direct (no scattering) amplitude, single scattering, double scattering, etc. We will use the notation as follows to describe each of these terms:

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This result will be expanded in terms of free spherical waves about the origin (absorber) to determine the amplitudes of each partial wave. Let’s do that for the first term (direct wave)

## Direct term

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

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Comparing this to the unscattered wave from partial wave theory:

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We obtain the amplitudes of the partial waves for the direct term:

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## Single scattering

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Here we are introducing the notation

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We introduce the notation

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I’m going to assert:

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In coordinate representation this is:

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Comparing this to the unscattered wave from partial wave theory:

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We obtain the amplitudes of the partial waves for the direct term:

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Now, by Rehr and Albers,

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So

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I’m disturbed by this – the free-space propagator contains r as a vector – this complicates the comparison to the unscattered form, and makes the coefficients functions of r (vector) – since we don’t know where on the sphere we will match. Essentially what this is saying is that the field at the muffin-tin boundary is non-uniform. Need to impose spherical symmetry on what is essentially a non-spherical problem. Options to match to the spherically symmetric muffin-tin interior:

1. Average the incident field over the muffin-tin boundary (easy)
2. Treat the problem as non-spherical symmetry (hard)

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Strategy – expand in spherical harmonics and integrate.

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Now what makes me wonder is that Rehr doesn’t do this for his calculation of EXAFS, which should be subject to the same termination condition. How does he do it? Another thing I just thought of – averaging won’t work for the amplitude, since it is complex – need to average the amplitude squared… but that loses phase information! Something wrong here…

# Requirements

## Inputs

* Cluster (a file input, able to load)
  + Position (x, y, z) (QuantityOfLength)
  + Element
  + Include/Exclude flag
  + Electronic Configuration
    - Optional, if null assume default atomic configuration
* Incident energy (in eV preferable, use QuantityOfEnergy?)
* Inner potential (QuantityOfEnergy)
  + Need a flag to indicate to use custom value or computed value.
* Absorber atom ID (must be a member of the cluster, throw an error otherwise)
* ThetaMin, ThetaMax, ThetaDelta (QuantityOfAngle)
  + Oriented such that +z (Theta = 0) is normal to the surface, pointing away. Normal incidence, pointing inwards, is Theta = Pi.
* PhiMin, PhiMax, PhiDelta (QuantityOfAngle)
* Temperature (QuantityOfTemperature)
* Muffin-tin calculation algorithm (optional, future)
* Free atom calculation algorithm (optional, future)
* Voptical (QuantityOfEnergy)
* Threading (Boolean)
* Lmax – maximum angular momentum
* RAOrder – dimension of matrices
* PathCut, MaxPathLength (QuantityOfLength)

Pop-up property grid in Nunit to set properties

Nice-to-have: Save all calculation parameters as a file

## Outputs

* Output to console (text)
* Table:
  + Theta
  + Phi
  + Intensity
  + Direct intensity
  + Chi (Intensity / Direct intensity – 1)
* Overall time of calculation (QuantityOfTime)
* List of contributing paths, ranked by amplitude (Optional)
* Phase shifts (Optional)
* Inner Potential