Software Spec - PhaseShift and PhaseShiftLookup Class

From Pendry:

The phase shifts can be calculated by integration of the Schrodinger equation starting at the origin, where we have the boundary condition that the wave function must not be singular, and proceeding out to the boundary of the muffin-tin sphere. Once out of range of the potential we know that the wave function has the form:

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The r-multiplied wave function has the form:

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And has the derivative:

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And from details of the integration we calculate the logarithmic derivative at the boundary of the muffin-tin sphere, radius *R*,

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The logarithmic derivative for the r-multiplied wave function is:

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Solving eq. 2 for the exponential including the phase shift,

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Or

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Alternate form – assume the wave function in the zero potential region has the form (from <http://galileo.phys.virginia.edu/classes/752.mf1i.spring03/Scattering_II.htm>):

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Rearranging to solve for terms in delta l,

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If we know the phase shifts for a real energy E, we can compute the (complex) phase shift for the imaginary energy E (including the optical potential) as follows:

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# Temperature Effects

The phase shift is further modified to include temperature effects.

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K is the electron momentum = sqrt(E) in Rydberg units.

Where

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(I am assuming the L = l,m)

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Alpha has units of 1/E. Here I’m using the symbol to represent the Debye temperature, m is the mass of the atom in electron mass units, kb is Boltzmann’s constant in Hartrees/Degree Kelvin, T is temperature in Kelvin. In Rydberg units (*ħ* = 2*m*e = *e*2/2 = 1), and Eq 17 is:

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Where M is the (dimensionless) ratio of the mass of the atom to the mass of the electron.

Kb has units [Energy/K] = 3.166815E-6 Hartrees/K

Since 1 Hartree = 27.211 eV = 2Ry, Kb = 6.33363E-6 Ry/K

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* Need to find out what phase convention for Ylm Pendry is using.

On the atomic mass term: M is the mass of the atom in electron mass units. For example, for Si, atomic weight is 28.0855 g/mol. The electron mass is 9.10938215x10-31 kg. Avogadro’s constant is 6.022142E23/mol. So the mass of a Si atom is 28.0855 [g/mol] / 6.02143E+23 [mol-1] = 4.66425E-23 g or 4.66425E-26 kg. In electron mass units this is 4.66425E-26 / 9.10938215E-31 = 5.12027E+4, which is a dimensionless number.

Method PhaseShift.GetComplexValue(L,T, Voptical, E) as Complex

Strategy:

1. Solve the (unbound) Schrodinger equation for real energy and angular momentum l.
2. Compute the logarithmic derivative at the muffin-tin radius
3. Apply equation (4) to compute the phase shift.
4. Use the optical potential to compute complex E .
5. Phase shifts are modified slightly for complex E according to eq. 5.

Implementation

PhaseShift

Sub New(energy as double, muffintin as MuffinTinPotential, opticalPotential as double, temperature as double)

Sub New(energy as complex, muffintin as MuffinTinPotential, temperature as double)

(+ overloads for no temperature and no optical potential)

(IMuffinTin needs to expose mesh, potential, and Rmt/Imt)

(Energy must be relative to the zero of the muffin-tin potential).

Computes a single phase shift at a single E. Exposes the IRadialMesh used to compute, the wave function, and both the real-valued and complex-valued phase shift. Real-valued phase shifts do NOT include temperature or optical potential effects.

PhaseShiftLookup Class

This class stores a table of phase shifts at different energies and encapsulates routines to interpolate on that table to produce phase shifts for any E. Since DESD is an angle-dependent phenomenon at fixed E, this class might not be of value.