Software Spec – HermanSkillmanPotential Class

The HermanSkiillmanPotential class is a Factory that exposes shared methods for generating an array containing a potential function V(r) enumerated on an IRadialMesh.

# Background

In the central field approximation (following Herman and Skillman),

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Where the radial charge density is

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Where *Nnl* is the occupation number for the orbital (n,l) with both spins, and the spherically averaged radial charge density is

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Note that the free-electron approximation for the exchange potential exactly cancels out the self-potential due to the electron, so that the radial charge density includes contribution from all electrons, including the one whose wave function is being solved for.

Since the functions s(r) and p(r) are both negative, they form repulsive (positive) potential terms. The nuclear potential and the exchange potential terms are both attractive (negative).

## Latter Tail Correction

The correct potential to use in Eq 1 is slightly modified from that given in Eq 4:

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Where Z is the atomic number and N is the number of electrons. The switching radius *r*0 is chosen such that

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## V(r) function for Numerov

The differential equation to solve is:

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Numerov’s method is useful for solving DEs of the form:

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When expressed in this form, the Numerov function *v*(*r*) is:

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Note that since *V*(*r*) is only a function of the total radial charge densities summed over n and l, it does not need to be modified as E changes or as the identity of the electron orbital being computed changes. E can be changed independently, which is very convenient for the energy eigenvalue solver.

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# Implementation Spec

Public Class HermanSkillmanPotential

Public Shared Function GetPotential(mesh as IRadialMesh, Z as Integer, orbitals as IList(Of Orbital), useStatisticalExchange as Boolean) as Double()

Public Shared Function GetPotential(mesh as IRadialMesh, Z as Integer, nE as Double) as Double()

This class computes the potential function v0nl(r) for use in

Inputs – the collection of Pnl(r) functions for all orbitals, their occupancies (configuration object), the atomic number Z, and the radial mesh.

Alternate constructor – omits the Pnl(r) functions, signaling that an initial potential is desired.

Outputs –v0(r)

Requires: A routine to integrate a given radial function on the mesh.