Pendry’s Method for Phase Shift Calculation

Let us look at one of the muffin-tin spheres in isolation. It contains a modified neutral atom and we have established all of the quantities needed to calculate the potential of the isolated atom. We are looking for a Schrodinger equation governing the motion of an incident electron, but initially it must be recognized that the problem is really a many-body one. We should be solving the complete Schrodinger equation that includes all electrons in the total wave function for an atom with N electrons having positions and spin coordinates , plus an incident electron with position and spin

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is the potential due to the screening charge (see p. 40 for a discussion). I *think* the screening charge represents the charge folded back into the muffin-tin.

We begin the approximations by expressing the as the product of core-state wavefunctions, modified if necessary by the muffin-tin potential. At the same time, we must be sure to make the resulting wavefunction is asymmetric under exchange of particles because electrons are fermions:

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