4. Hartee approximation

Goal: solve

$$\left[-\frac{1}{2}\frac{d^2}{dr^2} - \frac{2}{r} + V_H(r)\right]u(r) = \varepsilon u(r)$$

where $V_H(r)$ depends on $u(r)$:

$$\frac{d^2}{dr^2}U = -\frac{u^2}{r}, \quad U(0) = 0, \quad U(r_{max}) = 1$$

$$V_H(r) = V_{SH}(r) = U(r)/r$$

Procedure:

$$\begin{array}{ll}
1. \text{ Guess} & u(r) = \sqrt{4\pi n_s(r)} \\
2. \text{ Solve} & D^2 U_0 = -u^2/r \\
3. \text{ Compute} & U(r) = U_0(r) + \dfrac{r}{r_{max}} \\
4. \text{ Compute} & V_{SH}(r) = U(r)/r \\
5. \text{ Compute} & V_H(r) = V_{SH}(r)
\end{array}\right\} P2$$

6. Solve $\left(-\frac{1}{2}D^2 - 2r^{-1} + V(r)\right)u = \varepsilon u \}$ P3
7. Compute $E_0 = 2\varepsilon - 2\int dr\, u^2(r)\frac{1}{2}V_H(r)$
8. Repeat from 2 until convergence