Exchange forces in He atom

spin eigenfunction	s	m_s	space eigenfunction	Exchange force
antisymmetric: $\frac{1}{\sqrt{2}}[\sigma(\uparrow\downarrow) - \sigma(\downarrow\uparrow)]$	**0**	0 (singlet)	symmetric; maximal for $\vec{r_1} \approx \vec{r_2}$	attractive
symmetric: $\sigma(\uparrow\uparrow)$ $\frac{1}{\sqrt{2}}[\sigma(\uparrow\downarrow) + \sigma(\downarrow\uparrow)]$ $\sigma(\downarrow\downarrow)$	**1**	$+1$ 0 -1 (triplet)	antisymmetric; vanishes for $\vec{r_1} \approx \vec{r_2}$	repulsive

Hartree method

° Estimate net potential $V(r)$ for typical electron subject to:

$$V(r) = \begin{cases} \frac{-Z\,e^2}{4\pi\epsilon_0\,r}, & r \to 0 \\ \\ \frac{-e^2}{4\pi\epsilon_0\,r}, & r \to \infty \end{cases}$$

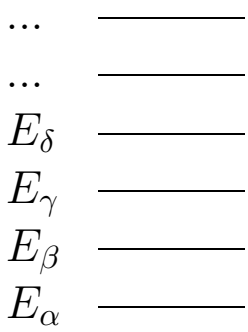
¸ Solve TISE for typical electron:

$$\frac{-\hbar^2}{2m}\,\nabla^2\,\psi(r,\theta,\phi) + V(r)\,\psi(r,\theta,\phi) = E\,\psi(r,\theta,\phi)$$

yielding the eigenfunctions and eigenvalues:

$$\begin{matrix} \psi_\alpha(r,\theta,\phi), & \psi_\beta(r,\theta,\phi), & \psi_\gamma(r,\theta,\phi), \ldots \\ E_\alpha, & E_\beta, & E_\gamma, \ldots \end{matrix}$$

Ì Obtain the ground state of the atom:
(minimize total energy, obeying P.E.P.)



˝ Compute charge distribution seen by typical electron:

$$Q(r) = \underbrace{+Ze}_{\text{nucleus}} \underbrace{-e\psi_\alpha^*\psi_\alpha - e\psi_\beta^*\psi_\beta - e\psi_\gamma^*\psi_\gamma - ...}_{Z-1 \text{ electrons}}$$

˛ Determine the net potential that generates this charge distribution using Gauss's law and integrating the electric field $E(r)$:

$$Q(r) \rightarrow E(r) \rightarrow V^{'}(r)$$

ˇ Is the potential self-consistent?

$$V^{'}(r) \simeq V(r)?$$

NO	YES
iterate $V^{'}(r)$ ¸ $\rightarrow$Ì $\rightarrow$˝ $\rightarrow$ ˛ $\rightarrow$ˇ	$E_\alpha, \psi_\alpha, E_\beta, \psi_\beta, ...$ describe the electrons in atom's ground state