

Engel 10.6

Problem. Write a Slater determinant for the ground state of Be.

Answer. The ground state configuration of Be is $1s^2 2s^2$. Because all of the shells are "closed" (electrons have been assigned to all available orbitals and spins), the Hartree-Fock wave function can be represented by a single Slater determinant.

To construct a Slater determinant, write a different spin-orbital in each column (for simplicity, write "1s" in place of ϕ_{1s}), and write a different electron's coordinates (label) in each row. If the atomic orbital functions are drawn from an orthonormal set, the normalization constant N equals $1/\sqrt{4!}$.

$$\psi(1, 2, 3, 4) = N \begin{pmatrix} 1s(1)\alpha(1) & 1s(1)\beta(1) & 2s(1)\alpha(1) & 2s(1)\beta(1) \\ 1s(2)\alpha(2) & 1s(2)\beta(2) & 2s(2)\alpha(2) & 2s(2)\beta(2) \\ 1s(3)\alpha(3) & 1s(3)\beta(3) & 2s(3)\alpha(3) & 2s(3)\beta(3) \\ 1s(4)\alpha(4) & 1s(4)\beta(4) & 2s(4)\alpha(4) & 2s(4)\beta(4) \end{pmatrix}$$