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 \( \phi_{1s} \)), 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 \( 1/\sqrt{4!} \).

\[
\psi(1, 2, 3, 4) = N \begin{pmatrix}
1 \ s(1) \ a(1) & 1 \ s(1) \ \beta(1) & 2 \ s(1) \ a(1) & 2 \ s(1) \ \beta(1) \\
1 \ s(2) \ a(2) & 1 \ s(2) \ \beta(2) & 2 \ s(2) \ a(2) & 2 \ s(2) \ \beta(2) \\
1 \ s(3) \ a(3) & 1 \ s(3) \ \beta(3) & 2 \ s(3) \ a(3) & 2 \ s(3) \ \beta(3) \\
1 \ s(4) \ a(4) & 1 \ s(4) \ \beta(4) & 2 \ s(4) \ a(4) & 2 \ s(4) \ \beta(4)
\end{pmatrix}
\]