Integrals Involving S Functions

Overlap:

$$\langle S_A | S_B \rangle = (ab)^{3/4} \left(\frac{2}{a+b} \right)^{3/2} e^{-\frac{ab}{a+b} \overline{AB}^2}$$

Kinetic Energy:

$$\left\langle S_A \left| -\frac{1}{2} \nabla^2 \right| S_B \right\rangle = \left(\frac{3ab}{a+b} - \frac{2a^2 b^2 \overline{AB}^2}{(a+b)^2} \right) \langle S_A | S_B \rangle$$

Electron-Nuclear Attraction:

$$\left\langle S_A \left| \frac{1}{r_c} \right| S_B \right\rangle = 2 \sqrt{\frac{a+b}{\pi}} F_0(Z) \langle S_A | S_B \rangle$$

$$F_0(Z) = \int_0^1 e^{-Zt^2} dt \qquad \text{and} \qquad Z = (a+b) \overline{PC}^2$$

Electron-Electron Repulsion:

$$\left\langle S_A(1)S_B(1)\left|\frac{1}{r_{12}}\right|S_C(2)S_D(2)\right\rangle = \frac{2F_0(Z)}{\sqrt{\frac{\pi}{a+b}+\frac{\pi}{c+d}}}\left\langle S_A\middle|S_B\right\rangle\left\langle S_C\middle|S_D\right\rangle$$

$$Z = \frac{(a+b)(c+d)}{a+b+c+d}\overline{PQ}^2 \quad ; \quad \vec{P} = \frac{a\vec{A}+b\vec{B}}{a+b} \quad ; \quad \vec{Q} = \frac{c\vec{C}+d\vec{D}}{c+d}$$