

Let $\psi(x, y)$ be the wave function of two electrons in a one dimensional box of length L .

$$\psi(x, y) = \frac{1}{\sqrt{2}}(\phi_1(x)\phi_2(y) - \phi_1(y)\phi_2(x))$$

$$\phi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

Wave function $\psi(x, y)$ is antisymmetric under exchange of electrons.

$$\psi(x, y) = -\psi(y, x)$$

For $L = 10^{-9}$ meter the expected potential energy is

$$V = \frac{e^2}{4\pi\epsilon_0} \int_0^L \int_0^L \frac{\psi^*(x, y)\psi(x, y)}{|x - y|} dx dy = 4.67 \text{ eV}$$

Next calculate the potential energy for a wave function that is symmetric.

$$V_s = \frac{e^2}{4\pi\epsilon_0} \int_0^L \int_0^L \frac{\phi_1^*(x)\phi_2^*(y)\phi_1(x)\phi_2(y)}{|x - y|} dx dy = 12.80 \text{ eV}$$

The difference is the exchange energy.

$$V_{ex} = V - V_s = -8.13 \text{ eV}$$

Note that the formula for V_s has a singularity at $x = y$. The computed value shown above is the result of an arbitrary cutoff in numerical integration. The actual value of V_s goes to infinity.

Note also that there is a singularity at $x = y$ in the formula for V . However, due to antisymmetry we have $\psi(x, x) = 0$ and hence the integral converges.