Energy as a Function of Atom Separation

The even and odd states behave similarly to the square well, but there is also repulsion between the nuclei that prevents them from coming too close.

Schematic picture for the total energy of two nuclei and one electron:



Let's consider what happens when there is more than one electron:

- 2 electrons (two neutral H atoms): Both electrons occupy the bonding state (with different m_s). This is neutral H₂.
- 4 electrons (two neutral He atoms). Two electron must be in the anti-bonding state. The repulsive force cancels the bonding, and the atoms don't stick. The He₂ molecule does not exist!