# ORIGIN OF HUND'S MULTIPLICITY RULE IN SINGLY-EXCITED TWO-ELECTRON SYSTEMS

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Origin of Hund's multiplicity rule has been a source of active theoretical studies since the beginning of quantum mechanics till today [1]. A significant part of those previous efforts has been focused on singly-excited states of the helium and helium-like atomic ions, which is the simplest example to which Hund's multiplicity rule applies: For a given orbital configuration of $(1s)(nl)$ with $n$ and $l$ denoting the principle and angular momentum quantum numbers, respectively, there arises only one singlet-triplet pair of states, and according to the rule, the triplet is always lower in energy than the singlet. Even for this simplest example the reason why the triplet has a lower energy than the corresponding singlet has turned out to be significantly involved. One of the major puzzling observations is that the helium atom has a *larger* electron repulsion energy than does the corresponding singlet, as opposed to the traditional interpretation based on Slater's paper in 1929. This implies that unlike the traditional interpretation the reason why the triplet has a lower energy is not due to the smaller electron repulsion but must be ascribed to a more compact electron density distribution of the triplet state than the singlet, which then results in a much larger energy decrease due to the nuclear attraction potential that compensates the energy increase by the electron repulsion. On the one hand, in our earlier study the origin of Hund's multiplicity rule in two-electron artificial atoms or quantum dots was studied [2]. It has been found in the study that the electron density distribution of the triplet state is indeed more compact than the corresponding singlet state as in the case of the helium atom but that the electron repulsion energy of the triplet state *never becomes larger* than that of the corresponding singlet state in contrast to the helium case. Motivated by these earlier analyses, the present study focuses on the origin of how the electron repulsion energy is always smaller for the triplet state than the corresponding singlet for quantum dots while its relation gets inverted for the He-like atomic systems for small values of the nuclear charge $Z$. The observed trends are rationalized on the basis of a new concept of the so-called *conjugate Fermi holes* [1].

[1] T. Sako et al. Phys. Rev. **A83**, 032511 (2011).

[2] T. Sako et al. Phys. Rev. **A81**, 022501 (2010).