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Origin of Hund's multiplicity rule: Genuine and conjugate Fermi holes

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The lowest singlet-triplet pair of states of the two-electron two-dimensional quantum dots and the corresponding pair of states of the two-dimensional helium-like systems have been studied by the full configuration interaction method focusing on the origin of the first Hund rule. The one- and two-electron components of the singlet-triplet energy gap show distinct trends for the systems studied in the regime of small nuclear charge Z_n or of small confinement strength ω. The $(0\sigma_g)(1\pi_u)$ singlet state in quantum dots is characterized by a larger electron repulsion than its counterpart triplet state for all values of ω while this relationship gets inverted for the corresponding $(1s)(2p)$ singlet-triplet pair of He-like systems for small values of Z_n, such as $Z_n = 2$ or 3. The internal part of the full configuration interaction wave functions has been extracted and visualized in the three-dimensional internal space (r_1,r_2,ϕ_-) to rationalize the observed trends. The singlet probability density of He-like systems located originally near the Fermi holes is shown to migrate into regions where r_1 or r_2 are large while the corresponding singlet probability of quantum dots stays close to the Fermi holes. Their differences and their observed trends are rationalized on the basis of the structure of the genuine and *conjugate Fermi holes*.