

Angular Correlation and Independent Particle Model in Two-Electron Atomic Systems

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Abstract : The ground and low-lying singly-excited states of He and He-like atomic ions have been studied by the Full Configuration Interaction (FCI) method focusing on the angular correlation between two electrons in the studied systems. The two-electron angle density distribution obtained by integrating the square-modulus of the FCI wave function over the coordinates other than the interelectronic angle shows a distinct trend between the singlet-triplet pair of states for different values of the nuclear charge Z . Further, both of these singlet and triplet distributions tend to show an increasingly stronger dependence on the interelectronic angle as Z increases, in contrast to the well-known fact that the correlation energy approaches towards zero for increasing Z . This controversial observation has been rationalized on the basis of the recently introduced concept of so-called conjugate Fermi holes.

Keywords : He-like systems, angular correlation, configuration interaction wave function, conjugate Fermi hole

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