Max-Planck-Institut für Astrophysik
Garching, Germany
http://www.mpa-garching.mpg.de

Origin of Hund's multiplicity rule in singly excited helium.

Tokuei Sako
Nihon University, Funabashi, Chiba, Japan
Josef Paldus
Waterloo University, Waterloo, Ontario, Canada
and
Geerd HF Diercksen
Max-Planck-Institut für Astrophysik, Garching, Germany

The origin of Hund's multiplicity rule in the low-lying excited states of the helium atom has been studied by considering the two-dimensional helium atom. The internal wave function of the singlet states *without* electron repulsion has a significant probability around the origin of the internal space while the corresponding probability of the triplet wave function is negligible in this region due to the presence of a Fermi hole. The electron-electron repulsion potential has been visualized also in the internal space. It manifests itself by three striking poles penetrating exactly into the spatial region defined by the Fermi hole. Because of the existence of these strong potential poles in the vicinity of the Fermi hole a major part of the singlet probability migrates out of this region. In contrast, the corresponding triplet wave function is less affected by these poles due to the presence of the Fermi hole. The singlet probability is shown to migrate from its original region close to the origin to a region far away where either r_1 or r_2 are large. This results in a more diffuse electron density distribution and a smaller electron repulsion energy of the singlet state than of the corresponding triplet state. The mechanism of the evolution of the singlet probability towards the region of large r_i ($i = 1, 2$) in the presence of the electron repulsion potential has been rationalized on the basis of a new concept called *conjugate Fermi hole*.