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Antiferromagnetism and superconductivity in the iron vacancy ordered $A_yFe_{1.6}Se_2$

Shin-Ming Huang[1] and Chung-Yu Mou[1,2,3]
[1]Department of Physics, National Tsing Hua University, Hsinchu 30043, Taiwan
[2]Institute of Physics, Academia Sinica, Nankang, Taiwan
[3]Physics Division, National Center for Theoretical Sciences, P. O. Box 2-131, Hsinchu, Taiwan

We investigate the electronic structure of the $\sqrt{5}\times\sqrt{5}$ iron-vacancy-ordered $A_yFe_{2-x}Se_2$ by constructing an effective tight-binding model as the vacancy order is explicitly treated. It is shown that the constructed band model, when combined with generalized Hubbard interactions, yields a spin susceptibility which exhibits both the block-checkerboard anti-ferromagnetism instability and the stripe antiferromagnetism instability. In particular, for large Hund's rule couplings, the block-checkerboard antiferromagnetism wins over the stripe antiferromagnetism, in agreement with the observation in experiments.

For the superconducting state assumed by the antiferromagnetic fluctuations, due to the broken reflection symmetry induced by the iron vacancies, new superconducting states with C_{4h} symmetry emerge. In the C_{4h} symmetry, there is no symmetric axis in the plane, such that the relative orientation of the pairing wave function to the lattice forms another degree of freedom for characterizing the superconducting gap and can further help in gaining the condensation energy. Nonetheless, similar to other iron-based superconductors, the singlet ground state is still dominated by *s*-wave or *d*-wave, which are nearly degenerate with anisotropic gaps. Furthermore, *s*-wave and *d*-wave superconducting states are separated by a quantum critical point controlled by the Hund's rule coupling J_H.

References:

[1] Shin-Ming Huang and Chung-Yu Mou, Phys. Rev. B 84, 184521 (2011).

[2] Shin-Ming Huang and Chung-Yu Mou, Phys. Rev. B 85, 184519 (2012).