Excited states beyond Mott gap in half-filled Hubbard model

Hisatoshi Yokoyama [1], Kenji Kobayashi [2], Tsutomu Watanabe[2], and Masao Ogata[3,4]

[1] *Department of Physics, Tohoku University, Sendai, Miyagi 980-8578 Japan*
[2] *Department of Natural Science, Chiba Institute of Technology, Narashino, Chiba 275-0023 Japan*
[3] *Department of Physics, University of Tokyo, Bunkyo-ku, Tokyo 113-0033 Japan*
[4] *Trans-scale Quantum Science Institute, University of Tokyo, Bunkyo-ku, Tokyo 113-0033 Japan*

In connection with recent experiments on excitation in which Mott insulators change to conductors, we study the properties of excited states beyond the Mott gap as quasi-stationary states for a two-dimensional Hubbard model at half-filling. Variational Monte Carlo methods are used with several kinds of trial wave functions for paramagnetic or normal state (PM), superconducting state with d-wave order parameter (d-SC), isotropic s-wave superconducting state, extended s-wave state, and antiferromagnetic state (AF) [1]. To study the excited states, we impose a minimum number of the doubly occupied states (doublons) on the variational states. In the region where the on-site interaction U is larger than the band width, the doublon density (d_L) will correspond to the intensity of the excitation. A semi-quantitative phase diagram in the U / t- d_L space is shown below.

When the doublon density is larger than 0.14, the PM state is stabilized, while the doublon density is less than 0.14, the insulating AF state is the most stable among the states we studied. On the other hand, the d-SC state becomes more stable than the PM state for $0.02< d_L <0.11$, but it is always unstable toward the AF order. The d-SC may appear if the AF order is destroyed by some reason. The PM state in the region $d_L >0.14$ is conductive since the free doublons and holons are generated in excitation. The s-wave-type superconducting states are not stabilized for any parameter set.

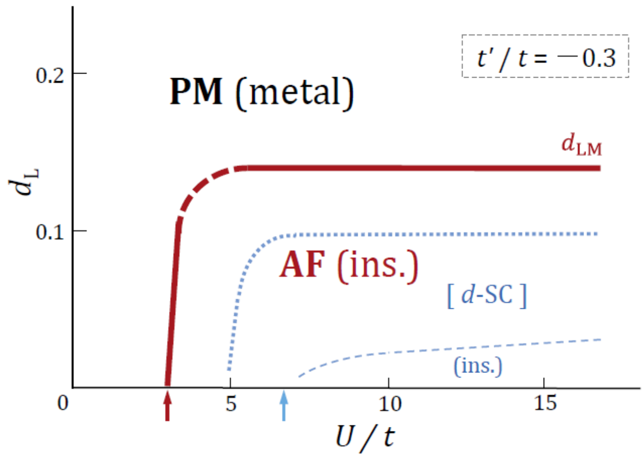

Figure: Semi-quantitative phase diagram of stationary doublon-holon excited state in the space of doublon density (d_L) and the interaction strength U / t. [1]

[1] H. Yokoyama, K. Kobayashi, T. Watanabe, and M. Ogata, J. Phys. Soc. Jpn. **91**, 124705 (2022).