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Variational Monte Carlo Study of Excited States in Strongly Correlated Hubbard model

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

Department of Physics, Tohoku University, Japan[1]
Department of Natural Science, Chiba Institute of Technology, Japan[2]
Department of Physics, University of Tokyo, Japan[3]

In recent experimental research, excited states were artificially produced by irradiating various (doped) Mott insulators with pulsed light or by modulating the periodic potential of optical lattices in cold atom systems, and relaxation processes from them were actively studied. For example, it was discussed that when one excites parent compounds (antiferromagnetic Mott insulators) of cuprate superconductors, the features of metallization are different between the compounds for hole-doped and electron-doped systems [1]. So far, most theoretical studies have addressed dynamical relaxation processes, but it is also important to elucidate static properties of many-body excited states because they are not necessarily what are expected from the band theories. For example, how much doublon density, namely, light intensity is needed to make a Mott insulator metallic.

In this work, we study static properties in the initial quasi-steady states after an excitation beyond the Hubbard gap, by applying a variational Monte Carlo (VMC) method to a two-dimensional Hubbard model with diagonal transfer (t'). We can make a trial wave function for an initial excited state by regulating the lowest number of doublons D_L to $D_L>0$, legitimately at least in the Mott insulating regime; for the ground state, $D_L=0$. We primarily consider fundamental features of excited states at half filling for intermediate and strong correlations, for instance, the threshold of doublon density to metallize a Mott insulator as a function of U/t and t'/t [2] or how superconducting (SC) correlation is enhanced immediately below the Mott transition point U_c/t, as compared to the ground state. Secondly, how this SC correlation evolves as doping rate increases. In the presentation, we explain the details of formalism and discuss basic results.

[1] H. Okamoto *et al.*, Phys. Rev. B **82**, 060513(R) (2010), ibid. **83, 125102** (2011).
[2] H. Yokoyama, T. Miyagawa, M. Ogata, J. Phys. Soc. Jpn. **80**, 084607 (2011).

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