Variational Monte Carlo study of Mott transitions in two dimensions

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In connection with high-T_c cuprates and κ-ET salts, mechanisms of Mott transitions and *d*-wave superconductivity (SC) are studied in the half-filled-band Hubbard model on square lattices with a diagonal hopping term (t'), using an optimization (or correlated) variational Monte Carlo method. In the trial wave functions, a doublon-holon binding effect is introduced in addition to the onsite Gutzwiller projection. We mainly treat a *d*-wave singlet state and a projected Fermi sea. In both wave functions, first-order Mott transitions without direct relevance to magnetic orders take place at $U=U_c$ approximately of the bandwidth for arbitrary t'/t. These transitions originate in the binding or unbinding of a doublon to a holon. *d*-wave SC appears in a narrow range immediately below U_c. The robust *d*-wave superconducting correlation are necessarily accompanied by enhanced antiferromagnetic correlation; the strength of SC becomes weak, as t'/t increases.[1] Regarding SC, we would like to take up the relation to the doping cases.[2,3]

[1] H. Yokoyama, M. Ogata, and Y. Tanaka, submitted to J. Phys. Soc. Jpn.
[2] H. Yokoyama, M. Ogata, and Y. Tanaka, in preparation.
[3] K. Kobayashi, and H. Yokoyama, in preparation.