Variational wave functions for multiband Hubbard models

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I give a review on the possibility to describe strongly-interacting systems by variational wave functions that are obtained by inserting electron-electron correlation on top of Slater determinants. In this regard, Jastrow factors are considered,[1] which generalize the on-site Gutzwiller term to include long-range density-density correlations. I discuss the accuracy of this approach for both weak and strong couplings and how it is possible to describe the metal-insulator transition, as well as the Mott insulator.

Generalizations to multiband models are straighforward and represent an on-going line of research: the case of the orbital-selective Mott transition in a two-band Hubbard model with different hopping amplitudes t_1 and t_2 is discussed.[2] The phase diagram at half filling (as a function of t_1/t_2 and the on-site Coulomb repulsion U) is worked out. The results are in good agreement with previous dynamical mean-field theory calculations, demonstrating that the non-magnetic phase diagram is only slightly modified from infinite to two spatial dimensions. Finally, I present recent calculations on a two-band model that is designed to capture the low-energy properties of charge-transfer insulators, such as κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Cl.[3] This model takes into account the presence of two organic BEDT-TTF molecules, which form a dimer on each site of the lattice, and includes short-range intramolecular and intermolecular interactions and hoppings. Charge-ordered insulating phases are stabilized in the strongly correlated limit and their actual charge pattern is determined by the relative strength of intradimer to interdimer couplings. Our results suggest that ferroelectricity is not driven by magnetism, since these polar phases can be stabilized also without antiferromagnetic order.

[1] M. Capello, F. Becca, M. Fabrizio, S. Sorella, and E. Tosatti, Phys. Rev. Lett. **94**, 026406 (2005).

[2] L.F. Tocchio, F. Arrigoni, S. Sorella, and F. Becca, J. of Phys.: Condens. Matter **28**, 105602 (2016).

[3] R. Kaneko, L.F. Tocchio, R. Valenti, and F. Becca, arXiv:1705.08915 (to be published).