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DMFT calculations of materials properties using the continuous time QMC method[1]

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The combination of DFT with DMFT has proven to be an instrumental method for describing realistic strongly correlated electron systems. In essence, DMFT treats the strongly correlated electrons near the Fermi surface while DFT treats the electrons which are less correlated. DMFT effectively maps the intractable lattice many-body problem onto a tractable impurity many-body problem. The DMFT impurity problem must be solved using numerical methods or approximate analytical methods, and this is the bottleneck of the entire procedure. Continuous time QMC has recently emerged as a dominant method to solve the DMFT impurity problem. We present applications of DFT+DMFT(CTQMC-atomic-limit) to the cobaltates and Pu. In Pu, a variety of physical properties are calculated such as the Photoemission spectra, magnetic susceptibility, and the heat capacity. These physical properties are probed as a function of temperature and volume, and compared with experimental measurements. Additionally, we demonstrate the effect of the full on-site exchange interaction on the physical observables. In the cobaltates, the Fermi surface and heat capacity are calculated for $Na_{0.3}CoO_2$. We demonstrate that the topology of the Fermi surface depends sensitively upon the bare Hamiltonian. It is shown that consistent agreement with heat capacity measurements and ARPES experiments can only be achieved if the e'_g satellite pockets are not present at the Fermi surface.

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