Development of a Lanczos-ED DMFT Method for Multiorbital Electron–Phonon Systems

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Electron–phonon interactions can substantially modify the low-energy properties of strongly correlated electron systems, particularly when electronic and lattice interactions act on comparable energy scales. In the single-orbital Hubbard–Holstein model, the competition between the local Coulomb interaction and phonon-mediated attraction gives rise to metallic, Mott-insulating, and bipolaronic regimes [1,2]. In multiorbital systems, the situation becomes richer because phonons with different symmetries couple to distinct electronic degrees of freedom. In particular, Jahn–Teller phonons couple to orbital degrees of freedom and may compete with Hund's coupling, as demonstrated in correlated fulleride systems [3].

We develop a dynamical mean-field theory (DMFT) framework with a Lanczos exact-diagonalization impurity solver to investigate strongly correlated multiorbital electron–phonon systems. As a first benchmark, we have applied the method to the half-filled single-orbital Hubbard–Holstein model. By systematically varying the Hubbard interaction U and electron–phonon coupling, we reproduce the characteristic competition among the correlated metallic, Mott-insulating, and bipolaronic regimes reported in previous DMFT studies [1,2]. The evolution of the system is characterized using the quasiparticle weight, double occupancy, and real-frequency spectral function, which provide complementary diagnostics of correlation-driven and phonon-driven localization.

We are currently extending the framework to a two-orbital Hubbard–Hund model coupled to Jahn–Teller phonons. The implementation will first be benchmarked against previously reported multiorbital DMFT results [4], allowing us to examine the competition between Hund's coupling and phonon-induced orbital fluctuations. After establishing this multiorbital benchmark, an additional breathing phonon mode coupled to the local charge density will be introduced. This extension enables a systematic comparison between charge-channel fluctuations induced by the breathing mode and orbital-channel fluctuations induced by Jahn–Teller phonons. Our goal is to determine how these competing electron–phonon coupling channels modify quasiparticle coherence, local electronic configurations, spectral properties, and the metal–insulator phase boundaries in strongly correlated multiorbital systems.

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