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Intersite correlations and the metal insulator in cluster dynamical mean field theory: cluster size, interaction strength, and the location of the transition line[1] C. LIN, A. MILLIS, Columbia University — To gain insight into the physics of the metal insulator transition and the effectiveness of cluster dynamical mean field theory we have used one, two and four site dynamical mean field theory (both CDMFT and DCA) to solve a model of electrons coupled to a classical phonon field. A partial density of states is defined encoding a generalized nesting property of the band structure; variations in this density of states account for differences between dynamical cluster approximation and cellular-DMFT implementation of cluster DMFT, and for differences in behavior between single band (cuprate-like) and multiband (manganite-like) models. The cluster size dependence of the metal to polaronic insulator phase boundary is determined along with electron spectral functions and cluster correlation functions. Over most of the interaction strength regime the single-site and multi-site approximations are found to yield similar results. Important cluster size effects occur only in the metal insulator transition region, where short-ranged orrelations are found to significantly reduce the critical interaction strength required to drive a metal polaron insulator transition. In the cluster approximations the physics of the metal-insulator transition is shown to be Slater-like (driven by band filling). The minimal cluster size required to capture the metal-polaron insulator transition is shown to depend sensitively on the carrier concentration. Implications for the theoretical treatment of doped manganites are discussed.

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