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Quantum Monte Carlo simulations of ARPES spectra on correlated materials with electron-phonon coupling ELIZABETH NOWADNICK, Stanford University and SLAC National Accelerator Laboratory, STEVEN JOHNSTON, University of British Columbia, BRIAN MORITZ, Stanford University and SLAC National Accelerator Laboratory, RICHARD SCALETTAR, University of California at Davis, THOMAS DEVEREAUX, Stanford University and SLAC National Accelerator Laboratory — Results from a variety of experiments have revealed the importance of the electron-phonon interaction in strongly correlated electron materials. In particular, ARPES experiments on the cuprates have observed signatures of polaron formation in the underdoped regime, indicative of strong electron-phonon coupling, as well as “kinks” in the dispersion in the doped compounds, which have been interpreted in a phonon picture. In order to study the role of electron-phonon coupling in strongly correlated systems, we simulate the single-band Hubbard-Holstein model using determinant quantum Monte Carlo, an approach that allows the non-perturbative study of strongly interacting systems, and treats the electron-electron and electron-phonon interactions on an equal footing. We present electronic spectral functions, which can be compared to ARPES results, as well as phonon spectral functions, which shed light on phonon renormalizations. In particular, we focus on an antiferromagnetic—charge density wave transition that occurs in the Hubbard-Holstein model at half filling, and present signatures of an emergent intermediate metallic phase that occurs between the two insulating phases. We also discuss the influence of phonons on the electronic dispersion.

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