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Luttinger, Peierls or Mott? Quantum phase transitions in 1D strongly correlated electron-phonon systems

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The challenge of understanding metal-insulator and insulator-insulator quantum phase transitions 1D has stimulated intense work on generic microscopic models of interacting electrons and phonons. Combining Lanczos diagonalization with Chebyshev moment expansion and density matrix renormalisation group techniques we present unbiased results for ground-state and spectral properties of the Holstein-Hubbard model at half-filling. For the spinless fermion case, we identify four distinct regimes of the phase diagram, corresponding to an attractive or repulsive Luttinger liquid at weak electron-phonon (EP) coupling, and an band-insulator or polaronic superlattice at strong coupling. Electron and phonon spectra reveal substantially different physics in these regimes and beyond indicate that the size of the phonon frequency significantly affects the nature of the Peierls transition. For the spinful case, with respect to the metal the the electron-electron interaction favours a Mott insulating state, whereas the EP interaction tends to establish a Peierls state with true CDW long-range order. While polaronic features emerge only at strong EP couplings, pronounced phonon signatures, such as multi-quanta bound states, can be found in the Mott insulating regime as well. In order to corroborate the Mott to Peierls transition scenario, we determine the spin and one- and two-particle charge excitation gaps and comment on the possibility of an intervening metallic phase in the weak-coupling regime.