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Percolative Mott Metal-Insulator Transition in the Doped Hubbard-Holstein model: Theoretical Results from Hartree-Fock and Slave Boson Approaches

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— Motivated by the current interest in the understanding of the Mott insulators away from half filling, observed in many perovskite oxides, we study the Mott metal-insulator transition in the doped Hubbard-Holstein model using the Hartree-Fock and slave-Boson approaches. The model contains both the Coulomb and the electron-lattice interactions, which are important ingredients in the physics of the perovskite oxides. In contrast to the half-filled Hubbard model, which always results in a single phase (either metallic or insulating), our results show that away from half-filling, a mixed phase of metallic and insulating regions occur. As the dopant concentration is increased, the metallic part progressively grows in volume, until it exceeds the percolation threshold, leading to percolative conduction. This happens above a critical dopant concentration, which, depending on the strength of the electron-lattice interaction, can be a significant fraction of unity. This means that the material could be insulating even for a substantial amount of doping, in contrast with the Nagaoka theorem, where a single hole destroys the insulating behavior of the half-filled Hubbard model. Our theory provides a framework for the understanding of the density-driven MIT observed in many complex oxides.

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