Abstract Submitted
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Quantum phase transitions arising from competing electron-electron and electron-phonon interactions in a two-orbital single-molecule junction[1] LILI DENG, KEVIN INGERSENT, U. Florida, GISELLE LUIZ, EDSON VERNEK, U. Fed. Uberlandia, Brazil, ENRIQUE ANDA, PUC-Rio, Brazil — Electron-electron and electron-phonon interactions both play important roles in determining the transport properties of nanostructures such as single-molecule junctions. We use the numerical renormalization group to study a molecule with two active electronic orbitals connecting a pair of metallic leads. We focus on quantum phase transitions (QPTs) that can be accessed by varying couplings to a local vibrational mode, particularly the strength of phonon-assisted tunneling between the two molecular orbitals. One type of QPT arises in situations where, in the absence of electron-phonon interactions, one of the molecular orbitals manifests the many-body Kondo effect with its characteristic zero-bias anomaly in the electrical conductance through the junction. At a critical coupling, the system undergoes a first-order QPT to a low-conductance phase in which the electron-phonon interaction overwhelms the strong bare electron-electron repulsion and Kondo physics is completely destroyed. A second type of first-order QPT is found in cases where there is also a Holstein coupling of local phonons to the molecular charge. We will explain the conditions that give rise to QPTs, as opposed to crossovers, between different ground states of this system.

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