Mott Transitions: Transition Orders, Unstable Heavy Fermi Liquid, and Quantum Criticality

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Dynamical mean-field theory (DMFT) has revealed that the quasiparticle weight of a metal gets suppressed upon increasing interaction strength and vanishes at a Mott metal-to-insulator transition. Despite the success established in the early 2000s, fundamental questions remain open about the DMFT scenario of Mott transitions. In this work, we answer these questions using the numerical renormalization group (NRG)—a tensor network method specialized in quantum impurity problems—as the DMFT impurity solver with direct access to real-frequency spectral functions and zero temperature. First, we find that the local ground-state degeneracy of a lattice site determines whether the quasiparticle weight has either a first- or second-order metal-to-insulator transition at zero temperature. Second, we demonstrate that the unstable solution, located in the coexistence region of two stable solutions (metal and insulator), is a heavy Fermi liquid with peculiar interaction and temperature dependencies. The unstable solution is a potential origin of the quantum critical scaling of the resistivity, which was first proposed using DMFT and then confirmed in the experiment on quasi-2D organic salts.