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Effects of Particle-Hole Asymmetry on the Mott-Hubbard Metal-Insulator Transition[1]

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The Mott-Hubbard metal-insulator transition (MIT) is one of the most important problems in correlated electron systems. In the past decade, much progress has been made on examining a particle-hole symmetric form of the transition in the Hubbard model with dynamical mean field theory (DMFT) where it was found that the electronic self energy develops a pole at the transition. However, since most real materials are not at half filling one would like to examine the particle-hole asymmetric MIT. Here we analyze this problem using Falicov-Kimball (or simplified Hubbard) model. It is believed to describe correlated electron behavior and MIT in materials that can be fit into a binary alloy picture. Unlike the Hubbard model, which has a metal-insulator transition only at half filling, the Falicov-Kimball model exhibits a MIT for asymmetric particle densities. An example of the system that fits this picture is Ta_xN, which exhibits the MIT away from half filling at $x = 0.6$. We find that away from half filling a number of features change when the noninteracting density of states has a finite bandwidth. First, we compare the nature of Mott-Hubbard transition at zero temperature in the Falicov-Kimball model for the lattices with finite and infinite bandwidths within the DMFT. We derive simple formulas for the critical interaction strength U for both the development of a pole in the self energy and for the opening of a gap in the single-particle density of states. While the critical U values are the same at half filling on both lattices, and for arbitrary filling on infinite bandwidth lattice, they are different for the particle-hole asymmetric cases on the finite bandwidth lattice. We discuss what role the development of the pole has on the physical properties of the MIT and the consequences these results have for the MIT in real materials. As an illustration we calculate a number of thermal transport properties and show how they are influenced by the bandwidth and the MIT for different fillings. [1] D.O.Demchenko, A.V.Joura, J.K.Freericks, Phys.Rev.Lett. **92**, 216401 (2004).

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