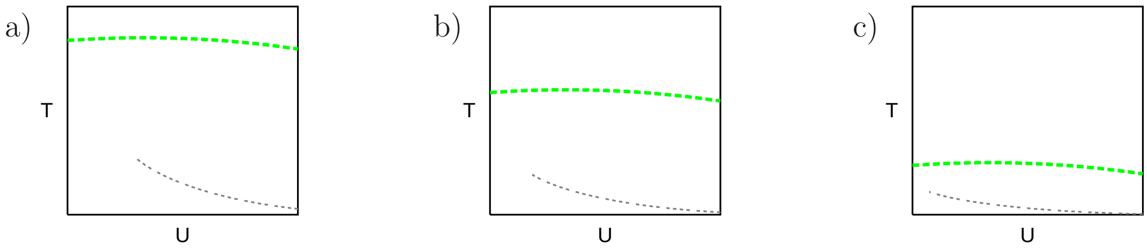

Figure 3.57: Schematic phase diagram for frustration by longer-range hopping. **a)** In the unfrustrated case, a paramagnetic MIT line (faint thin line) is present only for a calculation restricted to the paramagnetic phase; in an unrestricted calculation, it is hidden by the low-temperature AF phase (below the Néel curve, dashed). **b)** and **c)**: Increasing frustration suppresses both the AF phase and the MIT line (obtained in a restricted calculation) so that the latter never becomes thermodynamically relevant.

phase) and a smooth crossover develops for any $|t'^*| > 0$.

2. The first-order Mott transition survives sufficiently strong finite microscopic frustration with no or only a minor change of the critical temperature T^* so that $T_\mathrm{N} < T^*$.

3. The Mott transition coexists with NNN hopping, but with $T^* < T_\mathrm{N}(U^*)$ for all hopping strengths t^* as illustrated in Fig. 3.57 (with increasing frustration from left to right). The MIT line (computed in the enforced homogeneous phase) never reaches the true homogeneous phase.

Since the first suggestion implies changes of order one in solutions of the DMFT equations for an infinitesimal change of the DOS, it may be safely excluded. The second scenario leads to the same conclusions as the case of frustration at constant DOS studied above. The third scenario comprises only a single phase transition line, the Néel curve. In fact, this least interesting possibility seems to apply at least for the DMFT treatment of the cubic lattice with NNN hopping. Here, T^* is strongly suppressed (from about $T^* = 1/25$ to $T^* = 1/35$) by introducing moderate frustration ($t'^*/t^* = -0.25$) according to recent QMC results (Knecht, 2002).

3.7 Landau Theory and Criticality

In this section, we will study some implications of Landau theory. In subsection 3.7.1, we introduce an explicit representation of the lattice contribution to the Ginzburg-Landau free-energy functional for semi-elliptic DOS. Using this formalism, we show that each step of a direct iteration of the DMFT equations proceeds downhill, i.e., opposite to the gradient (with respect to the hybridization function) of the free energy. Based on this finding, a new method for evaluating free energy differences between coexisting phases within the DMFT is proposed in subsection 3.7.2. In subsection 3.7.3, we discuss to which degree critical behavior should impact or become visible in numerical calculations as performed in this work.