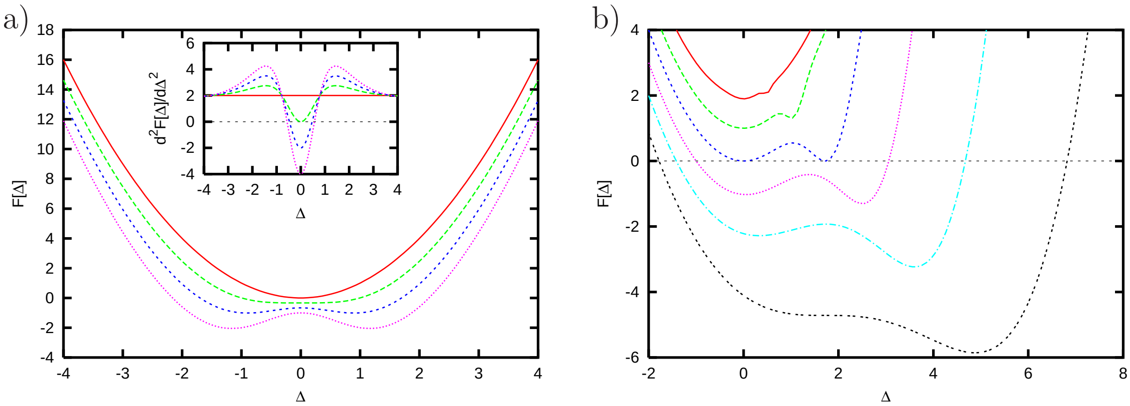

Figure 3.4: Schematic dependence of the free energy functional on an order parameter Δ near a first-order phase transition. **a)** For phase points above the critical point and along the transition line, one minimum splits into two minima of equal depth. The inset shows the second derivative of F. **b)** Evolution perpendicular to the transition line. The scenario in b) also serves as a cartoon of our concept of the Mott MIT; then, the right minimum corresponds to the metallic solution which exists almost until it equals the insulating solution while the insulating solution keeps its character until it disappears.

for the physical values of the mean field. Then, the physical solution is the one which minimizes F_{GL}. Supposed we can identify an one-dimensional order parameter Δ, the dependence of $F[U, T, \Delta]$ on Δ is similar to the curves shown in Fig. 3.4 for a first-order transition. The curves in Fig. 3.4 a illustrate the development along the first-order line (coming from above the critical point): a single minimum becomes flat (i.e., with zero curvature) at the second order end-point. It splits for lower T; the minima separate with increasing order parameter. Note that the region where the second derivative (inset of Fig. 3.4 a) is reduced may be quite small (cf. subsection 3.7.3). Therefore, asymptotically singular behavior may be visible only very close to the second-order end point. Figure 3.4 b depicts the evolution of the free energy functional perpendicular to the transition line: in the top curve, the left minimum corresponds to a stable solution while the right one is metastable. The third curve (from top) marks the MIT. In the bottom curve, only one minimum remains. Note the asymmetry in the coexistence region which will reappear in our results for the MIT.

Locating and characterizing phase transitions within the DMFT is potentially a two-step process. In a first step, solutions are obtained and observables are computed on a fine enough grid to identify nonanalytic behavior. If numerical discontinuities are detected, it is necessary to search for hysteresis effects with coexisting solutions. The result of the first step is then a diagram which indicates continuous transitions and/or coexistence regions. For the MIT on the Bethe lattice, such incomplete phase diagrams will be presented in Sec. 3.5. A second step is necessary for locating the first-order transition line within a coexistence region. This task is particularly difficult for QMC since this method is by construction unable to directly calculate the free