stable, i.e., this phase point is on the first-order line while in Fig. 3.58 b, the solution corresponding to $\lambda = 1$ is only metastable since the free energy is much higher (inset). Even though the comparatively more conventional method of pinpointing the first-order transition line used in our numerical calculations also worked well, the new method suggested here seems significantly superior since it is fully local in U and T and should be used in future work.[48]

Integrating the free energy in the solution space may also be useful for an absolute determination of F using some reference system. In particular, the impurity model corresponding to a Lorentzian DOS can be solved analytically and may serve as a reference point. Finally, the concept can obviously be generalized for arbitrary lattices. While for these cases, the lattice contribution to the free energy will have to be computed numerically, the additional cost is still negligible in comparison with the effort for solving the impurity model.

3.7.3 Critical Behavior Near the MIT

Two different aspects of criticality are potentially relevant in the context of studies of the Mott metal-insulator transition: On the one hand, observables may show singular behavior (i.e., have divergent slope as a function of T or U) near critical points or critical lines. On the other hand, critical slowing down of the iterative DMFT convergence process may arise within some regions of the parameter space.[49] In principle, "raw" QMC results (i.e., results for fixed finite $\Delta\tau$) could be negatively impacted by critical slowing down while the accuracy of extrapolations and fits could suffer from our neglect to take singular behavior explicitly into account. We will in this subsection discuss both effects and their relevance to the QMC studies presented earlier in this chapter.

As pointed out by Kotliar et al. (2000), a second-order critical end point is signaled within the DMFT by the appearance of a single zero eigenvalue m_0 of the fluctuation matrix (3.61) of the Ginzburg-Landau functional F_{GL}.[50] Under the assumption that this matrix smoothly depends on the hybridization function Δ_n and on the parameters T and U, the associated eigenvector is well-defined also in the vicinity of the critical end point where it represents a soft mode. The associated coefficient η_0 of an expansion of Δ_n in terms of the eigen basis of the fluctuation matrix then determines the critical behavior. In principle, critical exponents may be calculated from Taylor expansions in η_0. According to Kotliar et al. (2000), the parameter η_0 may be replaced by another parameter η which fulfills a cubic equation without quadratic term, $p\eta + c\eta^3 = h$, near the critical point. As a consequence, the double occupancy is predicted to show cubic-root behavior near the critical point

[48] As pointed out in more detail in Sec. 3.6, the transformation technique used by Tong et al. (2001) for determining the thermodynamic MIT line is directly related to the concepts of this subsection. In contrast to the method suggested here, however, the transformation technique incorporates an approximation.

[49] Note that only the first consequence is strictly a property of the model; critical slowing down could in principle be overcome by more advanced iteration techniques.

[50] All other eigenvalues are, then, negative since the minimum of F_{GL} is unique for temperatures at or above the critical point (cf. subsection 3.7.1).