3.9 Conclusion

In this chapter, we have studied the fully frustrated half-filled Hubbard model with a semi-elliptic noninteracting density of states in the limit of infinite dimensionality near the Mott metal-insulator transition (MIT).

We have computed the coexistence region of metallic and insulating phases with significantly higher accuracy than achieved previously in the literature. In the course of this study, we have discussed the signatures of a first-order transition within the DMFT and for the first time established a rigorous relation between the stability of fixed points in a DMFT iteration scheme and the thermodynamic (meta-) stability of phases. Using an improved method for the quantum Monte Carlo (QMC) calculation of the kinetic energy, we have presented the first accurate estimates of the full energy (per electron) and have shown that this observable is far better suited for the QMC determination of phase boundaries than other observables considered so far. We have explained the initial contradiction between QMC results regarding the possible extent of the coexistence region by identifying strengths and weaknesses of the QMC codes and strategies used by the major groups in the field. In particular, we have found and corrected a major flaw in the QMC code used previously by our group; while the original code was already correct in the limit of vanishing discretization $\Delta\tau \to 0$, it had introduced an unnecessary error at small frequencies which suppressed the coexisting insulating phase at attainable values of $\Delta\tau$. We have also parallelized the QMC code in order to efficiently use all available computing resources.

While the coexistence of metallic and insulating solutions indicates the presence of a first-order transition, the phase diagram is only complete with the determination of the thermodynamic first-order transition line $U_c(T)$. This task was previously regarded as too difficult for numerically exact methods that cannot directly compute the free energy of the impurity model (such as QMC and NRG); even the prediction of the iterative perturbation theory was initially unclear. We have derived a first-order differential equation for the phase boundary; its solution is more stable than a more direct comparison of free energies due to the cancellation of errors. On the basis of highly accurate measurements for the energy and the double occupancy, we have established that the differential equation may be linearized without loss of accuracy. We have derived the leading low-temperature asymptotics of $U_c(T)$ from Fermi liquid theory and have fixed a numerical coefficient by calculating the ground state properties of the metallic phase. This was possible by performing an interpolating fit of new (zero-temperature) second-order perturbation theory estimates with results for $U_c(T=0)$ previously obtained by ground state methods. The quality of this fit has been stabilized by demanding thermodynamic consistency and has been successfully tested by comparison with extrapolated QMC data. As a byproduct, we have calculated the coefficient $\gamma(U)$ of the low-temperature specific heat and checked the consistency with extrapolated estimates for the quasiparticle weight Z. Due to the high precision of the QMC data and the numerous independent checks, the accuracy of the resulting first controlled estimate of the thermodynamic first-order phase transition line is well established.

We have analyzed Tong et al.'s (2001) recently published independent estimates