3.5 Results: Coexistence Region

In this section, we will begin the systematic construction of the phase diagram of the fully frustrated Hubbard model with semi-elliptic DOS in $d \to \infty$ at half filling. For this purpose, only those observables need to be considered which can be directly computed from standard QMC solutions of the DMFT self-consistency equations. As shown in subsection 3.5.1, the internal energy E is very well suited for determining the metal-insulator transition in the physical limit $\Delta\tau \to 0$, much better than other observables considered so far. In subsection 3.5.2, we establish and parametrize universal, i.e., temperature-independent, properties of the insulating phase. Measurements of the energy E presented in subsection 3.5.3 are used for the construction of a preliminary phase diagram including a crossover region at high temperatures, a critical end point, and a region of coexisting metallic and insulating solutions at low temperatures in subsection 3.5.4.

Measurements of the double occupancy D and its (difficult) extrapolation for $\Delta\tau \to 0$ in the metallic phase are discussed in subsection 3.5.5. The very precise extrapolated QMC estimates for E and D obtained in this section will allow for an implicit comparison of the free energies of the metal and the insulator (within the coexistence region) and will lead to the full phase diagram in Sec. 3.6.

3.5.1 Choice of Observables and Extrapolation

In this subsection, we determine which of the observables introduced in subsection 3.2.3 are best suited for indicating and characterizing the metal-insulator transition. Using QMC results for the relatively high temperature $T = 1/15 \approx 0.067$ as a test case, we discuss in particular the difficulties of extrapolations to the physical limit $\Delta\tau = 0$.

The double occupancy for $T = 0.067$ is shown in Fig. 3.15 for a range of values of the discretization parameter $\Delta\tau$. Here, the symbols, which reflect QMC measurements, have been connected by straight line segments in order to guide the eye. As expected on physical grounds, the double occupancy decreases significantly with increasing U, i.e., with decreasing metallicity. Evidently, the slope $|\mathrm{d}D/\,\mathrm{d}U|$ reaches a maximum at $4.55 \lesssim U \lesssim 4.65$ (depending on $\Delta\tau$). One would be hard pressed, however, to decide if there is a continuous crossover or a sharp transition, even for finite $\Delta\tau$. Furthermore, the dependence of D on $\Delta\tau$ is seen to be very irregular: coming from the metallic side the $\Delta\tau$ error increases up to $U \approx 4.6$ while it is invisible on the insulating side.[21] One might suspect that the primary effect of a finite $\Delta\tau$ error is a horizontal shift of the curves towards larger values of U. Still, results of an extrapolation to $\Delta\tau = 0$ would strongly depend on the assumed (nontrivial) functional forms and, thus, be unreliable without additional input.

A similar picture emerges for the quasiparticle weight Z as defined in (3.6) and shown in Fig. 3.16. This observable is in principle a very good candidate for characterizing the metal-insulator transition since, within the Fermi liquid picture, the

[21]The absence of significant $\Delta\tau$ dependence for the QMC estimate of D in the insulator may be specific to the particular algorithms used in our code.