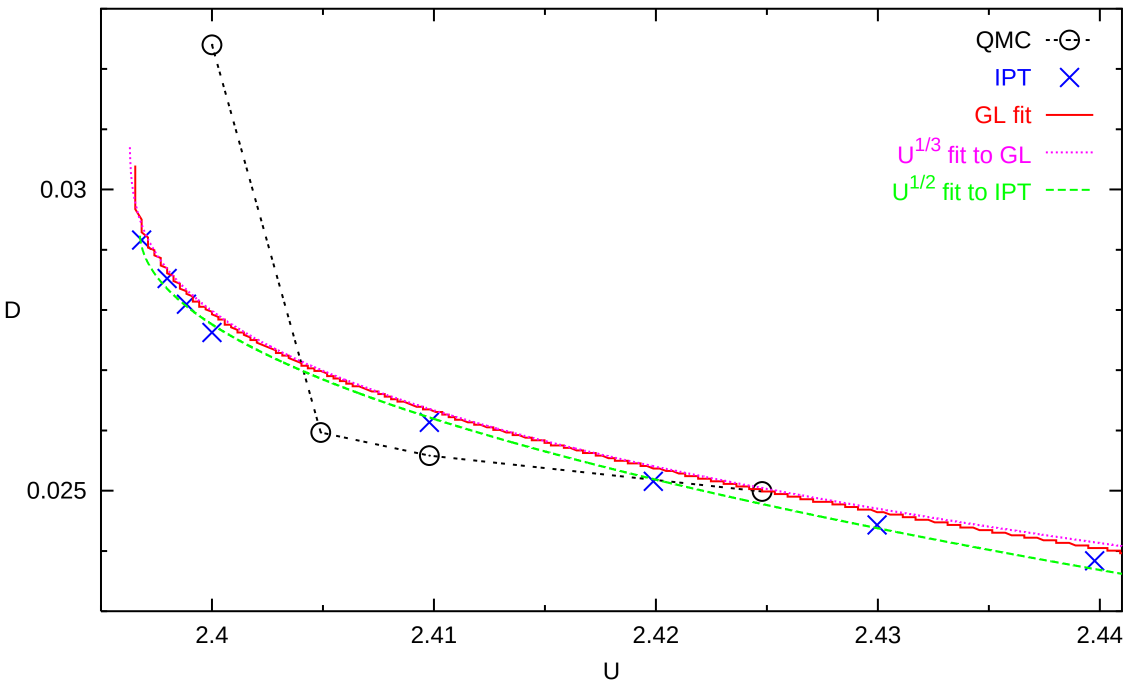

Figure 3.62: Double occupancy D versus U for $T \lesssim T^*$. Magnified view on top set of curves/circles shown in the main panel of Fig. 3.59 (Kotliar et al., 2000) for the insulator. In addition to the QMC and IPT data and to the Ginzburg-Landau fit, a cubic-root fit of the form $D(U) = 0.031 - 0.0195\,(U - 2.3963)^{1/3}$ (dotted lines) and a square-root fit of the form $D(U) = 0.0293 - 0.027\,(U - 2.39675)^{1/2}$ (dashed lines) to the asymptotic behavior of the insulating IPT solution is shown. Interactions are in units of the half bandwidth.

to the insulating phase at $U \approx 2.4$ at this temperature is incompatible with all other data or fit functions; a finer grid or an intensive convergence study would be needed to elucidate the irregular behavior of this single data point. The fit for $T = 1/32$, the highest temperature considered here, is perfect. Only for $T = 1/35$, just above the critical temperature T^*, a deviation in the transition region is clearly seen. The numerical significance of this discrepancy is not completely clear.[53] We conclude that potential problems arising from the fit functions used throughout this chapter are indeed limited to a very small region around the second-order end point. Since no results are reported for this region and since no signals for singular behavior are present, a negative impact on our results can be excluded.

Critical Slowing Down

All points in parameter space (here formed by U and T) where a new minimum of the free energy appears in the space of hybridization functions are critical in the

[53]Note that the deviation of the QMC data is of the same order of magnitude for $T = 1/32$ and $U = 2.3$ where the only viable explanation is the numerical Monte Carlo error.