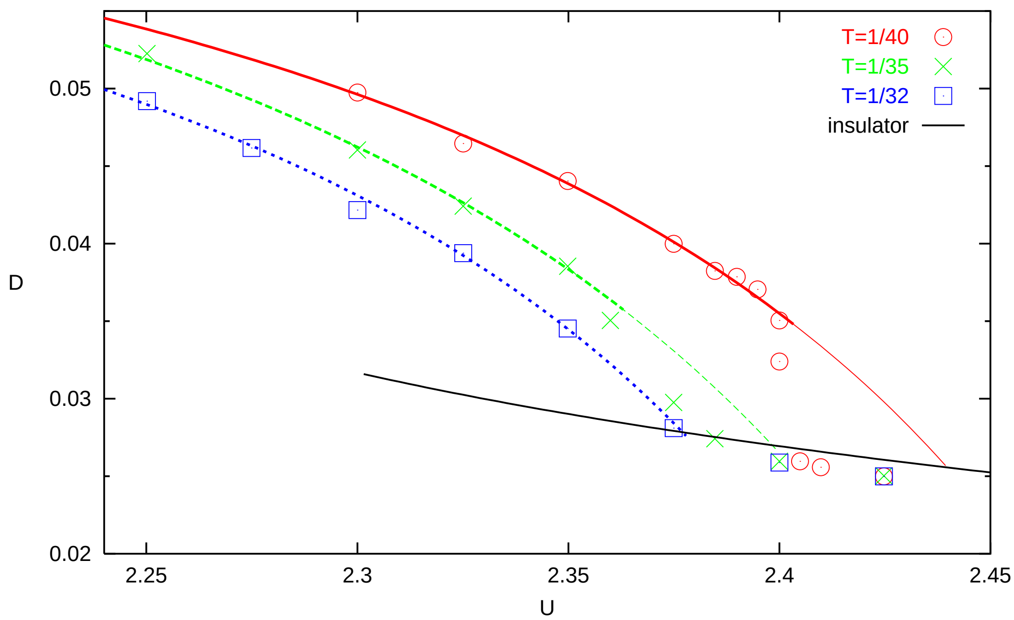

Figure 3.63: Double occupancy D versus U for $T \lesssim T^*$. QMC data for a selected set of temperatures extracted from the main panel of Fig. 3.59 (Kotliar et al., 2000) in comparison to fits with regular functions and to our result (3.19) for the double occupancy of the insulator. Thick portions of the lines indicate ranges of good agreement with the QMC data. All energies are in units of the half bandwidth.

sense that the fluctuation matrix has a zero eigenvalue.[54] Consequently, at least one component of the gradient of the free energy with respect to the hybridization function vanishes faster than linearly at its minimum. An iteration scheme that relies on linear behavior of the gradient thus slows down near the critical point; exactly at the critical point, the number of iterations necessary for decreasing the error of a solution by some factor may even diverge (in the limit of infinite target accuracy).

Therefore, difficulties in the DMFT iteration process may be expected near critical points and lines. It is not clear a priori, however, how large the problematic regions are and what accuracy can be reached at reasonable numerical cost. Joo and Oudovenko (2001) found themselves unable to present QMC estimates of the coexistence region for $T > 0.035$ due to critical slowing down.[55] Our experiences are less dramatic. We found slower convergence near critical points, in particular at higher temperatures close to the temperature of the second-order end point, both for $T \lesssim T^*$ and for $T \gtrsim T^*$. This is illustrated in Fig. 3.64 for $T = 1/15$ and $U = 4.55$ (in units of the variance of the DOS). Here, “traces” of the double occupancy D are shown

[54] In the context of the MIT, these points are the second-order end point and the stability edges of solutions at the boundaries of the coexistence region.

[55] These authors even found critical slowing down for the stable solution near the boundaries of the coexistence region. This claim is rather surprising in view of the fact that the zero eigen mode only appears when the free energy is evaluated at the hybridization function corresponding to the unstable solution. It is not supported by our data at all.