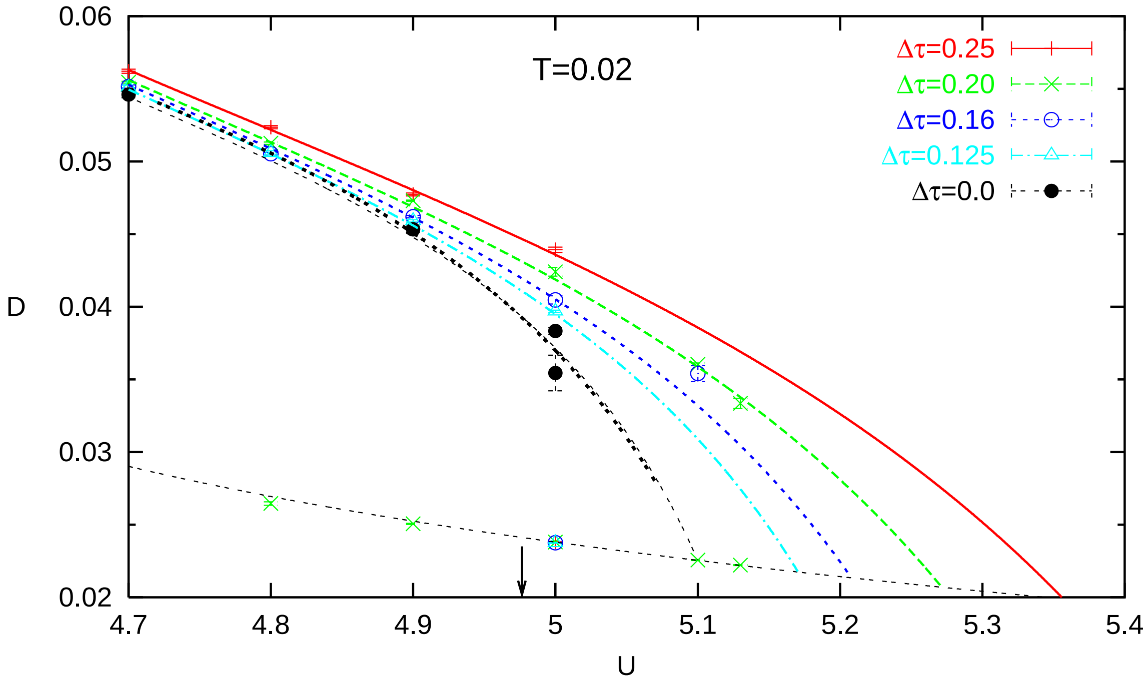

Figure 3.41: Double occupancy for $T = 1/50$, analogous to Fig. 3.37. For $U = 5.0$, where the quality of a purely quadratic least-squares fit for D in the metallic phase (upper solid circle) is already bad, a fit including a linear term has been added (lower solid circle). Both estimates bracket the fit functions for $\Delta\tau = 0.0$ (double-dashed lines).

with using only 120000 sweeps) and is too small to impact our final results visibly. Note the good agreement of the "linearized fit" (thick line) with the original fit across the range $U_c = 4.7$ to $U_{c2} = 4.99$.

In Fig. 3.41, we have again included the result both of a purely quadratic and linear+quadratic extrapolation, here for $U = 5.0$. Note that the quality of least-squares fits is generally worse in this plot since simulations at $\Delta\tau = 0.1$ could not be afforded. Longer and even more precise simulations would be required for understanding or correcting the deviation of the metallic solution for $\Delta\tau = 0.16$ at $U = 5.1$. Still, the accuracy of the $\Delta\tau$ extrapolated fits is very satisfactory, considering that we are looking at the strongly correlated region at very low temperatures.

The summary of our results for the double occupancy is given in Fig. 3.42, where the fit functions for the metal at $\Delta\tau = 0$ are drawn (thin colored lines) together with QMC data (symbols) for interactions deep enough in the metallic phase so that quadratic least-squares fits are reasonable. In analogy to our summarizing result Fig. 3.30 for the energy, the thick line shows the double occupancy for the insulating phase. The nearly straight thin line at the top indicates the result of an extrapolation to $T = 0$ for the metallic phase to be detailed in Sec. 3.6.

The relative error of the estimates for ΔD implied by the results shown in Fig. 3.42 is about 10^{-2} in the proximity of the first-order phase transition (see arrows in Fig. 3.36 – Fig. 3.41) for $T \leq 0.04$ and is only slightly larger for $T = 0.05$. Such a high