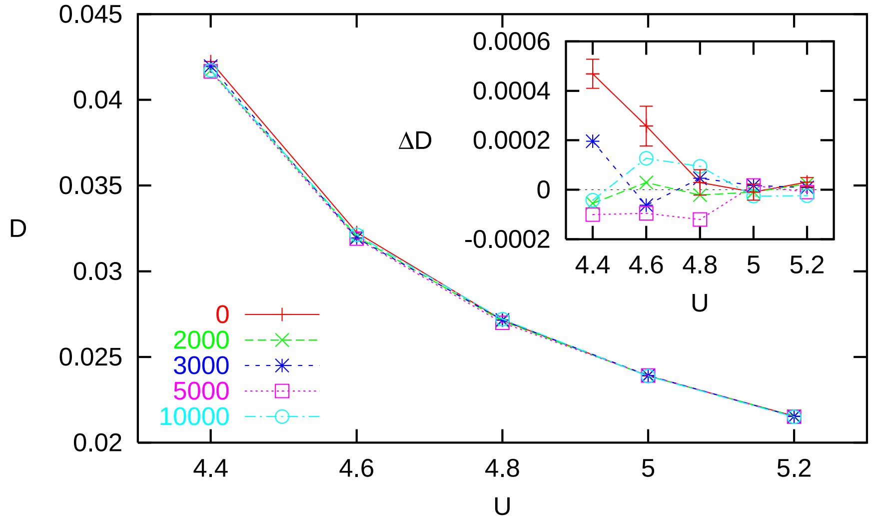

Figure 3.14: Double occupancy for $\beta = 10$ and $\Delta\tau = 0.125$: comparison of QMC runs with different number of warm-up sweeps (8 walkers with n warm-ups plus 20000 measurements each; about 20 iterations). In the inset, differences to the average (of all results with $n > 0$) are shown. No systematic dependence on n, except for $n = 0$ in the metallic phase.

deviations arise both from statistical and convergence errors. Only the production runs (with 2000 warm-up sweeps; crosses) were long enough to reduce the total error far below 10^{-4}.

The use of insufficiently converged solutions is potentially a very significant source of errors. It is important to realize that in principle measurements have to be performed exactly at the solution of the self-consistency equations, i.e., for the exact bath Green function. Averages over measurements performed for different impurity models corresponding to approximate solutions do not necessarily converge to the exact answer in the limit of an infinite number of models (i.e., iterations) and measurements.[19] Still, the most important practical point when computing observables is that only runs are included in averages which are close to the solution in comparison to the asymptotic statistical error. For higher precision, the number of sweeps (and not only the number of measurements) must be increased. In this work, we usually used between 10^5 and $5 \cdot 10^5$ sweeps, in particular cases more than 10^6 sweeps. If the convergence of solutions was unclear, we started new iteration chains; partially with the same initial self-energy (but different random numbers), partially using specially prepared self-energies.[20] The good convergence of our solutions will also become

[19] Trivially, a measurement of the free energy F itself (using a suitable impurity solver) is a good example. Since F is minimal for the true solution, all measurements taken for approximate solutions will be too large. The correct answer can, therefore, not be approached by averaging over many measurements, but only by reducing the deviations from the exact solution.

[20] We will prove in subsection 3.7.1 that the iteration process is convergent at least for the direct iteration scheme since (for an exact solution of the impurity problem) each step is downhill in the space of hybridization functions with the step length being proportional to the slope of the free