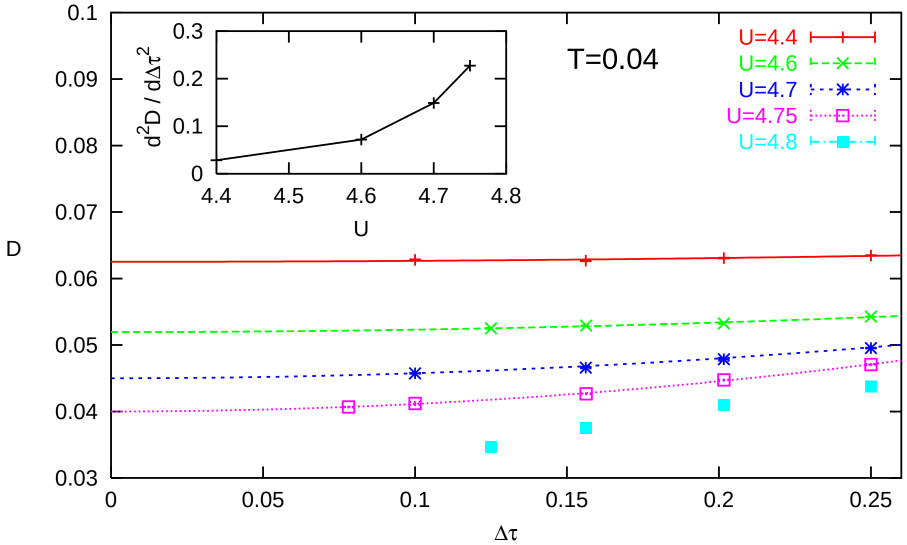

Figure 3.34: Extrapolation $\Delta\tau \to 0$ of double occupancy D in metallic phase for $T = 0.04$: At small enough U, the QMC data points agree with purely quadratic least-squares fits (lines). Since the quadratic (in $\Delta\tau$) extrapolation law is seen to break down for $U = 4.8$, it is also unreliable at slightly smaller U. The inset shows the (second order) fit coefficient which increases significantly for $U \to U_{c2}$.

estimate for the double occupancy in the metal, we will also indicate approximate functional forms for $D_{\text{m}}(T, U)$ within the coexistence region which correspond exactly to a linearized, interpolated version of this differential equation.

The difficulty in extrapolating D to the physical limit $\Delta\tau \to 0$ is illustrated for $T = 0.04$ in Fig. 3.34. Well within the metallic phase, the dependence of D on $\Delta\tau$ follows quadratic fit curves (i.e., without linear terms). Within the range of $\Delta\tau$ shown in the plot, this observation even remains true (with strongly increased $\Delta\tau$ dependence; see inset of Fig. 3.34) up to $U = 4.75$. This value of the interaction is just below $U_{c2} = 4.8$, where the metallic phase becomes unstable, and $U_{c2b} \approx 4.83$, where the extrapolated energy (see Fig. 3.25) meets that of the insulator. At $U = 4.8$, however, the purely quadratic extrapolation law for the double occupancy clearly breaks down for $\Delta\tau \lesssim 0.16$. The observed irregularity not only makes it impossible to perform the extrapolation $\Delta\tau \to 0$ for fixed interaction U very close to the MIT, but also makes the results of extrapolations for slightly smaller U suspicious. After all, deviations from the quadratic extrapolation law might occur for $\Delta\tau \ll 0.1$ so that the true value of D could be lower than the extrapolated value. Therefore, reliable extrapolations can only be performed on the basis of appropriate fit functions, each of which approximate the QMC estimates for $D(U)$ for some value of $\Delta\tau$ in the metallic phase. Extrapolations to the limit $\Delta\tau = 0$ are then no longer local in U and are thus much less affected by the difficulties discussed above.

As in subsection 3.5.3, we present the results for the double occupancy sorted from high to low temperatures, starting with $T = 0.1$. Due to the broad crossover at this