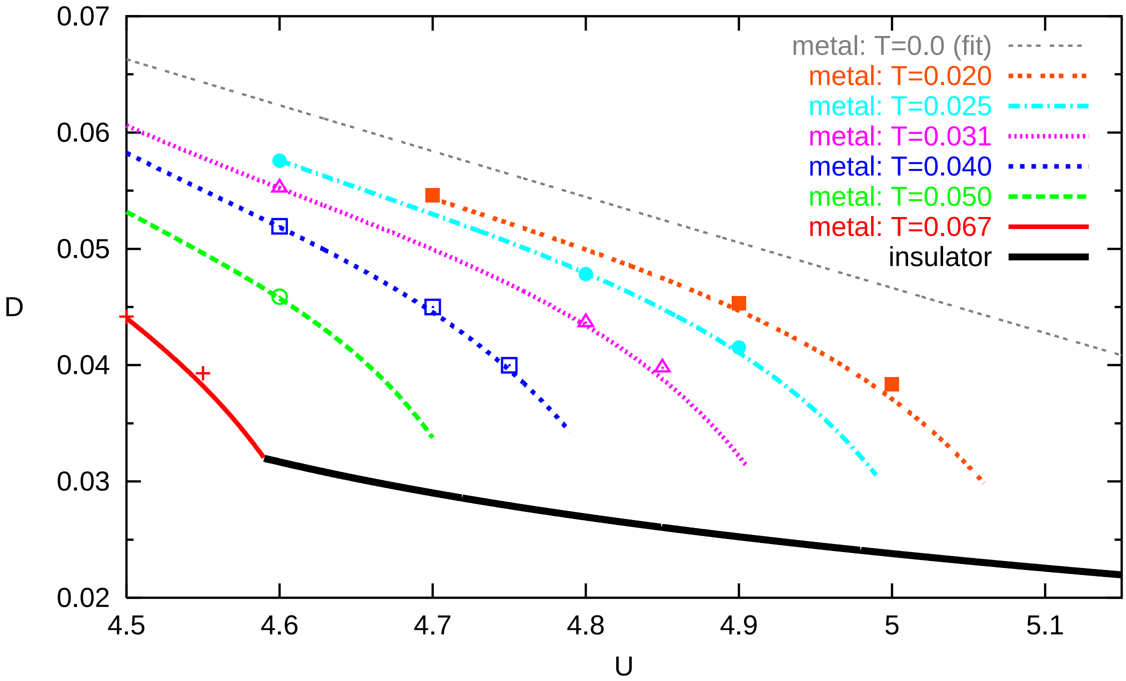

Figure 3.42: Double occupancy D vs. interaction U at $\Delta\tau = 0$. The symbols indicate extrapolated QMC data for the metallic phase; colored lines indicate “linearized” fit curves (thick lines in Fig. 3.36 – Fig. 3.41). The thick solid line denotes the double occupancy of the insulator within its T-dependent stability region. The thin top line marks the ground state double occupancy in the metal (to be determined in Sec. 3.6).

accuracy may seem surprising in view of our discussion initiated in subsection 3.5.1 and continued in the beginning of this subsection. However, the choice of suitable fit functions has made it possible to perform a nonlocal $\Delta\tau$ extrapolation (i.e., for all values of U at the same time for fixed T), including both physical intuition and prior knowledge that had been obtained in subsection 3.5.3. Thus, reliable estimates of D could be obtained even close to the MIT where naive, local extrapolations would have failed (as illustrated in Fig. 3.34).

3.6 Results: Thermodynamic Phase Transition Line

In this section, a differential equation will be derived for the transition line $U_c(T)$ between metal and insulator based on the fact that both phases have the same free energy along the transition line.

3.6.1 Differential Equation for $\mathrm{d}U_c/\mathrm{d}T$ and Linearization

For the Hubbard model, the free energy F and its differential $\mathrm{d}F$ can be expressed in terms of energy E, temperature T, entropy S, double occupancy D, and interaction