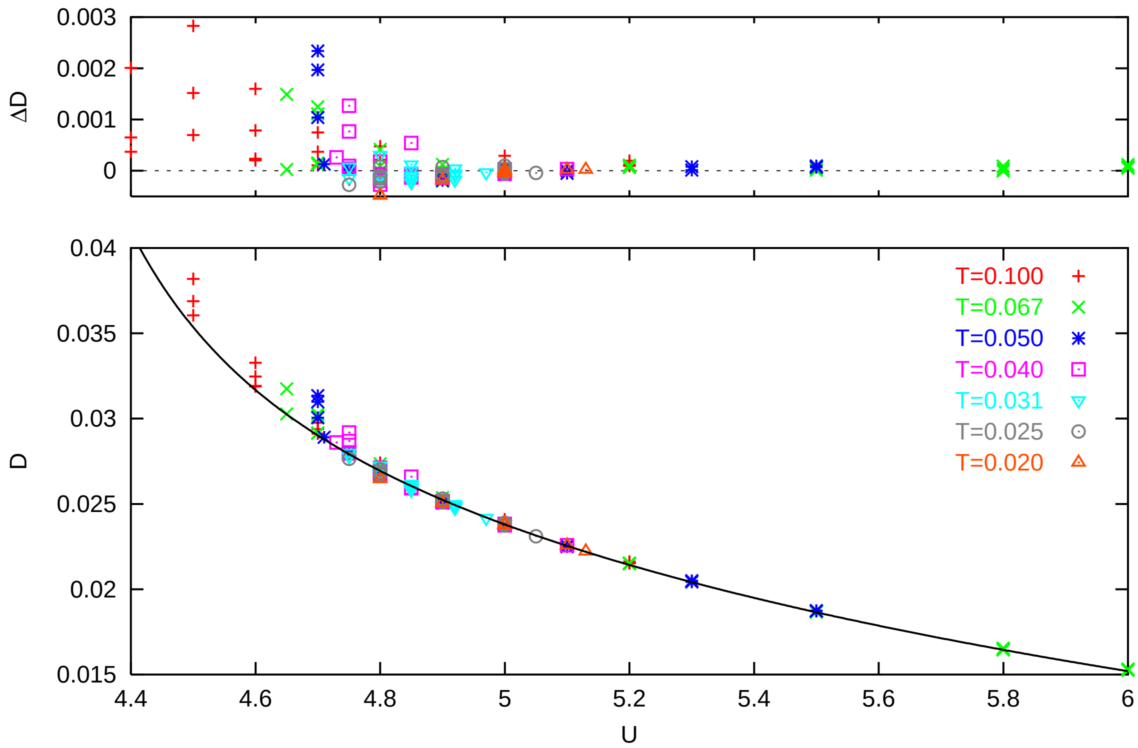

Figure 3.21: Double occupancy in insulating phase vs. U. The symbols in the lower part represent the QMC data (without extrapolation $\Delta\tau \to 0$). The fit curve (solid line), given by (3.19), is thermodynamically consistent with the fit for E shown in Fig. 3.20. The upper part shows the deviations of the QMC data from the fit curve which is significant only for small U [i.e., for $U \to U_{c1}(T, \Delta\tau)$] and dependent on $\Delta\tau$ (not encoded in the figure).

can be easily verified since the QMC measurements for D are practically free of $\Delta\tau$ errors in the insulating phase so that no extrapolation $\Delta\tau \to 0$ or scaling is necessary. The "raw" QMC estimates are shown in the lower part of Fig. 3.21; here, the solid line is given by the function

$$D_{\mathrm{i}}(U) = \frac{0.515}{U^2} + \frac{0.0027}{(U-3.95)^2} + 0.00325 - 0.0005\,U\,. \tag{3.19}$$

Again, the deviations of the measurements from the fitting function are magnified in the upper part of the figure. The overall agreement is very good; the deviations at small U indicate a strongly increased influence of the $\Delta\tau$ error near the phase boundary at not too low temperatures (see subsection 3.5.5).

As a result of this subsection, we have identified the internal energy E as an appropriate observable for a QMC study of the metal-insulator transition. In addition, we have established functional expressions for E and D within the insulating phase. These will not only be used for the determination of the "coexistence" phase diagram in the next subsection, but also help determine the low-temperature behavior of the thermodynamic phase transition line in Sec. 3.6.