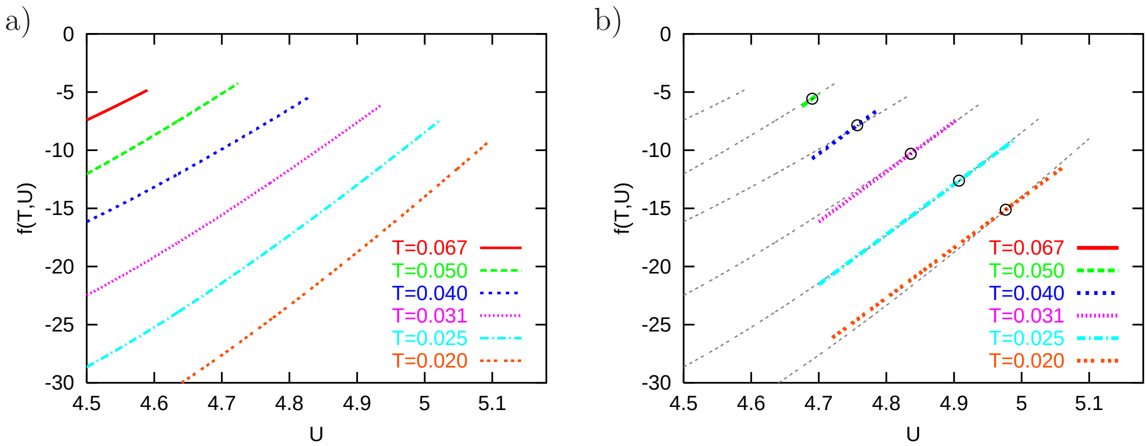

Figure 3.43: Function $f(T,U)$ which coincides with the derivative $\mathrm{d}U_\mathrm{c}/\mathrm{d}T$ on the phase transition line $U_\mathrm{c}(T)$. **a)** "Raw data" extracted from fits of QMC data for E and D. **b)** Linearized fits with the functional form $f(T,U) = A(T) + 43\,U$. Circles indicate $\mathrm{d}U_\mathrm{c}/\mathrm{d}T$ of the final solution.

Therefore, very accurate results in the whole coexistence region can only be achieved using the fit functions for $E_\mathrm{i}(U)$, $D_\mathrm{i}(U)$, $E_\mathrm{m}(T,U)$, and $D_\mathrm{m}(T,U)$ established in subsections 3.5.2, 3.5.3, and 3.5.5. Among these data sets, by far the largest error is associated with the double occupancy $D_\mathrm{m}(T,U)$ in the metallic phase. Figure 3.43 a shows "raw" results for $f(T,U)$ which follow from the QMC data when the best estimate for D_m according to the 2-parameter fits (3.20) (shown as thin lines in Fig. 3.36 – Fig. 3.41) are used. Here, the fit functions are not only shown within (our estimate of) the coexistence region, but extend up to $U = U_{\mathrm{c}2b}(T)$ (where the extrapolated energy of the metal crosses the energy of the insulator). Evidently, the dependence on U is almost linear for fixed T. Furthermore, the slope of the curves shown in Fig. 3.43 a is only very weakly dependent on T, at least within the coexistence region. Consequently, only a small error is made when these raw results are replaced by straight lines with identical slopes throughout the coexistence region. This is seen in Fig. 3.43 b, where the thick lines (shown only for U within the coexistence region) follow the form

$$f(T,U) = A(T) + 43\,U\,. \tag{3.32}$$

While the discrepancy between this linearized form and the original raw data is in the percent range throughout the coexistence region, it is even smaller near the most important points touched by the solution (circles) to be determined below. This fact alone ensures that the linearized form of $f(T,U)$ is a good interpolation for the purpose of finding the solution $U_\mathrm{c}(T)$. The particular practical advantage of the linear form (3.32) is that the solution of the corresponding differential equation $\mathrm{d}U_\mathrm{c}/\mathrm{d}T = A(T) + 43U_\mathrm{c}(T)$ is given by a regular integral which can even be performed analytically using the interpolation for $A(T)$ that will be established later in this section.