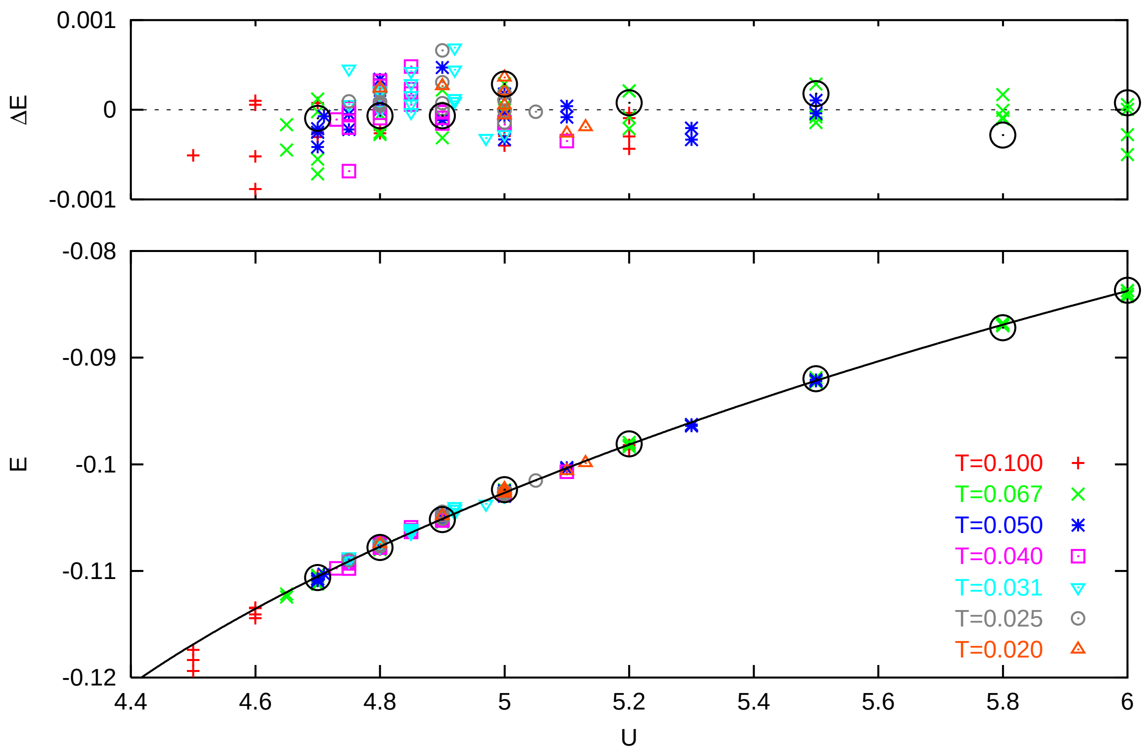

Figure 3.20: Total energy in insulating phase vs. U. In the lower plot, the large circles denote the results of the extrapolations shown in Fig. 3.19. The small symbols correspond to the rescaled QMC data, according to the extrapolation law (3.17) for $\Delta\tau \to 0$. The solid line indicates the (T-independent) fit function (3.18) which is consistent with the solid line for D shown in Fig. 3.21. The upper part gives a magnified view on the (small) discrepancies between data and fit curve.

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than about $4 \cdot 10^{-4}$. The deviations of the extrapolated data (large circles) are even smaller. In fact, we can trace the outliers at $U = 5.0$ and $U = 5.8$ to statistical deviations in the extrapolation process. This explanation is supported by the fact that the scaled data points [using the extrapolation law (3.17)] are much closer to the fit than the result of the free extrapolation. In summary, we expect the error of our fit (3.18) to be close to 10^{-4} at least for $4.75 \leq U \leq 6.0$.[22]

Such a high accuracy seems particularly impressive since the T-independent energy in the low-temperature insulating phase is a ground state property. This fact also allows for a numerical check since, at $T = 0$, the internal energy and the double occupancy are simply related: $D(T, U = 0) = \mathrm{d}E(T, U = 0)/\mathrm{d}U$. Therefore, the derivative of our fit (3.18) for $E(U)$ should represent the QMC data for $D(U)$. This

[22]The negative deviations for $T = 0.05$, $U = 4.7$ and for $U < 4.7$ are related to the proximity of the phase boundaries. It is unclear if the effects are fully physical; most probably, at least some part arises from a bias in the statistical error which may be significant for any almost unstable solution. On the other hand, the finite heat capacity implied by negative deviations with lower temperatures is also plausible on physical grounds. In any case, the effects are too small to affect our numerical results.