3.5.3 Internal Energy

In the following, we present QMC data for the internal energy E, fits for finite $\Delta\tau$, and extrapolations to the physical limit $\Delta\tau = 0$, ordered by decreasing temperature. The extrapolated data is summarized at the end of this subsection; the resulting phase diagram will be shown in the next subsection 3.5.4.

Since the insulating side has already been analyzed in the previous subsection, the remaining difficulty is the treatment of the metallic phase and the determination of the phase boundaries. Within the metallic phase, we use quadratic least-squares fits in $\Delta\tau^2$ for fixed U. Due to the small number of data points, the error in the quadratic coefficient (i.e., the $\Delta\tau^4$ term) is, however, of the same order of magnitude as the estimate itself. Furthermore, the estimate may shift depending on whether or not data points with small $\Delta\tau$ are included. In order to minimize the resulting errors, we have assumed slow variation of this coefficient as a function of U and T and have performed a global fit. The result is that the $\Delta\tau^4$ coefficient for the metal is always close to the value 0.95 computed for the insulating phase. The observation of a slight variation as a function of T lead to a linear interpolation with a value of 1.2 for $T = 0.1$ and 0.8 for $T = 0.02$.[23] This coefficient was then held fixed for all extrapolations within the metallic phase.

The results of such extrapolations to $\Delta\tau = 0$ at $T = 0.1$, the highest temperature considered here, are denoted as solid circles in Fig. 3.22. The $\Delta\tau = 0$ values for $U = 4.1$, $U = 4.2$, and $U = 4.3$ fall on a straight line which extends to $U = 4.4$ and is partially drawn as a thick and partially as a thin line. The parallel lines connecting data points for finite $\Delta\tau$ are offset according to a scaling law which not only includes the globally determined $\Delta\tau^4$ coefficient, but also a $\Delta\tau^2$ coefficient which has been averaged from the extrapolations for $U = 4.1$, $U = 4.2$, and $U = 4.3$. Each of these "metallic" lines crosses the corresponding "insulating" line (beginning as thick curve at large U and extending into a thin line towards the metallic phase) at some point. In this region, however, the QMC data deviates systematically from the fit curves, indicating a smooth crossover rather than a phase transition.[24]

An analogous plot for $T = 0.067$ (more accurately: $\beta = 15$, i.e., $T = 1/15$) is shown in Fig. 3.23.[25] Here, the transition is (almost) sharp within the numerical accuracy, i.e., the data follows linear fits in the metallic phase and the universal form (3.18) in connection with (3.17) in the insulating phase, respectively, for all values of the interaction U. Consequently, the transition points can be determined and extrapolated very accurately: $U_c = 4.59$. Only extremely close to the transition points, i.e., for $U = 4.65$ at $\Delta\tau = 0.15$ and $U = 4.7$ at $\Delta\tau = 0.2$, do slight deviations of the QMC data from the fits indicate some rounding effect. This observation, in combination with conclusions from lower temperatures, will later lead to the conclusion that $T = 0.067$ is close to, but slightly above, the critical temperature.

[23] Note that while the relative error for the coefficient is relatively large, its influence is small. The intrinsic uncertainty of about 0.2 translates, e.g., into a possible additional error in the energy estimates of $2 \cdot 10^{-5}$ for $\Delta\tau = 0.1$ and $3 \cdot 10^{-4}$ for $\Delta\tau = 0.2$.

[24] As the precise behavior of E in the crossover region will be irrelevant in the following, we only sketched the assumed form by manually adapting cubic splines (thick lines).

[25] Compare also the data for this temperature shown in the previous subsection.