the curves are again almost linear with significantly reduced slope; here, however, a small curvature remains visible. The comparatively sharp kinks unambiguously indicate the positions of phase transitions (or narrow crossover regions) for each value of the time discretization $\Delta\tau$. A detailed analysis using suitable fit functions will be presented in the next subsection. Furthermore, the dependence of the curves on $\Delta\tau$ is very regular both on the metallic and on the insulating side. While we will look at the precise extrapolation laws below, it is apparent from the figure that the $\Delta\tau$ error is about a factor of 3/2 larger in the metallic phase. This explains the irregularity of the $\Delta\tau$ dependence within the transition region where the phase transition (or crossover) line is passed upon varying $\Delta\tau$ for constant U. As long as this problematic region is excluded, very precise extrapolations $\Delta\tau \to 0$ can be expected. Finally, the regular shape of each curve also significantly reduces the convergence error since measurements obtained from unconverged solutions can be detected as deviations from the regular pattern and then corrected by performing additional simulations.

If high-frequency tail corrections in the energy estimators are properly taken into account (cf. subsection 3.2.3), low-frequency errors associated with the discrete Fourier transforms (cf. subsection 3.4.1) are avoided, and no phase transition lines are crossed, the error in the estimate for E is dominated by the Trotter error (cf. Sec. 1.3) which is $\mathcal{O}(\Delta\tau^2)$. Therefore, a reasonable starting point for a quantitative analysis is a purely quadratic extrapolation $\Delta\tau \to 0$ (i.e., a linear least-squares fit in $\Delta\tau^2$), both on the metallic and on the insulating side. The intersection of linear fits for $E_\mathrm{m}(U)$ and $E_\mathrm{i}(U)$ of the metallic and insulating solution then determines a first estimate of the transition point.

We found that the accuracy both in the estimates for energies and for transition points could be improved by an order of magnitude by extending the least squares fits to fourth order in $\Delta\tau$ (i.e., by using fits of the form $E_U(\Delta\tau) = E_U(0) + c_2\Delta\tau^2 + c_4\Delta\tau^4$) and by extracting a more complicated, more accurate, and thermodynamically consistent expression for the energy in the insulator.

3.5.2 Properties of the Insulating Phase

Leaving properties of the metallic phase for the next subsections, we will now take a detailed look at the insulating phase. The symbols in Fig. 3.19 represent all of our QMC measurements of E inside the insulating phase for various temperatures T and interactions U as a function of $\Delta\tau^2$. The most important observation is the absence of any significant dependence of E on T. Such universal behavior is expected deep inside the insulating low-temperature phase where a well-developed gap in the spectrum exists at the Fermi energy (cf. Sec. 3.8) and where thermal excitations are suppressed exponentially. Evidently, the specific heat is already reduced by several orders of magnitude compared to the metallic case in the low-temperature region of interest very close above the MIT as soon as a pseudo-gap appears. One practical consequence is that for fixed interaction U all QMC data points may be included in a least squares fit for the extrapolation $\Delta\tau \to 0$, irrespective of the associated temperature T. The solid lines in Fig. 3.19 reflect such extrapolations; here all three