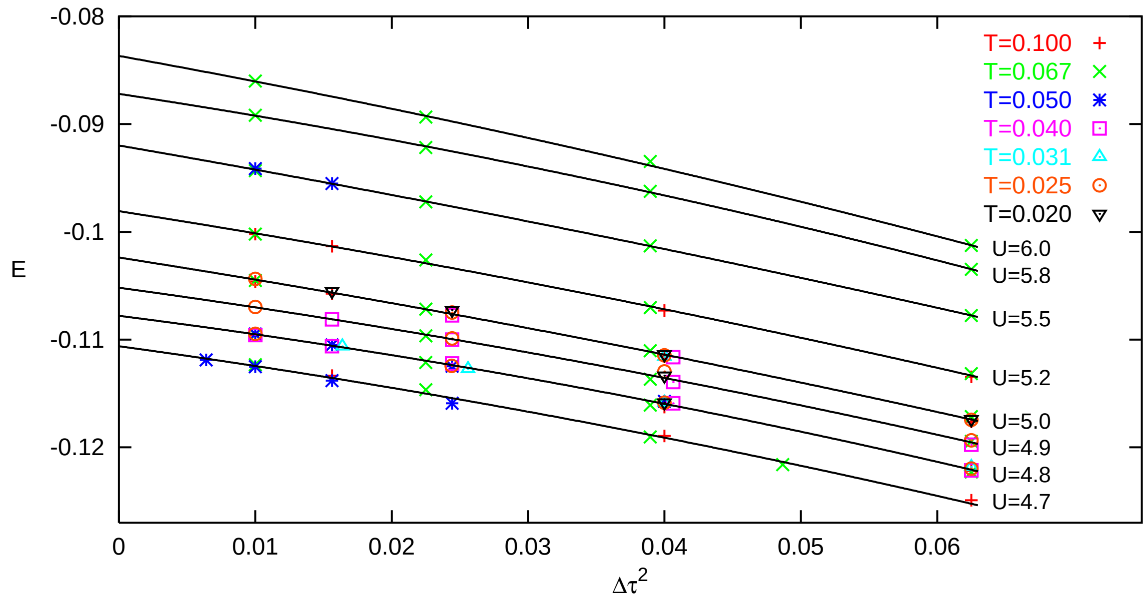

Figure 3.19: Total internal energy in insulating phase vs. $(\Delta\tau)^2$. Since the QMC estimates (symbols) do not significantly depend on the temperature T for fixed interaction U, they can be collectively extrapolated to $\Delta\tau \to 0$ in quadratic least squares fits in $(\Delta\tau)^2$ (solid lines) for each value of U.

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coefficients in the quadratic fit (in $\Delta\tau^2$) were taken as free parameters. Due to the small curvature, the extrapolations are well conditioned.

The extrapolated values for E are shown as large circles in the lower part of Fig. 3.20 as a function of U. The small colored symbols in the same plot represent a scaled version of the measurements shown in Fig. 3.19 according to the "average" extrapolation law

$$E_U(\Delta\tau) = E_U(0) - 0.036\,U\Delta\tau^2 - 0.9\,\Delta\tau^4 \quad \text{(insulator)}\,, \tag{3.17}$$

which was extracted from the data shown in Fig. 3.19. The solid line in the lower part of Fig. 3.20 indicates our best fit for the extrapolated data,

$$E_\mathrm{i}(U) = -\frac{0.515}{U} - \frac{0.0027}{U-3.95} - 0.0071 + 0.00325\,U - 0.00025\,U^2\,, \tag{3.18}$$

where the index i stands for "insulator". It is evident that this particular form was not chosen for elegance. Instead, we sought a curve that is smooth both within and near the parameter range $U = 4.7\ldots6.0$, is easily differentiable analytically, and accurately represents our extrapolated QMC data. As a slight bias we also tried to produce a reasonable approximation to data for the crossover region ($T = 0.1$, $U \lesssim 4.5$). The success is evident from the upper part of Fig. 3.20 where only the difference of the extrapolated or rescaled data to the fit function is plotted. Except for very small U [where the scaling function (3.17) for the dependence on $\Delta\tau$ is no longer expected to hold], the vast majority of scaled data points deviates by less