the PSCT, NRG, and ED estimates for U_c^0 are correct (cf. Table 3.1), the MIT occurs for values of U, D, and E indicated by the large circles. These points are evidently missed by the 2OPT solutions (faint thin lines); when compared to the noninteracting values, the deviations both in D and E are, however, quite small (about 4% and 2%, respectively). Since the curves $E(U)$ and $D(U)$ are also related nontrivially by $D(U) = \mathrm{d}E(U)/\mathrm{d}U$, the construction of a consistent, smooth fit that coincides with 2OPT for small U and agrees with the insulating solutions for $U = U_c^0$ is a well-conditioned task. The correction to E has to be of third order in U (or higher) in order not to change the asymptotically correct 2OPT result for $U \to 0$. Using a plain 3rd order correction, the requirement that both E and D match for metal and insulator at a single point U_c is fulfilled for $E_m(U) = E_{2OPT}(U) + 0.0000715\, U^3$, $D_m(U) = D_{2OPT}(U) + 0.0000715 \cdot 3\, U^2$ with $U_c^0 = 5.76$ (dotted line in Fig. 3.45). A smooth modification that also satisfies that $U_c^0 \approx 5.85$ (as computed within NRG, PSCT, and ED) is given by

$$E_m(U) = E_{2OPT}(U) + 0.000062\, U^3 \big(1 + \frac{0.1}{6.5 - U}\big) \tag{3.44}$$

$$D_m(U) = D_{2OPT}(U) + 0.000062 \left(3\, U^2 \big(1 + \frac{0.1}{6.5 - U}\big) + 0.1 \frac{U^3}{(6.5 - U)^2}\right). \tag{3.45}$$

These fits are shown as short-dashed lines in Fig. 3.45. Both fit curves agree very well with extrapolations of QMC data for E to $T \to 0$ and reasonably well with extrapolations for D. The change of slope of D at U_c implied by (3.45), (3.43), and (3.19) is $a = 0.0207$. Consequently, the asymptotic behavior of the fit function $A(T)$ defined via (3.30) and (3.32) is

$$A(T) = -4.1\, T^{-1/2} + \mathcal{O}(T^0)\,. \tag{3.46}$$

Low-Temperature Specific Heat and Quasiparticle Weight

Before we construct a global fit for $A(T)$ and, ultimately, for $U_c(T)$ in subsection 3.6.3, we would like to detail the extrapolation of the QMC data to $T = 0$ which was used in Fig. 3.45. The symbols in Fig. 3.46 show QMC estimates for E in the metallic phase at low temperatures for various values of the interaction U. The solid lines represent fits of the form

$$E_m(T, U) \approx E_m^0(U) + \frac{1}{2}\gamma(U) \frac{T^2}{1 + 125\, T^2}\,, \tag{3.47}$$

i.e., with the two free parameters E_m^0 and γ for each curve. The numerical parameter 125 which controls the curvature was determined for $U = 4.6$ where the QMC data is particularly precise; the resulting functional form is clearly consistent with the remaining data as well.

The accuracy of the estimate for the linear coefficient $\gamma(U)$ of the specific heat obtained by this procedure may be checked by a comparison with the quasiparticle weight Z using the Fermi-liquid relation (valid for semi-elliptic DOS)

$$Z(T = 0, U) = \frac{2\pi}{3\, \gamma(U)}\,. \tag{3.48}$$