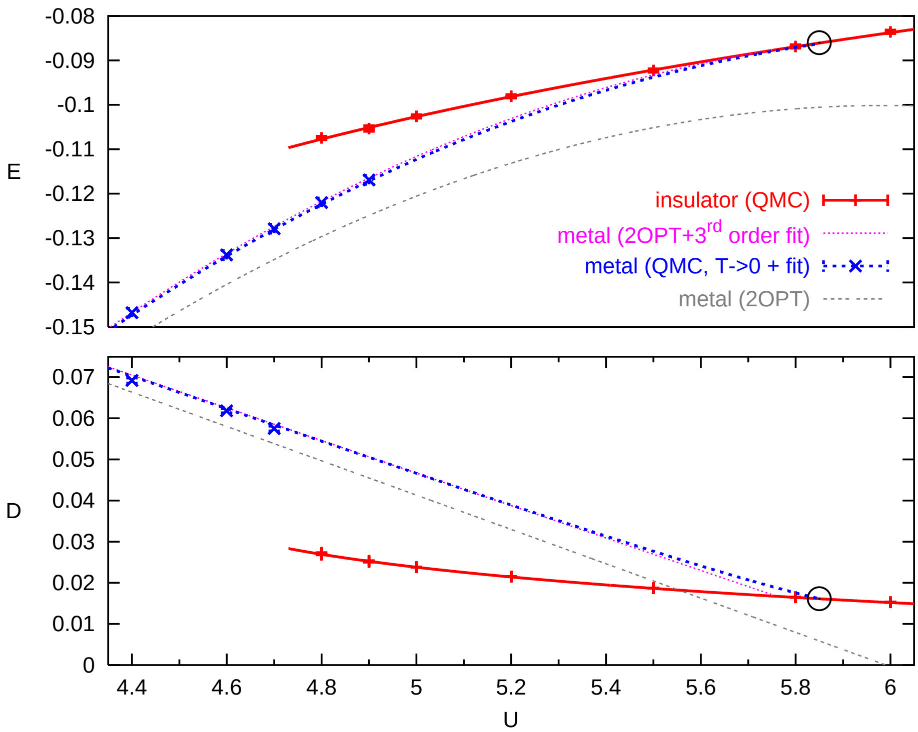

Figure 3.45: Ground state energy E and double occupancy D near the MIT. Due to the temperature-independence in the insulator, both observables can be measured using QMC without extrapolation for T in the insulating phase (upright crosses and solid lines). The accuracy of second-order perturbation theory (2OPT, thin lines) for the metallic phase can be improved significantly by using the third-order fit (3.44) for $E_{\mathrm{m}}(U)$ and the consistent expression (3.45) for $D_{\mathrm{m}}(U)$ (short-dashed lines) so that D and E match for insulator and metal at $U = U_c^0 \approx 5.85$ (circles) as predicted by PSCT. At these points, the fits yield $D = 0.01613$ and $E = -0.086$. These fits are supported by extrapolations of the QMC data for the metallic phase to $T = 0$ (slanted crosses). The dotted lines correspond to single-parameter plain third order fits (see text).

where all digits are significant and corrections are $\mathcal{O}(U^3)$. The corresponding estimate for the double occupancy is

$$D_{\mathrm{2OPT}}(U) \approx 0.25 - 0.041732\, U\,, \tag{3.43}$$

with corrections of $\mathcal{O}(U^2)$.

The important and somewhat surprising observation that we are heading for is that bare second-order perturbation theory gives a quantitatively reasonable description for E and D in the metallic phase at $T = 0$ almost up to the transition at $U_c^0 \approx 5.84$.[43] This is seen in Fig. 3.45. Here, the solid lines represent the (temperature-independent) QMC estimates for the energy and double occupancy (upper and lower plot, respectively) discussed in the previous section. Assuming that

[43] More precisely, 2OPT would break down at $U = 5.9905$ where the its estimate for D becomes negative.