Since the U dependence in (3.37) is regular for $T \to 0$ (as long as U_c^0 is finite), the same must apply to the fit function $A(T)$ defined via (3.30) and (3.32), i.e.

$$A(T) = -\sqrt{\frac{S_o}{2a}}\,T^{-1/2} + \mathcal{O}(T^0)\,. \tag{3.39}$$

Using the value of $S_0 = \ln 2$, this form can be made quantitative by evaluating the parameter a defined in (3.35) which equals the change of slope of D at $T = 0$ and $U = U_\mathrm{c}^0$ $(= U_\mathrm{c2}^0)$. The PSCT yields a parameterization for the double occupancy of the metal as $D_\mathrm{m}(T = 0) \approx 0.015 + 0.235(1 - U/U_\mathrm{c}^0) \approx 0.25 - 0.0402\,U$, where $U_\mathrm{c}^0 = 5.84$ [Georges et al. (1996), p. 71]. Since a similar parameterization for the insulator is not published, one might neglect the corresponding (much smaller) slope of $D_\mathrm{i}^0(U)$ in a first approximation.[41] We found discrepancies when trying to reconcile the corresponding estimate for a with our QMC estimates for $A(T)$ at higher T, even when realistic estimates for the slope of the double occupancy in the insulator were used. In fact, it is hardly conceivable that the above ground state estimate for D_m could be correct. The problem is that it extrapolates exactly to the correct value $D = 0.25$ for $U = 0$, but not with the correct slope -0.0417 to be derived below. Thus, the correctness of the cited parameterization near U_c^0 would imply the existence of at least two turning points of $D(U)$ within the metallic phase which appears unlikely.

Second Order Perturbation Theory and Beyond

Before we derive an independent estimate for the coefficient a on the basis of our finite-temperature QMC data, we would like to evaluate $D(U)$ within 2OPT. For a general symmetric DOS, the ground state energy at half filling is given by (van Dongen, 2000)

$$E(U) = -\frac{8}{2\pi} + \frac{U}{4} - U^2\int_0^\infty \mathrm{d}x\, g^4(x) + \mathcal{O}(U^3); \qquad g(x) := \int_0^\infty \mathrm{d}\omega\rho(\omega)\mathrm{e}^{-\omega x}\,. \tag{3.40}$$

For the Bethe DOS, the function $g(x)$ can be expressed in terms of the modified Bessel function of the first kind and the modified Struve function,

$$g(x) = \frac{I_n(2x) - L_1(2x)}{2x} \overset{x\to\infty}{\longrightarrow} \frac{1}{\pi x}\,. \tag{3.41}$$

The asymptotic behavior of g [which is most easily seen directly from (3.40)] can be used in the integral for $x_0 \gtrsim 8$.[42] The remaining finite integral is easily evaluated numerically with the total result

$$E_\mathrm{2OPT}(U) \approx -0.848826 + 0.25\,U - 0.020866\,U^2\,, \tag{3.42}$$

[41] This approach was apparently chosen when Joo and Oudovenko (2001) interpolated $T = 0$ ED data and rescaled IPT data for deriving an approximate fit form for $U_\mathrm{c}(T)$.

[42] We checked the accuracy of this approach by computing estimates for the total integral with different integer intermediate points x_0 above which the approximation for the Struve function is used. For $x_0 = 1\ldots 10$, the quadratic coefficient of $E(U)$ converges as -0.022, -0.0209, -0.02087, -0.020868, -0.020867, -0.0208663, -0.0208662, -0.0208662, -0.0208662.