tion down to $T = 0$. More precisely, we will first derive the asymptotic form of $U_c(T)$ for $T \to 0$ analytically [which implies corresponding asymptotics for $f(T,U)$] and fix its numerical parameter in a second step using various extrapolated QMC data. This procedure will not only allow for a controlled construction of the full phase diagram, but validate the internal consistency of our results and some underlying assumptions at the same time.

Consequences of Fermi Liquid Theory

As we have established in subsection 3.5.3, the energy in the (low-temperature) insulating phase is independent of the temperature.[40] By virtue of (3.21), the same applies to the entropy in this phase. In addition, S_i is independent of U; its value per lattice site equals $S_0 = \ln 2$ (Georges et al., 1996; Gebhard, 1997; Kalinowski and Gebhard, 2002). Thus, the free energy of the insulator at low T is determined by

$$E_i(T,U) = E_i^0(U); \quad S_i(T,U) = S_0 \, . \tag{3.33}$$

Fermi liquid properties imply for the metallic phase that

$$E_m(T,U) = E_m^0(U) + \frac{1}{2}\gamma(U)T^2; \quad S_m(T,U) = \gamma(U)T \, , \tag{3.34}$$

where $\gamma(U)$ is the linear coefficient of the zero-temperature specific heat. Using the projective self-consistent technique (PSCT), Moeller established that $U_c(0) = U_{c2}(0)$, i.e., that the metallic solution is always stable within the coexistence region at $T = 0$ (Moeller et al., 1995; Georges et al., 1996). According to the PSCT, the energy difference between metal and insulator vanishes quadratically for $U \to U_c^0$ while the specific heat diverges,

$$E_i^0(U) - E_m^0(U) = \frac{a}{2}(U - U_c^0)^2; \quad \gamma(U) = \frac{\gamma_0}{U_c^0 - U} \, . \tag{3.35}$$

Since the PSCT is reliable only for exponents, not for absolute prefactors, a and γ_0 should for the moment be regarded as unknown parameters. Equating the free energies, we conclude

$$0 = \Delta F(T, U_c) = \frac{a}{2}(U - U_c^0)^2 + \frac{1}{2}\gamma(U)T^2 - TS_0, \tag{3.36}$$

to obtain the low-temperature solution,

$$\boxed{U_c(T) = U_c^0 - \sqrt{\frac{2S_oT}{a}} + \mathcal{O}(T) \, .} \tag{3.37}$$

Consequently, the temperature derivative of the solution has a square root divergence at low T,

$$\frac{\mathrm{d}U_c(T)}{\mathrm{d}T} = -\sqrt{\frac{S_o}{2aT}} + \mathcal{O}(1) \, . \tag{3.38}$$

[40] Note that the temperatures under consideration are so small that exponential corrections can be safely neglected (cf. subsection 3.5.2).