3.7.1 Free Energy Functional for the Bethe Lattice

Within the DMFT, the free energy per particle can in the general homogeneous case be written as (Georges, Kotliar, and Si, 1992)

$$F = F_{\mathrm{imp}} - 2T \sum_n \Big[\ln G(i\omega_n) + \int_{-\infty}^{\infty} \mathrm{d}\epsilon\, \rho(\epsilon) \ln \big(i\omega_n + \mu - \Sigma(i\omega_n) - \epsilon \big) \Big] . \tag{3.53}$$

Here, F_{imp} is the impurity part corresponding to (1.34). We wish to extract an explicit expression for the lattice contribution. For the Bethe lattice, we have $i\omega_n + \mu - \Sigma(i\omega_n) = t^{*2}G(i\omega_n) + 1/G(i\omega_n)$. Therefore, the lattice contribution can be explicitly written in terms of the Green function $G_n \equiv G(i\omega_n)$. Its derivative reads

$$-\frac{1}{2T}\frac{\partial}{\partial G_n}(F - F_{\mathrm{imp}}) = \frac{1}{G_n} + \Big(t^{*2} - \frac{1}{G_n^2} \Big) \int_{-\infty}^{\infty} \mathrm{d}\epsilon\, \rho(\epsilon) \frac{1}{t^{*2}G_n + G_n^{-1} - \epsilon} = t^{*2} G_n . \tag{3.54}$$

Consequently, the free energy may be expressed for a semi-elliptic DOS as

$$F = F_{\mathrm{imp}} - t^{*2} T \sum_n G_n^2 . \tag{3.55}$$

For consistency with Kotliar et al. (2000) we continue the discussion in terms of the hybridization function $\Delta_n \equiv \Delta(i\omega_n) = i\omega_n + \mu - \mathcal{G}_n^{-1}$. The impurity equation (1.31) is then equivalent (at the self-consistency) to

$$G_n = \frac{1}{2T} \frac{\partial F_{\mathrm{imp}}[T, U, \Delta]}{\partial \Delta_n} . \tag{3.56}$$

Since for the Bethe lattice $\Delta_n = t^{*2} G_n$, the total free energy may also be written as a functional of the hybridization function

$$F[T, U, \Delta] = -T \sum_n \frac{\Delta_n^2}{t^{*2}} + F_{\mathrm{imp}}[T, U, \Delta] . \tag{3.57}$$

The important point is that this Ginzburg-Landau functional $F_{\mathrm{GL}} \equiv F[T, U, \Delta]$ is defined (and real valued) for an arbitrary hybridization function. While the following considerations apply for arbitrary filling, we find it convenient to introduce explicitly real-valued notation which is only valid for half filling. Using the short hand notation $O'' \equiv \mathrm{Im}\, O$ we then have

$$\big(\boldsymbol{\nabla}_{\Delta''} F \big)_n \equiv \frac{\partial F[T, U, \Delta'']}{\partial \Delta''_n} = -2T \Big(G''_n[T, U, \Delta''] - \frac{\Delta''_n}{t^{*2}} \Big) \tag{3.58}$$

$$= -2T \big(G''_{\mathrm{new}}(i\omega_n) - G''_{\mathrm{old}}(i\omega_n) \big) . \tag{3.59}$$

Here, $G''_n[T, U, \Delta''] \equiv G''_{\mathrm{new}}(i\omega_n)$ denotes the (new) solution of the impurity model for given $\Delta''_n/t^{*2} \equiv G''_{\mathrm{old}}(i\omega_n)$. Eqn. (3.59) implies that each step of a direct iteration scheme (cf. subsection 3.2.2) advances G exactly opposite to the gradient of F, i.e.,