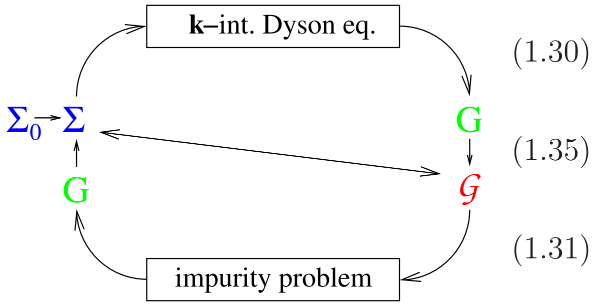

Figure 1.1: DMFT self-consistency cycle in conventional form: starting, e.g., with an initial guess for self-energy Σ, the $\boldsymbol{k}$ integrated Dyson equation (1.30) yields the lattice Green function G. Both Σ and G are used to compute the bath Green function $\mathcal{G}$ via (1.35) which defines the impurity problem (1.31). Its solution using QMC (or IPT, NCA, ED, NRG, etc.) provides a new estimate for G. The cycle is then closed by application of (1.35) to the new G and the *old* Σ. For an alternative iteration scheme, see Sec. 3.2.

in the homogeneous phase. Here, properties of the lattice only enter via the DOS $\rho(\epsilon)$ of the noninteracting electrons. The thermal average $\langle\hat{C}\rangle_{\mathcal{A}}$ of some observable $\hat{C}$ is defined as a functional integral over Grassmann variables ψ, ψ^*,

$$\langle\hat{C}\rangle_{\mathcal{A}} = \frac{1}{\mathcal{Z}}\int \mathcal{D}[\psi]\,\mathcal{D}[\psi^*]\,C[\psi,\psi^*]\,\mathrm{e}^{\mathcal{A}[\psi,\psi^*,\mathcal{G}]}, \tag{1.32}$$

using the partition function

$$\mathcal{Z} = \int \mathcal{D}[\psi]\,\mathcal{D}[\psi^*]\,\mathrm{e}^{\mathcal{A}[\psi,\psi^*,\mathcal{G}]} \tag{1.33}$$

and the single-site action

$$\mathcal{A}[\psi,\psi^*,\mathcal{G}] = \sum_{\sigma,n}\psi^*_{\sigma n}\mathcal{G}^{-1}_{\sigma n}\psi_{\sigma n} - \frac{U}{2}\sum_{\sigma\sigma'}\int_0^\beta \mathrm{d}\tau\,\psi^*_\sigma(\tau)\psi_\sigma(\tau)\psi^*_{\sigma'}(\tau)\psi_{\sigma'}(\tau)\,. \tag{1.34}$$

Here, $\beta = 1/k_{\mathrm{B}}T$ is the inverse temperature (in the following, we set $k_{\mathrm{B}} \equiv 1$) and

$$\mathcal{G}^{-1}_{\sigma n} = G^{-1}_{\sigma n} + \Sigma_{\sigma n} \tag{1.35}$$

is the effective local propagator.[20] Functions related by a Fourier transformation (here from imaginary time τ to fermionic Matsubara frequencies ω_n or vice versa) are denoted by the same symbol, but can be distinguished by their indices.

The solution of the DMFT problem by iteration is illustrated in Fig. 1.1. Here, the solution of the $\boldsymbol{k}$–integrated Dyson equation (1.30) is straightforward and can

[20] $\mathcal{G}_{\sigma n}$ may be regarded as a Weiss field in a (frequency-dependent) generalization of the usual static mean field. In contrast with spin models, for which the Weiss field replaces all (NN) interactions, the bath propagator replaces the hybridization of one site with the rest of the lattice.