a given self-energy. At a fixed point, we have

$$G[\mathcal{G}^{-1}] = \tilde{D}\big(\mathcal{G}^{-1} - \frac{1}{G[\mathcal{G}^{-1}]}\big) \tag{3.2}$$

which is equivalent to

$$\mathcal{G}^{-1} = \tilde{D}^{-1}(G[\mathcal{G}^{-1}]) + \frac{1}{G[\mathcal{G}^{-1}]}\,. \tag{3.3}$$

Eqn. (3.3) involves the inversion of the Dyson equation and (using $\mathcal{G}^{-1} = \Sigma + 1/G$) is equivalent to the self-consistency equations. Therefore, no artificial solutions are introduced in scheme (3.1). Note that (3.3) can also be read as the prescription for the "direct" iteration scheme

$$\mathcal{G}^{-1} \longrightarrow \tilde{D}^{-1}(G[\mathcal{G}^{-1}]) + \frac{1}{G[\mathcal{G}^{-1}]}\,, \tag{3.4}$$

which is illustrated in Fig. 3.5 b.

The remaining question is whether the fixed points of both iteration schemes are also (locally) stable. Only then can the iteration schemes be expected to converge at least for a sufficiently high accuracy of the impurity solver. As we will see in subsection 3.7.1, the direct scheme (3.3) can be rigorously shown to be a downhill method. It is, thus, locally convergent at least in combination with underrelaxation. While the same has not yet been shown for the scheme (3.1) used throughout this work and in most of the literature, its stability is established empirically. Numerical tests performed in this work did not indicate an enhanced stability of the metallic solution for the direct scheme. Therefore, the ability to follow metastable solutions up to their stability edge seems primarily limited by the numerical accuracy of the impurity solver.

3.2.3 Observables

Evidently, the observables most directly available within the DMFT framework are the solutions $\Sigma(i\omega_n)$ and $G(i\omega_n)$ of the self-consistency equations themselves. One closely related quantity is the quasiparticle weight also known as mass renormalization factor Z, which is defined in terms of the real-frequency self-energy,

$$Z = \frac{m}{m^*} = \frac{1}{1 - \frac{\partial}{\partial\omega}\mathrm{Re}\,\Sigma(\omega)\big|_{\omega=0}}\,. \tag{3.5}$$

In the context of QMC simulations, one usually approximates this quantity by its discrete Eliashberg estimate

$$Z \approx \frac{1}{1 - \frac{\mathrm{Im}\,\Sigma(i\omega_1)}{\pi T}}\,. \tag{3.6}$$

Due to the rules for complex derivatives, both definitions agree in the limit $T \to 0$ as long as the Luttinger theorem is fulfilled, i.e., for $\mathrm{Im}\,\Sigma(\omega = 0) = 0$. For $U \to 0$, no mass renormalization takes place so that $Z = 1$. With increasing U, Z decreases until the quasiparticle peak (in the spectrum) vanishes. Extending the Fermi liquid picture,