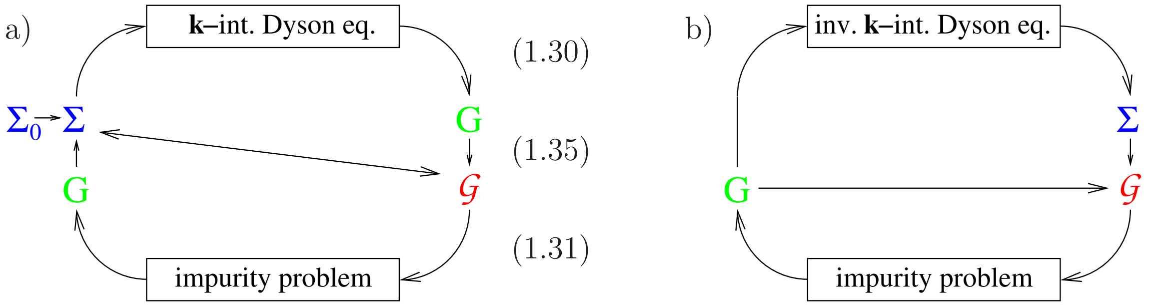

Figure 3.5: a) Conventional DMFT self-consistency cycle, replicated from Fig. 1.1. **b)** More direct iteration scheme, using the inverted lattice Dyson equation.

energy (which would be obtained by a full summation over the Hubbard-Stratonovich field). Our solution of this problem and its results will be discussed in Sec. 3.6.

3.2.2 Convergence of Fixed Point Methods

As discussed above and in Sec. 1.3, solutions are obtained within the DMFT in an iterative process. Evidently, there is a considerable degree of freedom for choosing a particular scheme. The conventional choice Fig. 3.5 a (here replicated from Fig. 1.1) is numerically convenient since an explicit inversion of the lattice Dyson equation is avoided. Its general usage in the literature implies the assumption that it converges to all solutions of the self-consistency equations if initialized appropriately and in the limit of high precision; i.e., that all solutions of the self-consistency equations are stable fixed points of the iteration scheme. This is, however, by no means guaranteed.[7] The only property that every iteration scheme fulfills by construction is that solutions of the self-consistency equations are (possibly unstable) fixed points. Hence, the iteration procedure for determining U_{c1} and U_{c2} can break down before the solutions themselves become thermodynamically unstable; as a consequence, the width of the coexistence region may be underestimated. At first sight, the iteration scheme Fig. 3.5 a might even imply the danger of introducing additional solutions since it incorporates a two-stage relaxation scheme: both the solution of the impurity problem and the solution of the Dyson equation are combined with old data for the next step in each cycle. Still, a full iteration may be written exclusively in terms of the "old" bath Green function which is updated as

$$\mathcal{G}^{-1} \longrightarrow \mathcal{G}^{-1} - \frac{1}{G[\mathcal{G}^{-1}]} + \frac{1}{\tilde{D}\big(\mathcal{G}^{-1} - \frac{1}{G[\mathcal{G}^{-1}]}\big)}\,. \tag{3.1}$$

Here, $G[\mathcal{G}^{-1}]$ denotes the solution of the impurity problem for given $\mathcal{G}^{-1}$, $\tilde{D}(\Sigma)$ denotes the solution of the lattice Dyson equation, i.e., the Hilbert transform for

[7] As a simple example, consider the reversal of any (locally) convergent scheme which clearly cannot converge to the same fixed point.