downhill.[46] If $\nabla_\Delta F$ changes slowly on the scale of the step length, we can approximate the change in F by the first term in a Taylor expansion:

$$F_{\rm new} \approx F_{\rm old} - 2\,T\,t^{*2} \sum_n \left(G''_{\rm new}(i\omega_n) - G''_{\rm old}(i\omega_n)\right)^2 < F_{\rm old}\,. \tag{3.60}$$

Consequently, the free energy of the new solution is lower for sufficiently small step size.

As a slightly alternative derivation of an equivalent result, let us consider the second derivative of the free energy functional:

$$\frac{t^{*2}}{2T}\frac{\partial^2 F[T,U,\Delta]}{\partial\Delta''_n\partial\Delta''_m} = -t^{*2}\frac{\partial G''_n}{\partial\Delta''_m} + \delta_{mn} \tag{3.61}$$

$$\frac{\partial G''_{\rm new}(i\omega_n)}{\partial G''_{\rm old}(i\omega_m)} = \delta_{mn} - \frac{t^{*2}}{2T}\left.\frac{\partial^2 F[T,U,\Delta]}{\partial\Delta''_n\partial\Delta''_m}\right|_{\Delta=G_{\rm old}}\,. \tag{3.62}$$

Since the matrix of the second derivatives on the right hand side has only positive eigenvalues[47] near a minimum of F, the fixed point method is contracting (as long as all eigenvalues are smaller than $4T/t^{*2}$) and is, thus, convergent to thermodynamically (locally) stable solutions. Another interesting consequence of these considerations for the iteration process is that the error decreases exponentially for the direct scheme in the neighborhood of a solution Δ_0 where the free energy is quadratic in $\Delta - \Delta_0$. We have derived, but omit, the equivalent to (3.62) for the conventional iteration scheme (3.1). In this case, the iteration definitely does not proceed downhill and, therefore, coexistence regions might indeed be underestimated. After noting the connection between convergence properties of iteration schemes and the behavior of the free energy functional, we performed additional numerical simulations in the coexistence region using the direct scheme. These indicated, however, no significant increase in the resulting estimate for U_{c2} in comparison to the conventional iteration scheme.

3.7.2 Direct Evaluation of Free Energy Differences

Another important consequence of the discussion of subsection 3.7.1 is that the gradient of the free energy with respect to the hybridization function Δ may be integrated along a line between two solutions (for fixed U and T). The result is then nothing but their free energy difference. The integration curve is arbitrary (within a subspace compatible with analytic constraints on $\Delta(i\omega_n)$); a convenient choice is a straight line, i.e., a convex linear combination of the converged Green functions. For metallic and insulating solutions denoted by subindex "m" and "i", respectively, we define

$$\Delta_\lambda := t^{*2}G_{\rm m} + \lambda t^{*2}(G_{\rm i} - G_{\rm m}); \quad 0 \le \lambda \le 1\,. \tag{3.63}$$

[46] While this is strictly true only for an exact solution of the impurity model, the statistical noise cancels out on average due to the linear dependence for a numerically exact method like QMC. The asymptotic noise in the solution decreases with increasing accuracy, i.e., an increasing number of sweeps. Only in the case of multiple solutions, fixpoints may be lost due to too much noise.

[47] Note the advantage of our explicitly real-valued formalism at this point: written in terms of $\Delta_n = i\Delta''_n$ all eigenvalues would be negative, which we found counter-intuitive.