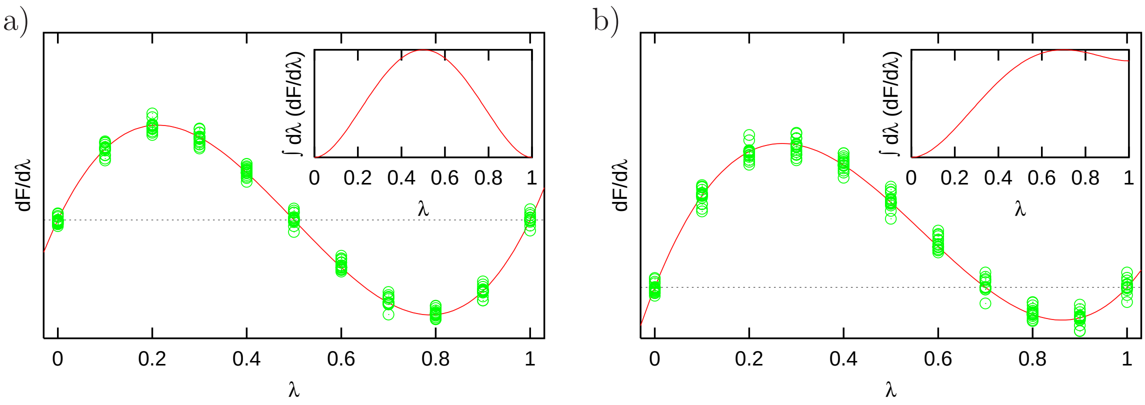

Figure 3.58: Illustration of an algorithm for direct evaluation of the free energy difference between two solutions A and B. Intermediate solutions are generated on a line $0 \leq \lambda \leq 1$, where $\lambda = 0$ corresponds to solution A and $\lambda = 1$ to solution B. The derivative $\mathrm{d}F/\mathrm{d}\lambda$ is computed on a grid λ_i (circles) by solving a series of specially constructed impurity models using, e.g., QMC. Integration (insets) then yields the difference in free energy (measured from solution A). **a)** Possible result for a phase point on the first order line, where both solutions A and B have the same free energy; **b)** for a phase point where A has the higher free energy.

Then, the free energy difference is given by the integral

$$F_\mathrm{i} - F_\mathrm{m} = \int_0^1 \mathrm{d}\lambda \, \frac{\mathrm{d}F}{\mathrm{d}\lambda} \,, \tag{3.64}$$

where

$$\frac{\mathrm{d}F}{\mathrm{d}\lambda} = -2T \sum_n \left(t^{*2} G''[T, U, \Delta_\lambda](i\omega_n) - \Delta''_\lambda(i\omega_n) \right) \left(G''_\mathrm{i}(i\omega_n) - G''_\mathrm{m}(i\omega_n) \right) \tag{3.65}$$

and which may be evaluated on a grid. When on each grid point multiple QMC measurements $G[T, U, \Delta_\lambda]_i$ are performed, even the error of the projection of the gradient in the "solution direction" may be evaluated so that a corresponding (statistical) error for the free energy difference is easily computed. Note that given the two converged solutions, the computation of the free energy difference within this scheme is completely parallel since no more self-consistency is involved. Another practical advantage of this method is that it checks the convergence of the existing solutions. This is illustrated in Fig. 3.58, a made-up example. Green circles indicate QMC estimates of the true derivative (solid line) of the free energy along the integration line. The limiting solutions (at $\lambda = 0$ and $\lambda = 1$) are indeed stable (gradient vanishes with positive slope), at least along the interpolation direction. The position of the intermediate fixed point only indicates a maximum of F in the one-dimensional subspace under consideration; in general it will not correspond to a true maximum of F. Integrating up the solution (insets) shows that in Fig. 3.58 a both solutions are