3.4.1 Fourier Transformation and Smoothing

A QMC simulation within the DMFT framework consists of a simultaneous solution of two principal equations: the lattice Dyson equation (1.30) and the defining expression for the impurity Green function (1.31). The IPT and QMC solutions of the impurity problem are formulated in imaginary time, i.e., the bath Green function $\mathcal{G}$ is needed as function of τ and the result is expressed as $G(\tau)$. In contrast, the Dyson equation is formulated (and is local) in the frequency domain, here for Matsubara frequencies $i\omega_n = i(2n+1)\pi T$. Therefore, two Fourier transformations (from frequency to imaginary time and vice versa) per self-consistency cycle are necessary, which for G read

$$G(i\omega_n) = \int_0^\beta d\tau \, e^{i\omega_n \tau} \, G(\tau) \tag{3.12}$$

$$G(\tau) = \frac{1}{\beta} \sum_{n=-\infty}^{\infty} e^{-i\omega_n \tau} \, G(i\omega_n) \, . \tag{3.13}$$

Note that (3.13) implies antiperiodicity of $G(\tau)$ for translations β (since $e^{i\omega_n \beta} = -1$) and allows for a discontinuity of $G(\tau)$ (at $\tau = 0$) since the number of terms is infinite. The spectral representation of G implies a decay of $G(i\omega_n)$ as $1/i\omega_n$ for $|n| \to \infty$ like for any normalized analytic function. Furthermore, $G(i\omega_n)$ is purely imaginary when $G(\tau) = G(\beta - \tau)$ as in the case of interest.

Discretization Problem

Numerically, however, the integral in (3.12) needs to be discretized and the Matsubara sum in (3.13) has to be truncated. Since the numerical effort in QMC scales with the number $\Lambda = \beta/\Delta\tau$ of discretized time slices at least[14] as Λ^3, this method is presently restricted to $\Lambda \lesssim 400$. Typically, 200 time slices and less are used. A naive discrete version of the Fourier transform,

$$\tilde{G}(i\omega_n) = \Delta\tau \Big(\frac{G(0) - G(\beta)}{2} + \sum_{l=1}^{\Lambda-1} e^{i\omega_n \tau_l} \, G(\tau_l) \Big); \quad \tau_l := l\Delta\tau \tag{3.14}$$

$$\tilde{G}(\tau_l) = \frac{1}{\beta} \sum_{n=-\Lambda/2}^{\Lambda/2-1} e^{-i\omega_n \tau_l} \, G(i\omega_n) \, , \tag{3.15}$$

fails for such a coarse grid. The problems are that the Green function $\tilde{G}(\tau)$ estimated from a finite Matsubara sum can not be discontinuous at $\tau = 0$ (as required analytically for $G(\tau)$) while the discrete estimate $\tilde{G}(i\omega_n)$ oscillates with periodicity $2\pi i\Lambda/\beta$ instead of decaying for large frequencies. This implies a large error of $G(i\omega_n)$ when $|\omega_n|$ approaches or exceeds the Nyquist frequency $\pi\Lambda/\beta$. Both (related) effects would

[14] In practice, the scaling is even worse on systems with a hierarchy of memory systems of increasing capacity and decreasing speed.