through the full spin field, i.e., by attempting to flip spins s_0 through $s_{\Lambda-1}$ one after the other and then starting the next sweep. Roughly, the number of such sweeps has to be held constant (rather than the number of attempted single-spin flips) for constant statistical error when the number of spins Λ is varied. Since the systematic error depends on $\Delta\tau$, the necessary number of time slices is proportional to the inverse temperature, $\Lambda \propto \beta$, so that the total numerical cost for given accuracy is proportional to β^3.

In this work, up to $\Lambda = 400$ time slices and up to 10^7 measurement sweeps were used. A single iteration for $\Lambda = 400$ with 200000 sweeps took more than 7 CPU hours on a Cray T90. Since typically 10-20 iterations are needed for well-converged solutions (even when initializing the runs with data obtained for larger $\Delta\tau$), the computation of each such data point took several weeks of real time and used up about a monthly contingent of supercomputer time. No minus-sign problem was encountered, i.e., the sign in (1.51) and (1.52) was always positive.

1.4 Maximum Entropy Method

Within the DMFT, all single-particle properties can be expressed in terms of the local single-particle spectral function (also called "full" or "interacting" density of states) which is proportional to the imaginary part of the local retarded Green function,

$$A(\omega) = -\frac{1}{\pi}\,\mathrm{Im}\,G(\omega + i0^+)\,. \tag{1.54}$$

The spectral function $A(\omega)$ is accessible experimentally: measured (angular averaged) photoemission spectra (PES) can under certain simplifying assumptions (see subsection 5.4.1) be identified with $A(\omega)$ multiplied by the Fermi function $n_{\mathrm{f}}(\omega - \mu)$. Correspondingly, inverse photoemission spectra or X-ray absorption spectra (XAS) can be identified with $A(\omega)$ multiplied by $1 - n_{\mathrm{f}}(\omega - \mu)$. Furthermore, nonlocal spectral functions and the optical conductivity $\sigma(\omega)$ can, within the DMFT, be calculated from $A(\omega)$ (see chapter 4).

In QMC calculations, however, the Green function G (and thus the spectral function $A(\omega)$) cannot be directly computed on the real axis. Instead, real-time dynamical information has to be extracted from imaginary-time data $G(\tau)$ (or, equivalently, from the Fourier transformed Matsubara-frequency data $G(i\omega_n)$) via analytic continuation. This is in principle possible through inversion of the spectral representation for $G(\tau)$, i.e.,

$$G(\tau) \;=\; \int_{-\infty}^{\infty} \mathrm{d}\omega\; K(\tau, \omega - \mu; \beta)\; A(\omega)\,, \tag{1.55}$$

$$K(\tau, \omega; \beta) \;:=\; \frac{\exp(-\tau\omega)}{1 + \exp(-\beta\omega)}\,, \tag{1.56}$$

but poses an ill-conditioned problem since $G(\tau)$ is only measured on a grid $\tau_l = l\Delta\tau$ (where $\Delta\tau = \beta/\Lambda$) and since the kernel (1.56) becomes exponentially small for generic