1.3 Quantum Monte Carlo Algorithm

In this section, we will discuss the auxiliary-field quantum Monte Carlo (QMC) algorithm used in this work for solving the impurity model (1.31). It was originally formulated for treating a small number of magnetic impurities in metals (Hirsch and Fye, 1986) and later applied to arbitrary hybridization functions, i.e., in the form required for the solution of the DMFT problem (Jarrell, 1992; Rozenberg, Zhang, and Kotliar, 1992; Georges and Krauth, 1992; Ulmke, Janiš, and Vollhardt, 1995). Before we discuss technical details, let us point out some general important consequences of using this particular method for solving the impurity problem: First of all, the QMC method is formulated in imaginary time, i.e., $G(\tau)$ is evaluated (as a functional of $\mathcal{G}(\tau)$ and the model parameters) which implies that dynamical information can be obtained directly only for imaginary Matsubara frequencies and that analytic continuation is required for getting information, e.g., the spectrum, at real frequencies (see Sec. 1.4). A second implication is that Fourier transforms are necessary in order to connect the imaginary-time impurity part with the Dyson equations (1.30) and (1.35) which are diagonal in frequency space. Finally, the QMC method introduces a discretization $\Delta\tau$ of the imaginary time β which not only necessitates an extrapolation of all DMFT(QMC) results to the physical limit $\Delta\tau \to 0$ (using converged DMFT solutions for different values of $\Delta\tau$) and restricts the method to relatively high temperatures, but also complicates the Fourier transformations. Here, we will concentrate on the solution of the impurity problem and discuss problems related to the Fourier transforms in Sec. 3.4. We also specialize to the single-band homogeneous case; for the generalization to the multi-band cases used in chapter 5, we refer to the literature (Rozenberg, 1997; Han, Jarrell, and Cox, 1998; Held and Vollhardt, 1998).

1.3.1 Wick's Theorem for the Discretized Impurity Problem

The difficulty in solving the functional integral equation (1.31) arises from the non-commutativity of the kinetic term and the interaction term in the single-site action (1.34). These terms can be separated by use of the Trotter-Suzuki formula (Trotter, 1959; Suzuki, 1976) for operators $\hat{A}$ and $\hat{B}$:

$$\mathrm{e}^{-\beta(\hat{A}+\hat{B})} = \left(\mathrm{e}^{-\Delta\tau\hat{A}}\,\mathrm{e}^{-\Delta\tau\hat{B}}\right)^{\Lambda} + \mathcal{O}(\Delta\tau)\,, \tag{1.37}$$

where $\Delta\tau = \beta/\Lambda$ and Λ is the number of (imaginary) time slices.[23] Rewriting the action (1.34) in discretized form

$$\begin{aligned}\mathcal{A}_\Lambda[\psi,\psi^*,\mathcal{G},U] \;&=\; (\Delta\tau)^2 \sum_\sigma \sum_{l,l'=0}^{\Lambda-1} \psi^*_{\sigma l}(\boldsymbol{\mathcal{G}}_\sigma^{-1})_{ll'}\,\psi_{\sigma l'} \\ &\quad -\Delta\tau U \sum_{l=0}^{\Lambda-1} \psi^*_{\uparrow l}\,\psi_{\uparrow l}\,\psi^*_{\downarrow l}\,\psi_{\downarrow l},\end{aligned} \tag{1.38}$$

[23] Since $\beta = 1/k_B T$ is the inverse temperature, small $\Delta\tau$ on each "time slice" corresponds to a higher temperature, for which the operators effectively decouple. Thus, we may view the Trotter approach as a numerical extension of a high-temperature expansion to lower temperatures.