and the process is ergodic (i.e., all configurations can be reached from some starting configuration), the distribution of configurations of the chain approaches the target distribution in the limit of infinite chain length. Since the normalization remains unknown, importance sampling by a Markov process can only yield ratios of different observables evaluated on the same chain of configurations. Another consequence of using a Markov process is that initial configurations have to be excluded from averages since the true associated probabilities might be vanishingly small. They would otherwise be overrepresented in any run of finite length. Consequently, we will later distinguish "warmup sweeps" from "measurement sweeps".

For the computation of errors, one has to take into account the finite autocorrelation induced by the Markov process, i.e., correlation between subsequent measurements. This correlaton may be characterized by the autocorrelation time[26] $\kappa_o \geq 1$ which effectively reduces the number of independent samples, so that $\Delta X = c\sqrt{v_o \kappa_o / N}$. The numerical effort necessary to reach some target statistical accuracy ΔX nevertheless increases only as $(1/\Delta X)^2$.

Returning to the evaluation of the Green function using (1.43) and (1.44), the obvious choice is to sample configurations $\{s\}$ according to the (unnormalized) probability

$$P(\{s\}) = \left| \det \boldsymbol{M}_\uparrow^{\{s\}} \det \boldsymbol{M}_\downarrow^{\{s\}} \right| . \tag{1.50}$$

The Green function can then be calculated as an average $\langle \dots \rangle_s$ over these configurations:

$$G_{\sigma l l'} = \frac{1}{\tilde{\mathcal{Z}}} \left\langle \left(\boldsymbol{M}_\sigma^{\{s\}}\right)^{-1}_{ll'} \operatorname{sign}\left(\det \boldsymbol{M}_\uparrow^{\{s\}} \det \boldsymbol{M}_\downarrow^{\{s\}}\right) \right\rangle_s , \tag{1.51}$$

$$\tilde{\mathcal{Z}} = \left\langle \operatorname{sign}\left(\det \boldsymbol{M}_\uparrow^{\{s\}} \det \boldsymbol{M}_\downarrow^{\{s\}}\right) \right\rangle_s . \tag{1.52}$$

Here, $\tilde{\mathcal{Z}}$ deviates from the full partition function by an unknown prefactor which cancels in (1.51). The inability to compute the partition function is a consequence of the importance sampling and is thus a general characteristic of QMC methods. This will have severe consequences for the study of phase transitions (see chapter 3).

In this work, the transition probability is chosen according to the Metropolis transition rule (Metropolis, Rosenbluth, Rosenbluth, Teller, and Teller, 1953)[27]

$$\mathcal{P}(x \to y) = \min\{1, P(y)/P(z)\} \tag{1.53}$$

for transitions from a spin configuration x to a configuration y, which clearly fulfills detailed balance (1.49). Configuration updates are always performed by sweeping

[26] For a set $\{o_1, o_2, \dots, o_N\}$ of measurements, the autocorrelation function (for the observable o) is $c^o_l = \langle (o_k - \langle o \rangle)(o_{k+l} - \langle o \rangle) \rangle_k$. An associated autocorrelation time may then be defined as $\kappa_o = c^o_0 + 2\sum_{l=1}^{N_0} c^o_l$, where the cutoff N_0 is determined by $c^o_l > 0$ for $l \leq N_0$ and $c_{N_0+1} < 0$.

[27] Since in the present problem most of the computational cost is associated with the spin update and only has to be paid for accepted spin flips, the Metropolis rule, which has the highest acceptance ratio compatible with detailed balance, might not be optimal. Our tests with the symmetric heat-bath rule and generalizations of it which further suppress transitions between states with similar probability did not, however, lead to significant saving of computer time at constant accuracy.