9

Reptation Quantum Monte Carlo

9.1 A Simple Path Integral Technique

In Chapter 8, we described the Green's function Monte Carlo (GFMC) in which the ground-state wave function is filtered out by using the power method. There, the projection technique is statistically implemented by introducing walkers that are labelled by the electron configuration $|x\rangle$ and the weight w. Then, we have seen that it is possible to solve the problem of the exponential growth of the weights by considering many walkers and iteratively propagate them with approximately the same weight. Although this kind of Monte Carlo approach is largely used, it may become inefficient when the number of walkers, which are necessary to carry out the simulation, becomes too large. This usually happens when the wave function used for the importance sampling is not particularly accurate. In addition, an exceedingly large number of walkers may be necessary for a large number of forward projections. For these reasons, the reptation quantum Monte Carlo (RQMC) algorithm has been introduced, as a simple and efficient way to perform a projection method within a path-integral representation (Baroni and Moroni, 1998; Moroni and Baroni, 1999). The main advantage of the RQMC is that it requires only one walker without any weight, as in the variational Monte Carlo method, thus allowing us to compute correlation functions, even for large projection times. However, in this case, the autocorrelation time may become very large.

The aim of the RQMC approach is to define a Markov process that allows us to sample:

$$\mathcal{Z} = \langle \Psi_{\text{var}} | (\Lambda - \mathcal{H})^N | \Psi_{\text{var}} \rangle, \tag{9.1}$$

where $|\Psi_{\text{var}}\rangle$ is a given initial state (for example the best variational *Ansatz*) from which the projection with N steps is performed (as usual Λ is a diagonal operator with $\Lambda_{x,x} = \lambda$, where λ is a sufficiently large number to guarantee the convergence to the ground state). Notice that, in contrast to the GFMC method, which

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is defined by Eq. (8.2), here the projection is done for a *fixed* number N of steps (and then the overlap with the initial state is computed). Within RQMC, $\mathcal{Z}$ plays the role of a pseudo-partition function that defines *classical* averages. Indeed, a natural representation of $\mathcal{Z}$ is given by using a discrete path integral representation (where the integral over different paths is substituted by sums over configurations); then, physical quantities will be written as classical averages by using this pseudo-partition function.

As for the variational and the GFMC approaches (see Chapters 5 and 8), we fix a complete basis set $\{|x\rangle\}$ in the many-body Hilbert space:

$$\sum_x |x\rangle\langle x| = \mathbb{I}, \tag{9.2}$$

in which the states are taken to be *orthogonal* and *normalized*. Furthermore, we assume that the matrix elements of the Hamiltonian in this basis $\mathcal{H}_{x',x} = \langle x'|\mathcal{H}|x\rangle$ can be computed efficiently for each $|x\rangle$ and $|x'\rangle$. For a local Hamiltonian, the number of non-zero entries $\mathcal{H}_{x',x}$ is extremely small compared to their total number; indeed, for a given $|x\rangle$, the number of non-zero matrix elements is of the order of the system size L, and not of the full Hilbert space. Therefore, for a given state $|x\rangle$, all entries $\mathcal{H}_{x',x}$ can be computed with a reasonable computational effort.

By inserting $N+1$ completeness relations for the chosen orthonormal basis, the pseudo-partition function $\mathcal{Z}$ is written as a path integral over N time slices:

$$\mathcal{Z} = \sum_{x_0,\ldots,x_N} \mathcal{W}(x_N,\ldots,x_0); \tag{9.3}$$

here, the weight $\mathcal{W}(x_N,\ldots,x_0)$ is defined by:

$$\mathcal{W}(x_N,\ldots,x_0) = \mathcal{G}_{x_N,x_{N-1}}\ldots\mathcal{G}_{x_2,x_1}\mathcal{G}_{x_1,x_0}\Psi^2_{\text{var}}(x_0), \tag{9.4}$$

where $\Psi_{\text{var}}(x) = \langle x|\Psi_{\text{var}}\rangle$ and, in analogy with the GFMC approach, we have defined the Green's function $\mathcal{G}_{x',x}$ with importance sampling:

$$\mathcal{G}_{x',x} = \langle x'|(\Lambda - \mathcal{H})|x\rangle \frac{\Psi_{\text{var}}(x')}{\Psi_{\text{var}}(x)}. \tag{9.5}$$

Thereafter, in order to simplify the notation, we do not put a tilde over the various quantities with importance sampling.

Similarly to the GFMC approach, in order to have a non-negative weight $\mathcal{W}(x_N,\ldots,x_0)$, it is necessary to have that *all* matrix elements of the Green's function $\mathcal{G}_{x',x}$ are non-negative. Whenever some couples (x',x) give $\mathcal{G}_{x',x} < 0$, we face the *sign problem*, which will be discussed in Chapter 10.

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9.1.1 Ground-State Energy and Correlation Functions

The ground-state energy and correlation functions of local operators can be written in terms of the pseudo-partition function $\mathcal{Z}$. For example, the ground-state energy can be estimated (for large enough N) by:

$$E_0 \approx \frac{\langle \Psi_{\rm var}|\mathcal{H}\mathcal{G}^N|\Psi_{\rm var}\rangle}{\langle \Psi_{\rm var}|\mathcal{G}^N|\Psi_{\rm var}\rangle} = \frac{1}{\mathcal{Z}} \sum_{x_0,\ldots,x_N} e_L(x_N)\mathcal{W}(x_N,\ldots,x_0), \tag{9.6}$$

where, as for the GFMC technique, the local energy is defined by:

$$e_L(x) = \frac{\langle \Psi_{\rm var}|\mathcal{H}|x\rangle}{\langle \Psi_{\rm var}|x\rangle}. \tag{9.7}$$

A slightly better estimation of the ground-state energy can be obtained by noticing that $\mathcal{H}$ commutes with $\mathcal{G}$ in Eq. (9.6), so that:

$$E_0 \approx \frac{1}{\mathcal{Z}} \sum_{x_0,\ldots,x_N} \left[\frac{e_L(x_0)+e_L(x_N)}{2}\right] \mathcal{W}(x_N,\ldots,x_0). \tag{9.8}$$

Similarly, for local operators that are diagonal in the basis set, i.e., $\mathcal{O}|x\rangle = \mathcal{O}(x)|x\rangle$, where $\mathcal{O}(x)$ is the eigenvalue corresponding to the configuration $|x\rangle$, we have that:

$$\frac{\langle \Psi_{\rm var}|\mathcal{G}^M\mathcal{O}\mathcal{G}^{N-M}|\Psi_{\rm var}\rangle}{\langle \Psi_{\rm var}|\mathcal{G}^N|\Psi_{\rm var}\rangle} = \frac{1}{\mathcal{Z}} \sum_{x_0,\ldots,x_N} \mathcal{O}(x_{N-M})\mathcal{W}(x_N,\ldots,x_0). \tag{9.9}$$

Therefore, quantum expectation values are written in terms of a *classical* probability $\mathcal{W}(x_N,\ldots,x_0)$ that depends upon the *reptile* (or *polymer*) defined by all the configurations from x_0 to x_N along the projection:

$$\mathcal{R} \equiv (x_N,\ldots,x_0). \tag{9.10}$$

A picture of the reptile is reported in Fig. 9.1.

9.2 A Simple Way to Sample Configurations

In order to evaluate the ground-state energy and correlation functions, we can consider a Markov process with the Metropolis algorithm to sample the classical weight $\mathcal{W}(\mathcal{R})$. We define two basic moves $\mathcal{R} \to \mathcal{R}'$ that shift the reptile on the right or left, adopting the convention that the right (left) move is denoted by $d = +1$ ($d = -1$), see Fig. 9.1. In the simplest RQMC sampling, the variable d is chosen randomly at each step with equal probability for left or right moves. We denote by $T(\mathcal{R}', d'|\mathcal{R}, d)$ the transition probability that defines the proposed move within the

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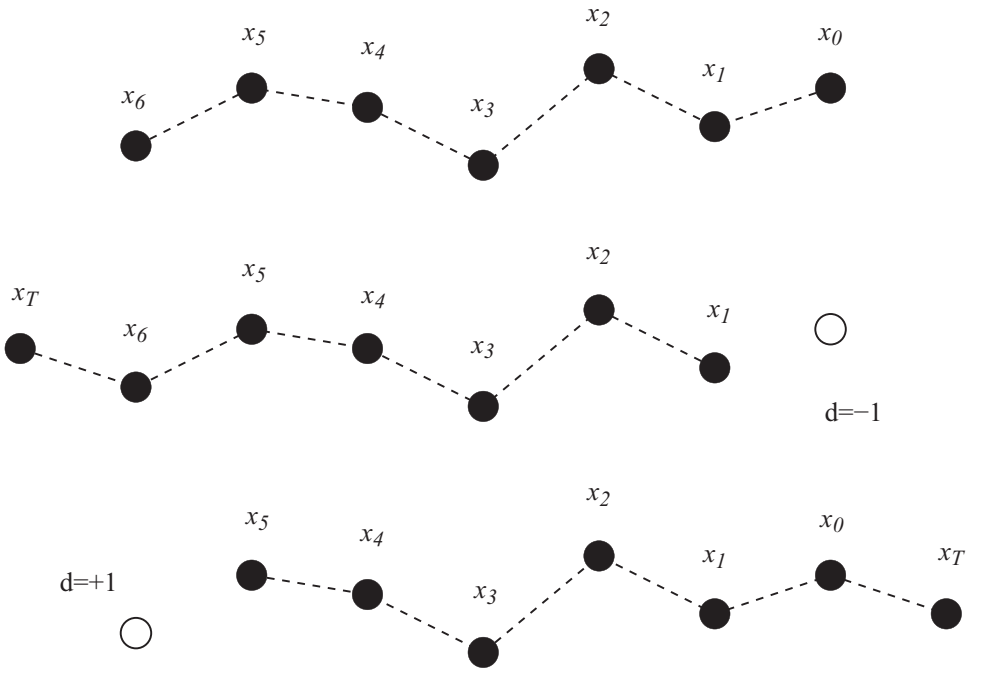

Figure 9.1 Pictorial representation of the reptile $\mathcal{R}$ defined by all the configurations from x_0 to x_N (here $N = 6$). The new reptile $\mathcal{R}'$ is generated from the old one performing left/right moves where a new head/tail is added and the old tail/head is discarded.

Metropolis algorithm. Since the new direction d' is chosen randomly with equal probability for left and right moves, regardless the actual value of d, we have:

$$T(\mathcal{R}', d'|\mathcal{R}, d) = \frac{1}{2} t^{(d')}(\mathcal{R}'|\mathcal{R}), \tag{9.11}$$

where $t^{(d')}(\mathcal{R}'|\mathcal{R})$ defines a change of the reptile $\mathcal{R} \to \mathcal{R}'$ for a given direction d'. The acceptance probability $a^{(d')}(\mathcal{R}'|\mathcal{R})$ can be obtained by exploiting the detailed balance condition:

$$t^{(d')}(\mathcal{R}'|\mathcal{R}) a^{(d')}(\mathcal{R}'|\mathcal{R}) \mathcal{W}(\mathcal{R}) = t^{(d)}(\mathcal{R}|\mathcal{R}') a^{(d)}(\mathcal{R}|\mathcal{R}') \mathcal{W}(\mathcal{R}'); \tag{9.12}$$

in this equation $d = -d'$ because the reverse move is possible only by changing the direction of the propagation d. Then, within the Metropolis algorithm, the acceptance probability is given by:

$$a^{(d')}(\mathcal{R}'|\mathcal{R}) = \text{Min}\left[1, r^{(d')}(\mathcal{R}', \mathcal{R})\right], \tag{9.13}$$

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where

$$r^{(d')}(\mathcal{R}', \mathcal{R}) = \frac{\mathcal{W}(\mathcal{R}')t^{(-d')}(\mathcal{R}|\mathcal{R}')}{\mathcal{W}(\mathcal{R})t^{(d')}(\mathcal{R}'|\mathcal{R})}. \tag{9.14}$$

Within this approach, the probability distribution of the reptile evolves along the Markov iteration n according to:

$$\mathcal{P}_{n+1}(\mathcal{R}', d') = \sum_{\mathcal{R},d} K(\mathcal{R}', d'|\mathcal{R}, d)\mathcal{P}_n(\mathcal{R}, d), \tag{9.15}$$

where the full transition probability is given by:

$$K(\mathcal{R}', d'|\mathcal{R}, d) = T(\mathcal{R}', d'|\mathcal{R}, d)a^{(d')}(\mathcal{R}'|\mathcal{R}). \tag{9.16}$$

Notice that the full transition probability satisfies the detailed balance:

$$K(\mathcal{R}', d'|\mathcal{R}, d)\mathcal{W}(\mathcal{R}) = K(\mathcal{R}, d|\mathcal{R}', d')\mathcal{W}(\mathcal{R}'), \tag{9.17}$$

which can be easily verified by using Eqs. (9.11) and (9.12). After a thermalization time, e.g., for large n, $\mathcal{P}_n(\mathcal{R}, d)$ converges to the desired equilibrium probability $\mathcal{P}_{\text{eq}}(\mathcal{R}) \equiv \mathcal{W}(\mathcal{R})/(2\mathcal{Z})$, see section 3.8.

In the following, we decompose the Green's function $\mathcal{G}$ as already done within the GFMC approach, i.e., $\mathcal{G}_{x',x} = p_{x',x}b_x$, such that the classical weight becomes:

$$\mathcal{W}(\mathcal{R}) = p_{x_N,x_{N-1}} \dots p_{x_2,x_1}p_{x_1,x_0}b_{x_{N-1}} \dots b_{x_1}b_{x_0}\Psi^2_{\text{var}}(x_0), \tag{9.18}$$

and discuss in detail the two right/left moves. Let us start with $d = +1$ (right move). In this case:

$$\mathcal{R}' = (x'_N, \dots, x'_0) \equiv (x_{N-1}, \dots, x_0, x_T), \tag{9.19}$$

where x_T is the trial move at the rightmost side of the reptile. The transition probability of this process is:

$$t^{(+1)}(\mathcal{R}'|\mathcal{R}) = p_{x_T,x_0}. \tag{9.20}$$

The corresponding weight on the new reptile $\mathcal{R}'$ is given by:

$$\mathcal{W}(\mathcal{R}') = p_{x_{N-1},x_{N-2}} \dots p_{x_1,x_0}p_{x_0,x_T}b_{x_{N-2}} \dots b_{x_0}b_{x_T}\Psi^2_{\text{var}}(x_T). \tag{9.21}$$

Thus in the ratio $\mathcal{W}(\mathcal{R}')/\mathcal{W}(\mathcal{R})$, which is required to implement the Metropolis algorithm, almost all factors cancel out, yielding:

$$\frac{\mathcal{W}(\mathcal{R}')}{\mathcal{W}(\mathcal{R})} = \frac{b_{x_T}p_{x_0,x_T}\Psi^2_{\text{var}}(x_T)}{b_{x_{N-1}}p_{x_N,x_{N-1}}\Psi^2_{\text{var}}(x_0)} = \frac{b_{x_0}p_{x_T,x_0}}{b_{x_{N-1}}p_{x_N,x_{N-1}}}, \tag{9.22}$$

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where we used that $\mathcal{G}_{x',x} = p_{x',x} b_x$ is the Green's function with importance sampling that satisfies $\mathcal{G}_{y,x} = \mathcal{G}_{x,y} \Psi^2_{\rm var}(y)/\Psi^2_{\rm var}(x)$. By contrast, for $d = -1$ (left move), we have:

$$\mathcal{R}' = (x'_N, \ldots, x'_0) \equiv (x_T, x_N, \ldots, x_1), \tag{9.23}$$

where now x_T is the trial move at the leftmost side of the reptile. The transition probability for this process is:

$$t^{(-1)}(\mathcal{R}'|\mathcal{R}) = p_{x_T,x_N}. \tag{9.24}$$

The corresponding weight on the new reptile $\mathcal{R}'$ is given by:

$$\mathcal{W}(\mathcal{R}') = p_{x_T,x_N} p_{x_N,x_{N-1}} \ldots p_{x_2,x_1} b_{x_N} b_{x_{N-1}} \ldots b_{x_1} \Psi^2_{\rm var}(x_1). \tag{9.25}$$

Thus the ratio $\mathcal{W}(\mathcal{R}')/\mathcal{W}(\mathcal{R})$, entering the Metropolis algorithm, acquires a simple form:

$$\frac{\mathcal{W}(\mathcal{R}')}{\mathcal{W}(\mathcal{R})} = \frac{b_{x_N} p_{x_T,x_N} \Psi^2_{\rm var}(x_1)}{b_{x_0} p_{x_1,x_0} \Psi^2_{\rm var}(x_0)} = \frac{b_{x_N} p_{x_T,x_N}}{b_{x_1} p_{x_0,x_1}}, \tag{9.26}$$

where, as before, we used the fact that $\mathcal{G}_{x',x} = p_{x',x} b_x$ is the Green's function with importance sampling, which satisfies $\mathcal{G}_{y,x} = \mathcal{G}_{x,y} \Psi^2_{\rm var}(y)/\Psi^2_{\rm var}(x)$.

We are now in the position to simplify the term appearing in the Metropolis algorithm of Eq. (9.14). For the right move, the opposite one that brings back $\mathcal{R}' \to \mathcal{R}$ is a left move with $x_T = x_N$:

$$t^{(-1)}(\mathcal{R}|\mathcal{R}') = p_{x_N,x_{N-1}}, \tag{9.27}$$

where we have used the fact that, after the first right move, the leftmost configuration of the $\mathcal{R}'$ reptile is x_{N-1}. Therefore, we obtain:

$$r^{(+1)}(\mathcal{R}', \mathcal{R}) = \frac{b_{x_0} p_{x_T,x_0}}{b_{x_{N-1}} p_{x_N,x_{N-1}}} \frac{p_{x_N,x_{N-1}}}{p_{x_T,x_0}} = \frac{b_{x_0}}{b_{x_{N-1}}}. \tag{9.28}$$

Analogously, for the left move, we have that the opposite move that brings back $\mathcal{R}' \to \mathcal{R}$ is a right move with $x_T = x_0$:

$$t^{(+1)}(\mathcal{R}|\mathcal{R}') = p_{x_0,x_1}, \tag{9.29}$$

where we have used the fact that the rightmost configuration of the $\mathcal{R}'$ reptile is x_1. Then, we get:

$$r^{(-1)}(\mathcal{R}', \mathcal{R}) = \frac{b_{x_N} p_{x_T,x_N}}{b_{x_1} p_{x_0,x_1}} \frac{p_{x_0,x_1}}{p_{x_T,x_N}} = \frac{b_{x_N}}{b_{x_1}}. \tag{9.30}$$

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In summary, Eqs. (9.28) and (9.30) completely define the rules for accepting or rejecting the new proposed reptile $\mathcal{R}'$ within the standard Metropolis algorithm (9.13).

9.3 The Bounce Algorithm

The main problem with the previous updating procedure is related to the presence of long correlation times. Indeed, choosing a different direction at every step makes the reptile shaking its head and tail (i.e., few configurations at the leftmost and rightmost positions) without changing its body (i.e., all the inner configurations). This is a particularly serious problem whenever a large number of time slices N is considered. The bounce algorithm has been proposed to achieve a small correlation time by performing many steps along one direction (right or left) before changing it (Pierleoni and Ceperley, 2005). In practice, the variable d is no longer randomly sampled but changes sign only when the move is rejected in Eq. (9.13). In this way, the detailed balance is no longer satisfied. However, the general theory of Markov chains (Meyer, 2000) guarantees the existence of a unique equilibrium distribution, provided ergodicity is satisfied. In the following, we will show that the bounce algorithm admits $\mathcal{W}(\mathcal{R})$ as an equilibrium distribution but we will not discuss the question about the convergence to it.

The full transition probability of the bounce algorithm is given by:

$$K_B(\mathcal{R}', d'|\mathcal{R}, d) = t^{(d')}(\mathcal{R}'|\mathcal{R})a^{(d')}(\mathcal{R}'|\mathcal{R})\delta_{d',d} + \delta(\mathcal{R}' - \mathcal{R})B^{(d)}(\mathcal{R})\delta_{d',-d}, \quad (9.31)$$

where $B^{(d)}(\mathcal{R})$ can be determined by the normalization condition:

$$\sum_{\mathcal{R}',d'} K_B(\mathcal{R}', d'|\mathcal{R}, d) = 1, \quad (9.32)$$

which leads to:

$$B^{(d)}(\mathcal{R}) = 1 - \sum_{\mathcal{R}'} t^{(d)}(\mathcal{R}'|\mathcal{R})a^{(d)}(\mathcal{R}'|\mathcal{R}). \quad (9.33)$$

The transition probability $K_B(\mathcal{R}', d'|\mathcal{R}, d)$ (that does not satisfy the detailed balance) determines both the new reptile $\mathcal{R}'$ and the new value of the direction d', e.g., $d' = d$ if the move $\mathcal{R} \to \mathcal{R}'$ is accepted (first term) or $d' = -d$ if the move is rejected (second term).

Then, the Master equation is given by:

$$\mathcal{P}_{n+1}(\mathcal{R}', d') = \sum_{\mathcal{R},d} K_B(\mathcal{R}', d'|\mathcal{R}, d)\mathcal{P}_n(\mathcal{R}, d), \quad (9.34)$$

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which admits as a stationary solution $\mathcal{P}_{\rm eq}(\mathcal{R},d) \equiv \mathcal{W}(\mathcal{R})/(2\mathcal{Z})$. Indeed, by using the explicit form of the transition probability of Eq. (9.31) with $\mathcal{P}_n(\mathcal{R},d) = \mathcal{W}(\mathcal{R})/(2\mathcal{Z})$, we get:

$$\mathcal{P}_{n+1}(\mathcal{R}',d') = \sum_{\mathcal{R}} t^{(d')}(\mathcal{R}'|\mathcal{R})a^{(d')}(\mathcal{R}'|\mathcal{R})\frac{\mathcal{W}(\mathcal{R})}{2\mathcal{Z}} + \frac{\mathcal{W}(\mathcal{R}')}{2\mathcal{Z}}B^{(-d')}(\mathcal{R}'); \quad (9.35)$$

then, by using Eq. (9.12) with $d = -d'$, we have:

$$\mathcal{P}_{n+1}(\mathcal{R}',d') = \frac{\mathcal{W}(\mathcal{R}')}{2\mathcal{Z}}\sum_{\mathcal{R}} t^{(-d')}(\mathcal{R}|\mathcal{R}')a^{(-d')}(\mathcal{R}|\mathcal{R}') + \frac{\mathcal{W}(\mathcal{R}')}{2\mathcal{Z}}B^{(-d')}(\mathcal{R}'). \quad (9.36)$$

Finally, by using Eq. (9.33), we obtain:

$$\mathcal{P}_{n+1}(\mathcal{R}',d') = \frac{\mathcal{W}(\mathcal{R}')}{2\mathcal{Z}}\left[1 - B^{(-d')}(\mathcal{R}')\right] + \frac{\mathcal{W}(\mathcal{R}')}{2\mathcal{Z}}B^{(-d')}(\mathcal{R}') = \frac{\mathcal{W}(\mathcal{R}')}{2\mathcal{Z}}, \quad (9.37)$$

which proves the fact that $\mathcal{W}(\mathcal{R})/(2\mathcal{Z})$ is a stationary solution of the stochastic process determined by $K_B(\mathcal{R}',d'|\mathcal{R},d)$.

9.4 The Continuous-Time Limit

As for the GFMC approach, it is possible to consider the limit of $\lambda \to \infty$ in the Green's function $\mathcal{G} = (\Lambda - \mathcal{H})$, e.g., by considering the imaginary time evolution of the exact propagator $\exp(-\beta\mathcal{H})$ applied statistically (see section 8.4). This can be done *without* any Trotter error (Trotter, 1959; Suzuki, 1976a,b). Within the RQMC method, we can take $\beta = N\tau$ and consider the path-integral representation with N time slices, each of them consisting into a projection with $\exp(-\tau\mathcal{H})$. Then, the previous updating schemes can be easily performed by propagating either the leftmost (rightmost) configuration $|x_N\rangle$ ($|x_0\rangle$) by using the transition probability of Eq. (8.62) for a time τ where $|x_T\rangle$ is eventually reached. Finally, the Metropolis algorithm is used to accept or reject the move (i.e., the entire propagation by τ); in this case, $r^{(d)}(\mathcal{R}'|\mathcal{R})$ is still given by Eq. (9.28) or (9.30), but the weights at numerator and denominator are the ones accumulated in the corresponding time slices, similarly to Eq. (8.66).

An example of the convergence with the number of time slices N is reported in Fig. 9.2. Here, we show the ground-state energy of the Heisenberg model on the square lattice for the 6×6 cluster (where the exact solution can be obtained by using Lanczos diagonalization).

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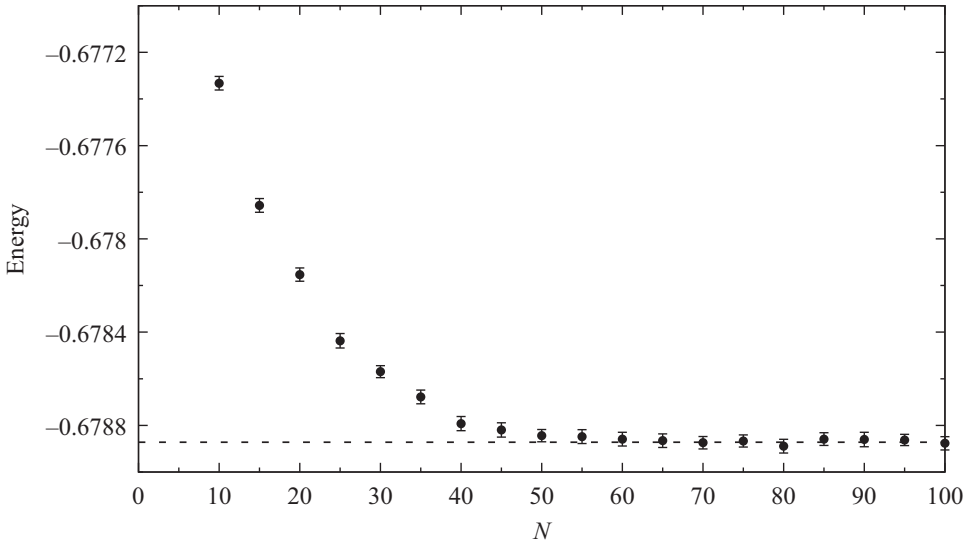

Figure 9.2 Energy per site for the Heisenberg model on the 6×6 cluster (square lattice) as a function of the number of the time slices N (the continuous-time approach with $\tau = 0.1$ is considered). The dashed line indicates the exact result obtained by Lanczos diagonalization.

9.5 Practical Implementation

We finally give a brief summary of the important steps in a practical implementation of the reptation quantum Monte Carlo algorithm.

1. **Initialization** at the beginning of the calculation.
   - Generate the same random configuration $|x_i\rangle$ for all the time slices. These configurations can be stored into a set of vectors $\texttt{iconf}(L, N+1)$, whose elements give the local state on each site $i = 1, \ldots, L$ and time slice, and $\texttt{kel}(2L, N+1)$, whose non-zero elements give, for each site, the position of the creation operators in the string defining the sampled configuration $|x\rangle$ of Eq. (5.44).
   - Verify that the initial configurations are not singular, i.e., $\langle x_i|\Psi_J\rangle \neq 0$, similarly to what has been discussed in the variational Monte Carlo method.
   - As for the variational Monte Carlo approach, compute the table of Eq. (5.33) to perform the fast update of the Jastrow factor and all the Green's functions that are necessary to perform the fast update. For the determinant case, only the static Green's function of Eq. (5.80) is necessary, while for the Pfaffian case both the standard Green's function (5.129) and the anomalous ones (5.130) and (5.131) are needed.

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2. **RQMC projection (with the continuous-time approach)**
   - Within the given direction $d = \pm 1$, propagate the leftmost (rightmost) configuration $|x_N\rangle$ ($|x_0\rangle$) by using the transition probability of Eq. (8.62) for an imaginary-time τ, until the trial configuration $|x'_T\rangle$ is reached. Accumulate the corresponding weight for the Metropolis algorithm, similarly to Eq. (8.66) to compute $r^{(d)}$. Accept or reject the trial move. If the trial move is accepted then keep the same d for the next one, otherwise change $d \to -d$.
   - Whenever the trial move is accepted, update the configuration, the table for the Jastrow factor (5.34) and all the Green's functions, i.e., Eq. (5.79) for determinants or Eqs. (5.125) and (5.128) for Pfaffians.
3. **Computation of observables**.

   Observables (e.g., the ground-state energy) can be computed every $O(L)$ steps.

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