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1. Introduction

The numerical treatment of many-body problems in solid state physics belongs to the realm of computer physics. Computer physics has evolved from 'number crunching' and 'dump data plotting' into a competitive field on a par with experimental an theoretical physics strongly entwined with both. Real experiments can be replaced by computer experiments as it is common practice in industry for monetary reasons. On the premises that an appropriate is simulated, the numerical experiment is often much faster, less expensive and in some cases even the only feasible alternative. With little extra effort, system parameters can be modified and novel material synthesized and the respective properties investigated.
As far as the links to theoretical physics are concerned the situation is similar. Computer physics has been disdained for many years by the 'pure theorists' claiming numerical results provide numbers and no insights. The situation has drastically changed over the last decade as testify by the significant and still increasing fraction of publications based essentially on computational techniques. Computer simulations from the theoretical viewpoint allow to scrutinies different models to figure out which fits the data best. Parameters can be modified with ease investigating wide parameter regimes with one and the same method. Otherwise different approaches have to be tailored for different parameter regimes, like week coupling strong-coupling etc.
A widely used approach is the density functional theory in various guises. The most famous approximation is the Local density approximation with various approximations to the unknown exchange-correlation potential. By definition, these one-particle approaches describe weekly correlated systems. Strongly correlated many-body systems are defined as those in which the simultaneous presence of all particles is essential for the respective phenomena. DFT is in principle exact in the sense that These techniques will not be discussed here.

2. Many Body Hamiltonians

The genuine ab-initio Hamiltonian describing condensed matter is the ab-initio Hamilton operator containing in the Oppenheimer-approximation. It forms the starting point for bandstructure calculations in the local-density-approximation (LDA), in which electronic correlations are treated on a mean-field level. The realm of LDA calculations are weakly correlated systems, as opposed to strongly correlated electronic systems in which the detailed electron-electron-interaction is responsible for correlation effects such as anti-ferromagnetism, Kondo-effect, fractional quantum-hall effect, Mott-transition and many more.
An exact treatment of ab-initio many-body problems is illusory. There are two options, either we stick to the ab-initio many-body Hamiltonian and are satisfied with uncontrolled approximations or we resort to model Hamiltonians which hopefully still contain the crucial essentials of the sought-for physical effect.
Model systems have the advantage that they can either be solved exactly by analytical means or they can be approached by numerical techniques. Numerical techniques are often the only feasible and reliable method for studying the really tough and long-standing problems of such systems.
We will begin with a concise description of the most important Hamilton operators for strongly correlated quantum systems, which have been the subject of intense numerical studies over the last 1-2 decades.

2.1 Hubbard model

We start out with the good old Hubbard model [**?**, **?**] a simple model for interacting electrons in narrow bands. Assuming localized orbitals and a strong screening of the Coulomb interaction, only the local density-density repulsion is allowed for. The mere on-site interaction is certainly a crude approximation to the Coulomb interaction, but, for certain phenomena, it bears already the essential features of strongly correlated electrons. The Hubbard model was originally introduced to study the metal-insulator transition and ferromagnetism of itinerant electrons in narrow bands. During the last decade it has re-gained considerable attention in connection with the high temperature superconductors.

Possible realizations of this model are atoms with partially filled 3d-shells. In these systems the physics at the Fermi-level is governed by electrons in localized (3d-) orbitals. The model is defined by

$$H = \underbrace{-t \sum_{\substack{\langle i,j \rangle \\ \sigma}} a^\dagger_{i\sigma} a_{j\sigma}}_{H_0} + \underbrace{U \sum_i n_{i\downarrow} n_{i\uparrow}}_{H_1} - \mu \hat{N} \,, \tag{2.1}$$

where $a^\dagger_{i\sigma}(a_{i\sigma})$ create (annihilate) fermions of spin $\sigma = \uparrow, \downarrow$ in a Wannier orbital centered at site i. $n_{i\sigma}$ denotes the occupation number operator $n_{i\sigma} = a^\dagger_{i\sigma} a_{i\sigma}$. The electrons move in tight binding bands, with a transfer integral t between nearest neighbor sites, as indicated by $\langle i, j \rangle$. The strength of the Coulomb interaction is U. The number of lattice-sites will be denoted by N. If not stated otherwise the underlying lattice will be "simple cubic" in 1-D, 2-D, or 3-D. For $U \gg t$ double-occupancies are energetically unfavourable. The dominant contributions to the low-lying eigenstate are those real-space configurations in which there are as few double-occupancies as possible. Of particular physical interested is the situation near half-filling. At half-filling there are as many electrons as there are site, namely N. Both spin directions get their equal share. The energetically favoured configurations are those with one electron per lattice site. The charge movement his hampered by a potential energy barrier of hight U. Unless there an applied voltage does not overcome this threshold there will be no significant current. The system is insulating. The reasons is merely the on-site Coulomb repulsion. Without U the system would be a perfect metal at half-filling. The same energy gap shows up in inverse photoemission. To bring an extra electron into the system an additional energy U has to be paid. In the insulating state only the spin degrees of freedom are dynamic and it can be shown in second order perturbation theory that the Hubbard model maps onto an Heisenberg model with antiferromagnetic nearest-neighbor spin-spin interaction.
For grand canonical calculations, in (2.1) a chemical potential μ is included which couples to the particle-number operator

$$\hat{N} = \sum_i \, n_{i\downarrow} + n_{i\uparrow} \,. \tag{2.2}$$

Besides the on-site repulsion some applications also include nearest-neighbor density-density repulsion, as well, or even long-ranged density-density interactions. The model

$$H = H_{\text{Hubbard}} + V \sum_{\langle ij \rangle} n_i n_j$$

is called the extended Hubbard model. We will also be interested in the negative-U (attractive) Hubbard model

$$H = -t \sum_{\langle i,j \rangle \, \sigma} a^\dagger_{i\sigma} a_{j\sigma} - |U| \sum_i \big(n_{i\downarrow} - \frac{1}{2}\big)\big(n_{i\uparrow} - \frac{1}{2}\big) - \mu \hat{N}$$

In this notation the chemical potential vanishes at half-filling $\langle n\rangle = 1$ which follows immediately from the invariance under particle-hole transformation. Particularly useful is the asymmetric particle-hole transformation

$$\begin{aligned} a_{i\uparrow}^\dagger &\to a_{i\uparrow}^\dagger & a_{i\uparrow} &\to a_{i\uparrow} \\ a_{i\downarrow}^\dagger &\to e^{i\boldsymbol{Q}\boldsymbol{x}_i} a_{i\downarrow} & a_{i\downarrow} &\to e^{-i\boldsymbol{Q}\boldsymbol{x}_i} a_{i\downarrow}^\dagger \end{aligned} \tag{2.3}$$

with $\boldsymbol{Q} = (\pi, \ldots, \pi)$. Equation (2.3) leaves the nearest neighbor hopping term of the Hamiltonian invariant, changes the sign of the onsite-Hubbard interaction and introduces a homogeneous magnetic field in z-direction

$$H \longrightarrow H_0 + |U| \sum_i \big(n_{i\downarrow} - \frac{1}{2}\big)\big(n_{i\uparrow} - \frac{1}{2}\big) - \mu \sum_i \underbrace{(n_{i\uparrow} - n_{i\downarrow})}_{2\sigma_i^z} - \mu N \; . \tag{2.4}$$

Hence, the negative-U model maps onto the repulsive Hubbard model in a homogeneous magnetic field of strength $h = 2\mu$. The latter vanishes only at half-filling. Interesting consequences of (2.3) are

$$\begin{aligned} \Delta_i^\dagger = a_{i\uparrow}^\dagger a_{i\downarrow}^\dagger \quad &\longleftrightarrow \quad e^{i\boldsymbol{Q}\boldsymbol{x}_i} a_{i\uparrow}^\dagger a_{i\downarrow} = e^{i\boldsymbol{Q}\boldsymbol{x}_i}\sigma_i^+ \\ \Delta_i = a_{i\downarrow} a_{i\uparrow} \quad &\longleftrightarrow \quad e^{-i\boldsymbol{Q}\boldsymbol{x}_i} a_{i\downarrow}^\dagger a_{i\uparrow} = e^{-i\boldsymbol{Q}\boldsymbol{x}_i}\sigma_i^- \\ n_i = n_{i\uparrow} + n_{i\downarrow} \quad &\longleftrightarrow \quad n_{i\uparrow} - n_{i\downarrow} + 1 = 2\sigma_i^z + 1 \end{aligned} \tag{2.5}$$

$\sigma_i^{(+,-,z)}$ are the Pauli matrices. Equation (2.5) can be used to deduce results for the negative-U Hubbard model from those of the repulsive one. For instance the staggered magnetization in x,y- direction in the repulsive case maps onto pair-field operators Δ_i and the staggered magnetization in z-direction translates into charge-density waves. Since at half-filling the repulsive Hubbard model in 2d exhibits long-ranged antiferromagnetic order at T=0K, there is a coexistence of superconductivity and charge-density waves in the attractive model.

2.2 Heisenberg model

The Hubbard type models describe itinerant electrons. If the charge degrees of freedom are bound to the atomic positions only the spin degrees of freedom remain active. They are described by the Heisenberg hamiltonian, the fundamental model in the theory of magnetism of local magnetic moments. It is defined by

$$H = \sum_{i,j} J_{ij}^z S_i^z S_j^z + J_{ij}^\perp \left(S_i^x S_j^x + S_i^y S_j^y\right) + B \sum_i S_i^z \tag{2.6}$$

where S_i^α ($\alpha = x, y, z$) is the α-th component of the spin-operator and J stands for the exchange integrals. The last term describes the coupling to an

external magnetic field B in z-direction. This model is particularly geared for magnetic insulators like the 3d-,4d-,4f-,5f-systems.
There are several special cases of the Heisenberg model

- $J^z = J^\perp$ ... isotropic Heisenberg model
- $J^\perp = 0$ ... Ising model
- $J^z = 0$ ... XY-model

The spin operators obey the well known commutator algebra

$$[S_i^\alpha, S_j^\beta] = i\,\delta_{i,j}\,\epsilon_{\alpha\beta\gamma}\,S_i^\gamma \ .$$

For numerical purposes it is convenient to introduce ladder operators

$$S_i^\pm = S_i^x \pm i\,S_i^y \ .$$

Therefore, the operators S^x and S^y can be written as

$$S_i^x = \frac{1}{2}(S_i^+ + S_i^-) \quad , \qquad S_i^y = \frac{1}{2i}(S_i^+ - S_i^-) \ .$$

Instead of S^x and S^y we use the operators S^+ and S^- to express the Hamiltonian

$$H = \sum_{ij}{}' \left\{ J_{ij}\,S_i^z S_j^z + \frac{1}{2}\,J_{ij}^\perp \underbrace{(S_i^+ S_j^- + S_i^- S_j^+)}_{F_{ij}} \right\} + B\sum_i S_i^z$$

where the summation is restricted to $i \neq j$.

2.2.1 Spin 1/2 Heisenberg Antiferromagnet

The isotrope spin-1/2 Heisenberg antiferromagnet ($J < 0$) attracts particular interest as being the strong coupling limit of the Hubbard model at half-filling ($N_\uparrow = N_\downarrow = N/2$) with $J = -4t^2/U$ [**?**]. Moreover, it is governed by quantum effects more than any other spin system.
However, the perfectly ordered Neel-state $|\uparrow\downarrow\uparrow\downarrow\rangle$ is not the ground state of the system.
The Hamiltonian has the special form

$$H = -J\sum_{\langle ij\rangle} \left\{ S_i^z\,S_j^z + \frac{1}{2}F_{ij} \right\} .$$

We have used the common sign convention for the exchange-integral. In the antiferromagnic case J is negative. The spin-spin interaction is restricted to nearest-neighbor sites, indicated by $\langle ij\rangle$. The so-called flip operator F_{ij} has a simple meaning for spin-1/2 particles. It swaps the spin-values of the neighboring sites i and j, if the spins have opposite sign. Otherwise, the application of F_{ij} yields the null vector.

$$\hat{F}_{i,j} \,|\ldots,\sigma_i,\ldots,\sigma_j,\ldots\rangle = \begin{cases} |\ldots,-\sigma_i,\ldots,-\sigma_j,\ldots\rangle & \text{if } \sigma_i = -\sigma_j, \\ |0\rangle & \text{otherwise.} \end{cases} . \quad (2.7)$$

A gauge-transformation can be invoked to map the spin-1/2 Heisenberg Hamiltonian onto a hard-core boson system with repulsive nearest neighbor interaction [**?**]. This representation is useful from the numerical and analytical point of view [**?**]. The transformation is defined by $S_i^+ = b_i^+$, $S_i^- = b_i$ and $S_i^z = 1/2 - b_i^+ b_i$, with the hard-core constraint $b_i^{+^2} = 0$. For $J < 0$ and a bi-partite lattice it is favorable to perform an additional gauge transformation $b_i \rightarrow e_i \cdot b_i$, with e_i being 1 on one sublattice and -1 on the other. The hard-core boson Hamiltonian then reads

$$H = -J \sum_{<ij>} b_i^+ b_i + J \sum_{<ij>} n_i n_j + E_0 \; . \quad (2.8)$$

In the above equation, $E_0 = -Jz(N - N_b)/4$, with N_b being the number of bosons and z the number of nearest neighbors. N_b is related to the z-component of the total spin via $N_b = N/2 - S_0^z$. Both, N_b and S_0^z are conserved quantities. It has been shown that the ground state of (2.8) is nodeless and unique [**?**, **?**].

2.2.2 Ising Model

The extrem unisotropic limit of the Heisenberg model is the Ising model, in which only the z-components of the spins are retained. Since no x- and y-components of the spins are involved, the Hamiltonian commutes with every S_i^z and the individual z-components are good quantum numbers. Therefore, the Ising model is a purely classical model, all operators commute and the only quantum-feature is the fact that only discrete values for S_i^z are allowed. The Hamiltonian of the Ising model reads

$$H = -J \sum_{<i,j>} S_i \, S_j + B \sum_i S_i \; , \quad (2.9)$$

where the spin-variables are restricted to ± 1. The Ising model is of particular interest for the theory of phase transitions since the 2d-Ising model has a second order phase-transition at a finite temperature and it can be solved analytically. There are various generalizations in the literature for a wide range of applications not only in physics but also in biology and in the field of pattern recognition. A particular class of generalizations leads to the so-called Potts-model. For a survey see [**?**].

2.2.3 The Potts Model

In the Potts–model the spins s_i can take on discrete values ranging from $1, 2, \ldots, q$. We restrict the discussion to periodic homogeneous systems where the Hamiltonian reads

$$H = -J \sum_{<i,j>} \delta_{s_i,s_j} \; . \tag{2.10}$$

As in the case of the Ising model, only nearest-neighbor spins interact and thus the sum is again restricted to nearest-neighbor sites i and j on the underlying lattice. Positive J values represent ferromagnetic coupling where, at $T = 0$, all spin values are equal. This ferromagnetic ground state is q-fold degenerate.
The Hamiltonian of the Potts model for $q = 2$ is related to that of the Ising model

$$H^I = -J^I \sum_{<i,j>} s_i \, s_j \tag{2.11}$$

via

$$\begin{aligned} H^I &= -J^I \sum_{<i,j>} \delta_{s_i,s_j} - (1 - \delta_{s_i,s_j}) \\ &= -2\, J^I \sum_{<i,j>} \delta_{s_i,s_j} + J^I \, N \, z \\ &= -J \sum_{<i,j>} \delta_{s_i,s_j} + J^I \, N \, z \, . \end{aligned} \tag{2.12}$$

Here, $J = 2\, J^I$ and z is the number of nearest neighbour pairs per lattice site. In the case of the Potts model, magnetic fields B couple via

$$H^1 = -B \sum_{i=1}^{N} \delta_{s_i,1} \tag{2.13}$$

where N denotes the number of spins. This formula relates to that for the Ising model via

$$\begin{aligned} H^{1I} = -B \sum_i s_i &= -B \sum_i \Big(\delta_{s_i,1} - (1 - \delta_{s_i,1}) \Big) \\ &= -2B \sum_i \delta_{s_i,1} + B \, N \; . \end{aligned} \tag{2.14}$$

Again, the coupling constant for the Ising model is twice that of the Potts model.

2.3 Kondo Model

The Kondo model was designed to describe the interaction of itinerant and localized (d, f) electrons of transition metal oxides such as $LaMaO_3$, which

are presently the subject of intense investigations. Due to strong Hund's rule coupling, the localized electrons are in a high spin state, which results in This means that at every lattice site i there is a localized spins $\mathbf{S}_i$. The sites i of these magnetic moments can either be distributed randomly to discribe magnetic impurities in metals or they can form a regular lattice. Like in the Hubbard model, the itinerant electrons are treated in the tight-binding approximation. They are subjected to strong exchange coupling with the localized spins. In its simplest form, the Kondo Hamiltonian reads

$$\hat{H} = -t \sum_{<i,j>,\,\sigma} a^{\dagger}_{i\sigma} a_{j\sigma} - J_H \sum_{i,\sigma,\sigma'} a^{\dagger}_{i\sigma'} \boldsymbol{\sigma}_{\sigma'\sigma} a_{i\sigma} \cdot \mathbf{S}_i \; + J \sum_{\langle ij \rangle} \mathbf{S}_i \mathbf{S}_j \; . \qquad (2.15)$$

Here, only one band of itinerant electrons is considered and electron–electron interaction are neglected. The coupling constant J_H has typical values of $J_H \approx 6\text{eV}$. Its influence is much greater than that of the hopping term.
Therefore, it is quite informative to consider the limit $J_H/t \to \infty$, where the itinerant spins are forced to align with the local ones. Then a misalignment of $\mathbf{S}_i$ and $\mathbf{S}_j$ suppresses the hopping, and, consequently a ferromagnetic ground state of the localized spins is favored. In this limit, an effective Hamiltonian can be derived. This is most easily done when considering the localized spins as classical vectors of equal length S pointing in the direction

$$\mathbf{n}_i = (\sin\theta_i \cos\varphi_i, \sin\theta_i \sin\varphi_i, \cos\theta_i) \; .$$

This simplification can be justified for large spins $S = 3/2,\, 5/2, \ldots$. In the case of classical localized spins, the effective Hamiltonian reads

$$H_{j_H=\infty} = - \sum_{<i,j>} t_{i,j}\, d^{\dagger}_{i\uparrow} d_{j\uparrow} \qquad (2.16)$$

with a hopping integral $t_{i,j}$ now depending on the relative orientation of the neighboring spins

$$t_{i,j} = t \left[\cos(\theta_i/2)\cos(\theta_j/2) + \sin(\theta_i/2)\sin(\theta_j/2) e^{-i(\varphi_i - \varphi_j)} \right] \; .$$

The operators $d^{\dagger}_{i\uparrow}(d_{i\uparrow})$ generate (annihilate) itinerant electrons whose spins point in the direction of the localized spin $\mathbf{S}_i$. We see that $t_{i,j} = 0$ for anti-parallel spins ($\theta_i = \pi - \theta_j$ and $\varphi_i = \pi + \varphi_j$) and $t_{i,j} = t$ for parallel spins ($\theta_i = \theta_j$ and $\varphi_i = \varphi_j$).
Another strategy is to to integrate out the effects of the itinerant electrons. This procedure yields the so–called *double exchange Hamiltonian*. In case of $S = 1/2$ it is of the Heisenberg form

$$H_{S=1/2} = -\frac{3}{8}\, t - \frac{1}{2}\, t \sum_{<i,j>} \mathbf{S}_i \cdot \mathbf{S}_j \, . \qquad (2.17)$$

In the general case, the double exchange Hamiltonian involves powers of the scalar product $(\mathbf{S}_i \cdot \mathbf{S}_j)^n$ up to $n = 2S$.

3. Numeric representation

There are four prerequisites a basis set should fulfill:

- It must be rapidly generated
- matrix elements are easy to compute
- modest need of memory
- fast access of states.

We will discuss the best basis sets and there numerical representation for spin and charge systems separately.

3.1 Spin-1/2 systems

Instead of the two spin values ± 1 we use the integers $n_i = \frac{\sigma_i+1}{2} \in \{0, 1\}$. One is prompted to identify the sequence of n_i values as bit-pattern of the integer $I = \sum_{l=1}^{N} n_l \, 2^{l-1}$. For instance the basis state $|\psi\rangle = |-1, +1, -1, +1\rangle$ is represented by $n = \{0101\}$, which again is mapped onto the integer 4. This representation has two advantages, it keep the memory requirements as small as possible and it speeds up certain numerical operations.
Since $S^z = \sum_{i=1}^{N} S_i^z$ commutes with the Hamiltonian, the Hamilton matrix is block-diagonal in the sectors with fixed S^z values, i.e. fixed numbers N^σ of σ-spins. For a given S^z-sector the number of ones in the bit-pattern is fixed, which reduces the number of basis states to

$$L = \binom{N}{N^\uparrow} , \tag{3.1}$$

where N is the number of lattices sites and

$$S^z = \frac{1}{2} \, 2N^\uparrow - N \, .$$

For instance, if the number of sites is $N = 16$ there are $2^{16} = 65536$ possible basis states in total, whereas there are merely $\binom{16}{8} = 12870$ for $S^z = 0$, i.e. $N^\uparrow = N^\downarrow = 8$, which is much less. Translation and Rotation could also be exploited which would reduce the number of basis state even further.

3.1.1 Generation of basis states

Not all integer values represent a permissible configuration, since the number of ones and zeros in the bit-pattern are fixed. We generate the basis states in such a way that the corresponding integer values are in increasing order. The basis states and there integer representations are therefore

$$
\begin{aligned}
|\varphi_1\rangle &= \{\overbrace{0,0,\ldots,0,0}^{N-N^\uparrow},\overbrace{1,1,1,\ldots,1}^{N^\sigma}\}; && I_1 = 2^{N^\sigma} - 1 \\
|\varphi_2\rangle &= \{0,0,\ldots,0,1,0,1,1,\ldots,1\}; && I_2 = 2^{N^\uparrow+1} - 1 - 2^{N^\uparrow-1} \\
|\varphi_3\rangle &= \{0,0,\ldots,0,1,1,0,1,\ldots,1\}; && I_3 = 2^{N^\uparrow+1} - 1 - 2^{N^\uparrow-2} \\
&\vdots \qquad\qquad \vdots \\
|\varphi_L\rangle &= \{\underbrace{1,1,1,\ldots,1}_{N^\uparrow},\underbrace{0,0,\ldots,0,0}_{N-N^\uparrow}\}; && I_L = 2^N - 2^{N-N^\uparrow}\ .
\end{aligned}
$$

As an example we consider a four-site cluster with $S^z = 0$, i.e. two up and two down spins. Since the basis states are ordered, basis states given in the

no	1	2	3	4	5	6
bit	0011	0101	0100	1001	1010	1100
integer	3	5	6	9	10	12

Table 3.1. *Example for the representation of spin pattern as integers.*

spin representation can be rapidly by bisection search.

3.2 Electronic systems

For the electronic systems described above, i.e. Hubbard, Anderson, Emery and t-J, we can construct a convenient basis in real space. Here we restrict the discussion to a single orbital per lattice site. A generalization is obvious. The vector in real space can be written as

$$
|\psi\rangle = \prod_{i=1}^{N\uparrow} a^+_{\Gamma_i^\uparrow} \prod_{j=1}^{N\downarrow} a^+_{\Gamma_j^\downarrow} |0\rangle \tag{3.2}
$$

where $|0\rangle$ denotes the vacuum state and $\Gamma_i^\uparrow$ is the lattice site of the i-th spin-up electron and $\Gamma_j^\downarrow$ is the lattice site of the j-th spin-down electron. For instance

$$\left| \begin{matrix} 1 & 2 & 3 & 4 \\ \uparrow & \sqcup & \downarrow & \uparrow\downarrow \end{matrix} \right\rangle \tag{3.3}$$

is represented by $\Gamma^{\uparrow} = \{1, 4\}$ and $\Gamma^{\downarrow} = \{3, 4\}$. Another way to represent this basis is by

$$|\psi\rangle = \prod_{i=1}^{N} (a_{i\uparrow}^{+})^{n_i^{\uparrow}} \prod_{i=1}^{N} (a_{j\downarrow}^{+})^{n_j^{\downarrow}} |0\rangle \tag{3.4}$$

where $n_i^{\uparrow}, n_j^{\downarrow} \in \{0, 1\}$ indicate whether or not site i is occupied by a spin-up or spin-down electron. The state (3.3) is represented by $n^{\uparrow} = \{1, 0, 0, 1\}$ and $n^{\downarrow} = \{0, 0, 1, 1\}$. N is the number of lattice sites. Yet another way to encode the same basis is

$$|\psi\rangle = \prod_{i=0}^{N} O_i |0\rangle \qquad O_i \in \{\hat{1},\ a_{i\uparrow}^{+},\ a_{i\downarrow}^{+},\ a_{i\uparrow}^{+} a_{i\downarrow}^{+}\}\ , \tag{3.5}$$

where the Operator O_i creates either an empty site, a site occupied by an up- or down-electron, or a doubly occupied site. The number of basis states is 4^N. Doubly occupied site are forbidden in the tJ model and the number of basis-states reduces in this case to 3^N. Since the electronic spin is conserve, $N_{\uparrow}$ and $N_{\downarrow}$ are good quantum numbers. The number of basis states in the sector of fixed N_{σ} values is therefore

$$\binom{N}{N_{\uparrow}} \binom{N}{N_{\downarrow}}$$

As an example take $N = 16$ and $N_{\uparrow} = N_{\downarrow} = 8$. The number of basis states is then $4^{16} = 4.294.967.296$, whereas $\binom{16}{8} \binom{16}{8} = 165.636.900$ In the t-J-model there is the additional constraint that there must not be any double-occupancy. The number of basis states reduces further to

$$\frac{N!}{N_{\downarrow}! N_{\uparrow}! N_h!}\ ,$$

where $N_h = N - N_{\downarrow} - N_{\uparrow}$ is the number of holes, or rather the number of empty sites. We implicitly assume that there are less electrons than sites, i.e. we are below half-filling. In the just mentioned half filling example the number of states is merely 12870. In all models, given the proper boundary conditions, translational invariance can be exploited which allows to reduce the number of basis states roughly by a factor N.

For the same reasons as before it is recommended to compress the representation. To this end representation (3.4) is favorable, since the two spin species are separately treated and for each spin-direction the sequence of values n_i^{σ} can be interpreted as a bit-pattern. In the previous example $n^{\uparrow} = \{1, 0, 0, 1\}$ corresponds to the integer $I^{\uparrow} = 9$ and $n^{\downarrow} = \{0, 0, 1, 1\}$ corresponds to $I^{\uparrow} = 3$. Each basis-state is therefore represented by a pair of integers $(I^{\uparrow}, I^{\downarrow})$.

3.2.1 Generation of basis states

The generation if the basis states is similar to that for the spin systems. The only difference is that we have to generate two integers fort the two spin species. For spin-σ there are

$$L^\sigma = \binom{N}{N^\sigma}$$

basis states. The total number of states for a given sector $N^\uparrow, N^\downarrow$ is $L = L^\uparrow L^\downarrow$.

3.3 Computation of the Hamilton matrix

Here we want to compute the matrix elements

$$h_{\nu'\nu} = \langle \Phi_{\nu'} | H | \Phi_\nu \rangle \tag{3.6}$$

of the Hamiltonian in suitable basis states $|\Phi_\nu\rangle$. To this end we split the Hamiltonian into individual contributions $H^{(l)}$

$$H = \sum_l H^{(l)} \tag{3.7}$$

such that the application of one such term $H^{(l)}$ to a basis state $|\Phi_\nu\rangle$ yields again a basis state or the null vector, i.e.

$$H^{(l)} |\Phi_\nu\rangle = h^{(l)}_{\nu'\nu} |\Phi_{\nu'}\rangle \ .$$

The full matrix element $\langle \Phi_{\nu'} | H | \Phi_\nu \rangle$ is obtained by summing up all contributions $h^{(l)}_{\nu'\nu}$. If there is only one term $H(l)$ in Hamiltonian that mediates between the two basis states $|\Phi_\nu\rangle$ and $|\Phi_{\nu'}\rangle$ than $h_{\nu'\nu} = h^{(l)}_{\nu'\nu}$.
For concreteness we consider the Hubbard Hamilton matrix in the real-space basis (3.4), characterized by the set of occupation numbers $|\Phi_\nu\rangle = \left|\{n^{(\nu)}_{i,\sigma}\}\right\rangle$ for all lattice sites i and the two spin directions, with $n^{(\nu)}_{i\sigma} \in \{0, 1\}$. The Hubbard interaction H_1 in (2.1) is diagonal in this basis, so we have

$$h_{\nu\nu} = U \sum_i n^{(\nu)}_{i\uparrow} n^{(\nu)}_{i\downarrow} \ .$$

There are no other contributions to the diagonal elements. Each summand in the kinetic energy of (2.1) represents an individual contribution to (3.7). It is, however, more sensible to combine the back-and-forth hopping processes for a particular nearest-neighbour pair

$$H^{(l)} = -t \left(a^\dagger_{i_0\sigma_0} a_{j_0\sigma_0} + h.c. \right) \ . \tag{3.8}$$

Application of one of these terms, $H^{(l)}$ say, to a basis state $|\Phi_\nu\rangle = \left|\{n_{i,\sigma}^{(\nu)}\}\right\rangle$ results either in the null vector, if $n_{i_0\sigma_0}^{(\nu)}$ and ${}^{(\nu)}n_{j_0\sigma_0}$ are both occupied or empty, i.e.

$$c_l = 0\,; \qquad \text{if } \; n_{i_0,\sigma_0}^{(\nu)} = n_{j_0,\sigma_0}^{(\nu)}\;.$$

Otherwise, the hopping process is possible and results in another basis state $|\Phi_{\nu'}\rangle = \left|\{n_{i,\sigma}^{(\nu')}\}\right\rangle$ which differs from $|\Phi_\nu\rangle$ only in the exchange of the occupation number $n_{i_0,\sigma_0}^{(\nu)}$ and $n_{j_0,\sigma_0}^{(\nu)}$, i.e.

$$n_{i,-\sigma_0}^{(\nu')} = n_{i,-\sigma_0}^{(\nu)} \qquad \forall i$$

$$\begin{aligned} n_{i,\sigma_0}^{(\nu')} &= n_{i,\sigma_0}^{(\nu)} \qquad \forall i \neq i_0, j_0 \\ n_{i_0,\sigma_0}^{(\nu')} &= n_{j_0,\sigma_0}^{(\nu)} \\ n_{j_0,\sigma_0}^{(\nu')} &= n_{i_0,\sigma_0}^{(\nu)}\;. \end{aligned} \tag{3.9}$$

There is only one hopping process $H^{(l)}$ mediating between the two basis states under consideration. The respective matrix element is therefor

$$h_{\nu'\nu} = \begin{cases} -t\;S & \text{if (3.9) is fulfilled,} \\ 0 & \text{otherwise.} \end{cases} \tag{3.10}$$

The hopping process can result in a sign S due to the fermi statistics of the electrons. E.g. consider a two-dimensional 4×4 lattice. The lattice sites are enumerated e.g. as follows

$$\begin{array}{cccc} 1 & 2 & 3 & 4 \\ 5 & 6 & 7 & 8 \\ 9 & 10 & 11 & 12 \\ 13 & 14 & 15 & 16 \end{array}\;.$$

There are many other ways of numbering the sites. The choice is arbitrary but fixed for the entire calculation. We consider the hopping between the adjacent sites 2 and 6 of one spin species. In the following we suppress the spin indices. The state $|\Phi_\nu\rangle$ be given by $\{n_{i\sigma}\} = \{0,0,1,1,\ 1,1,0,0,\ 0,0,0,0,\ 0,0,0,0\}$. The state reads according to (3.4)

$$|\Phi_\nu\rangle = a_3^\dagger a_4^\dagger a_5^\dagger a_6^\dagger |0\rangle\;.$$

Application of the hopping operator

$$-t(a_2^\dagger a_6 + a_6^\dagger a_2)$$

results in the state

$$|\Phi_\nu\rangle = a_3^\dagger a_4^\dagger a_5^\dagger a_2^\dagger |0\rangle = - a_2^\dagger a_3^\dagger a_4^\dagger a_5^\dagger |0\rangle \ .$$

The sign is given by

$$S = (-1)^{\Delta n} \ ,$$

where Δn is the number of electrons at the lattice sites between the sites i and j. In the above example $\Delta n = 3$.
What have we learned so far. We started out with an index $\nu \in \{1, \ldots, L\}$ for one of the basis states $|\Phi_\nu\rangle$, for which we know the representation $\{n_{i\sigma}^{(\nu)}\}$. The individual terms of the Hamiltonian couple to other basis states represented by a bit-pattern $\{n'_{i\sigma}\}$ or rather the corresponding integer representations $(I'_\uparrow, I'_\downarrow)$. We still need to know the corresponding index ν' of the basis state. Here it comes in handy that the basis states have been generated with increasing integer representation, so we can invoke a bisection search to find the respective indices ν. From the point of view of computer time this is crucial. The number of basis states one is interested in is typically $L = 10^8$ and more. A brute force search takes $O(L)$ steps, while the bisection search merely needs $O(\log_2(L))$ operations. For 10^8 the difference is a factor of 10^6. The index search has to be performed for each nonzero matrix element of the hamiltonian. In the Hubbard model there are roughly

$$N_{\mathrm{nz}} = L \ d \ N \ , \tag{3.11}$$

where d is the dimension of the underlying lattice and N the number of lattice sites.
The sign depends on the order in which electrons appear after the hopping process. For the interaction part, th prefactor is either U

3.4 Sparse matrices

In the above-mentioned representation the many-body Hamilton-matrices H_{ij} are sparse. We have seen that only a small fraction of all matrix elements is not zero. It is sensible to store only the nonzero matrix elements not only to save memory but also to speed up operations of the form $H\boldsymbol{x}$ which form the heart of the exact diagonalization schemes that will be discussed in

the next chapter. The most transparent algorithm to store sparse matrices is

Algorithm 3.4.1: COMPACT STORAGE$(H, H_c, ind, N_{\rm nz})$

---

initialize:
$L = \text{size}(H)$
$N_{\rm nz} = 0$

do $i = 1,\ L$
  do $j = 1,\ L$
    if $H(i,j) \neq 0$ **then**
      $N_{\rm nz} = N_{\rm nz} + 1$
      $H_c(k) = H(i,j)$
      $ind(k,1) = i$
      $ind(k,2) = j$
    endif
  end do
end do

The only operation the matrix will be used for is action on a vector. The compact storage can directly be used to perform only the nonzero multiplications as depicted in the following algorithm

---

Algorithm 3.4.2: MULTIPLY H $\boldsymbol{x}(H_c, ind, N_{\rm nz}, \boldsymbol{x}, \boldsymbol{y})$

---

initialize:
$\boldsymbol{y} = 0$

do $i = 1,\ N_{\rm nz}$
  $i_1 = \text{ind}(i,1)$
  $i_2 = \text{ind}(i,2)$
  $y(i_1) = y(i_1) + H_c(i) * x(i_2)$
end do

---

4. Exact diagonalization

In this chapter we describe methods for the exact evaluation of eigenvalues and eigenvectors of many-body Hamiltonians. There are very powerful exact diagonalization algorithms in the textbooks about numerical mathematics. A severe drawback of these schemes is there limitation to matrix sizes of the order $N = O(10^3)$. Strongly correlated many-body problems, however, start with $N = O(10^8)$ and go way beyond. It is obvious that conventional schemes are powerless in these cases. On the other hand there are no better algorithms for the full diagonalize of general hermitean matrices. The loop holes are the words 'full diagonalization' and 'general'. The interesting quantum features of strongly correlated many-body systems show up at very low temperatures. For the theoretical description of these temperatures, merely the ground-state and a few low-laying eigenvalues and the corresponding eigenvectors are required. Moreover, for most systems an appropriate basis can be found, in which the Hamilton-matrices are sparse. The number of nonzero matrix elements is typically $O(N)$ rather than $O(N^2)$.
A standard scheme from numerical mathematics, which allows to take advantage of the sparseness of a matrix and which allows to concentrate on the groundstate only, is the so-called power method or rather the vector-iteration due to von Mises.

4.1 The Power Method

The Power method is a simple and yet powerful technique to determine the eigenvector corresponding to the 'dominant' eigenvalue. The eigenvalue problem for the Hamilton operator H under consideration reads

$$\hat{H}\,|\varphi_l\rangle = \epsilon_l\,|\varphi_l\rangle \qquad \text{with} \quad \langle\varphi_l\,|\varphi_{l'}\,\rangle = \delta_{l,l'} \tag{4.1}$$

with real eigenvalue ε_l and mutually orthogonal and normalized eigenvectors $|\varphi_l\rangle$. The eigenvalues may be degenerate. We introduce a spectral shift

$$\hat{H} \to \hat{H}' = \hat{H} - E_s\hat{I} \qquad \text{and} \qquad \epsilon_l \to \epsilon_l' = \epsilon_l - E_s\ ,$$

which does not affect the eigenvectors $|\varphi_l\rangle$. Therefore, we can adapt E_s in such a way that the ground state yields the dominant eigenvalue, i.e.

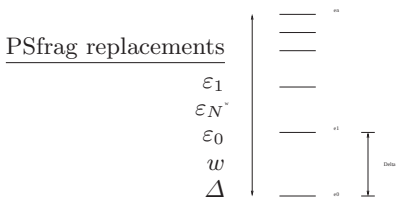

Fig. 4.1. Schematic representation of the eigenvalues of the Hamiltonian. The gap between the lowest two eigenvalues is denoted by Δ

$$|\epsilon'_0| \geq |\epsilon'_l| \quad \forall\, l\ .$$

To ensure that the groundstate energy ϵ'_0 has the greatest modulus of all eigenvalues the condition

$$\epsilon'_0 < -\frac{W}{2} = \frac{\epsilon_N - \epsilon_0}{2}$$

has to be fulfilled, which yields the condition

$$E_s > \frac{\epsilon_0 + \epsilon_N}{2}\ .$$

Next we want to apply the Power method to $\hat{H}'$ starting with an initial vector $|x_0\rangle$ chosen at random, possibly subject to suitable symmetry constraints. After n repeated applications of $\hat{H}'$ we obtain

$$|\tilde{x}_n\rangle \stackrel{\text{def}}{=} \hat{H'}^n\,|x_0\rangle = \sum_{l=0}^{N} |\varphi_l\rangle \epsilon_l'^n \underbrace{\langle\varphi_l\,|x_0\,\rangle}_{c_l}\ , \tag{4.2}$$

where we have inserted an expansion of the initial state $|x_0\rangle$ in the basis of eigenstates $\{|\varphi_l\rangle\}$ with the coefficients c_l. The normalization yields

$$|x_n\rangle \stackrel{\text{def}}{=} \frac{|\tilde{x}_n\rangle}{||\tilde{x}_n||} = \frac{\sum_l c_l \epsilon_l'^n |\varphi_l\rangle}{\left(\sum_l |c_l|^2 \epsilon_l'^{2n}\right)^{1/2}}\ , \tag{4.3}$$

or, equivalently, by dividing numerator and denominator by $c_0\,\epsilon_0'^n$

$$|x_n\rangle = \frac{\sum_l \frac{c_l}{c_0} \left(\frac{\epsilon'_l}{\epsilon'_0}\right)^n |\varphi_l\rangle}{\left(\sum_l \left(\frac{c_l}{c_0}\right)^2 \left(\frac{\epsilon'_l}{\epsilon'_0}\right)^{2n}\right)^{1/2}}\ . \tag{4.4}$$

We introduce the definition

$$q \stackrel{\text{def}}{=} \max_i \left|\frac{\varepsilon'_i}{\varepsilon'_0}\right|\ .$$

For the time being we assume that the groundstate energy is not degenerate and the initial vector has a non-vanishing overlap with the sought-for groundstate. In this case $q < 1$ and the Power method converges to the true groundstate

$$|x_n\rangle = |\varphi_0\rangle + O\left(q^n\right) \underset{n\to\infty}{\longrightarrow} |\varphi_0\rangle \ .$$

If the initial vector is orthogonal to the groundstate, the iteration converges to the lowest eigenstate which has a non-vanishing contribution in $|x_0\rangle$. This can be used directly to determine states with given symmetry, e.g. the dispersion relation of the lowest excitations. In order to guarantee the convergence towards the lowest energy for a given symmetry, one can choose an appropriate initial vector by imposing the desired symmetry on a random vector. The ratio q is either $\left|\frac{\varepsilon_1'}{\varepsilon_0'}\right|$ or $\left|\frac{\varepsilon_N'}{\varepsilon_0'}\right|$. The best convergence is achieved if

$$\left|\frac{\varepsilon_1'}{\varepsilon_0'}\right| = \left|\frac{\varepsilon_N'}{\varepsilon_0'}\right| \quad \Rightarrow q = \left|\frac{1-\Delta/W}{1+\Delta/W}\right| \ .$$

Obviously, the convergence is governed by the ratio Δ/W. The closer the excited states is to the groundstate, the longer it takes to get rid of its contribution in $|x_n\rangle$. If the lowest eigenvalue is degenerate

$$\varepsilon_0' = \varepsilon_1' = \ldots = \varepsilon_L' \ < \ \varepsilon_{L+1}$$

then then the Power iterates $|x_n\rangle$ converge towards the projection of the initial vector $|x_0\rangle$ onto the eigenspace of the first eigenvalue:

$$|x_n\rangle \ \underset{n\to\infty}{\longrightarrow} \ \frac{\mathbb{P}\,|x_0\rangle}{\langle x_0|\mathbb{P}\,|x_0\rangle}$$

where $\mathbb{P}$ is the projector onto the eigenspace of the ground state

$$\mathbb{P} = \sum_{l=0}^{L} |\varphi_l\rangle\langle\varphi_l| \ .$$

Using the expansion (4.2) for the energy-expectation value

$$\langle x_n|\hat{H}|x_n\rangle = \epsilon_0 + O\left(|\epsilon_1/\epsilon_0|^{2n}\right)$$

shows that the energy converges faster than the vector $|x_n\rangle$. On passing we note that the power-method allows also to determine excited states. Once the ground state is approximately determined a new sequence of iterations is started with an initial vector orthogonal to the approximate groundstate. Since the groundstate is approximate and due to the presence of numerical noise, the vectors $\boldsymbol{x_n}$ loose the orthogonality to the ground with increasing number of iterations and it is expedient to re-orthogonalize the vectors once in a while.

4.1.1 Eigenvalue Estimates

For the power method as well as for other numerical algorithms discussed in succeeding chapters it is advantageous to have a rough idea about the eigenvalue spectrum or to be able to give exact bounds for the individual eigenvalues.

Exact interval bounds. We will now derive a very useful exact expression for lower and upper bounds of individual eigenvalues. We assume that we have a reasonable approximation $|\psi\rangle$ for an normalized eigenvector, obtained e.g. by the Power method or Quantum Monte Carlo techniques. The corresponding approximate energy reads $\varepsilon = \langle\psi|H|\psi\rangle$. In addition we define the standard deviation $\sigma = \sqrt{< H^2 > - < H >^2}$. We will prove that there is at least one exact eigenvalue of $\hat{H}$ in the interval

$$I = [\varepsilon - \sigma, \varepsilon + \sigma] \; .$$

First, we expand the vector $|\psi\rangle$ in the basis $\{|\varphi_i\rangle\}$ of eigenvectors of $\hat{H}$

$$|\psi\rangle = \sum_i c_i \, |\varphi_i\rangle \; .$$

The variance can then be estimated by

$$\sigma^2 = \sum_i |c_i|^2 \, (\varepsilon_i - \varepsilon)^2 \geq (\varepsilon_m - \varepsilon)^2 \underbrace{\sum_i |c_i|^2}_{=1} \; ,$$

where ε_m denotes the exact eigenvalue that is closest to ε. We infer that $|\varepsilon_m - \varepsilon| \leq \rho$ and hence

$$\varepsilon_m \in [\varepsilon - \sigma, \varepsilon + \sigma] \; .$$

Different to the meaning of standard deviations in statistics, in the present context, the exact eigenvalue lies with certainty in the one-sigma regime. The standard-deviation can be used as convergence criterion for Quantum-Monte Carlo simulations or exact diagonalization techniques.

4.2 The Lanczos Method

The Power method uses only a small part of the information actually provided by the power method. One can do much better with only a little more computational effort. This goal is achieved by the Lanczos method.

4.2.1 The poor man's Lanczos scheme

To begin with, we analyze the information content of the first Power method iteration. After one step we have two normalized vectors $|x_0\rangle$ and $|x_1\rangle$, which are in general not orthogonal, and the corresponding energy-expectation values are

$$E_0^P = \langle x_0|\hat{H}|x_0\rangle$$
$$E_1^P = \langle x_1|\hat{H}|x_1\rangle \ .$$

The basic idea of the Lanczos method is to diagonalize the Hamiltonian in the subspace spanned by $\{|x_0\rangle, |x_1\rangle\}$, i.e. to minimize the energy of the variational Ansatz

$$\left|x_1^L\right\rangle = \alpha\,|x_0\rangle + \beta\,|x_1\rangle$$
$$E_1^L = \min_{\alpha,\beta} \frac{\left\langle x_1^L\middle|H\middle|x_1^L\right\rangle}{\left\langle x_1^L\middle|x_1^L\right\rangle} \leq \langle x_1|H|x_1\rangle \ .$$

The last inequality follows since $\langle x_1|H|x_1\rangle$ corresponds to the special case $\alpha = 0, \beta = 1$. It can easily be shown that the energy of the Lanczos method is actually lower than that of the Power method provided $\langle x_1|\hat{H}|x_0\rangle \neq 0$.
This procedure can be repeated by choosing the Lanczos vector x_1^L as initial vector of the subsequent iteration. The results of the Power method are compared with those of the simple Lanzcos scheme for a 10×10 tight binding matrix.

$$H = \begin{pmatrix} -1 & 1 & 0 & . & . \\ 1 & -1 & 1 & 0 & . \\ . & 1 & -1 & 1 & 0 \\ . & . & 1 & -1 & 1 \\ . & . & . & 1 & \ddots \end{pmatrix}$$

where an appropriate spectral shift has been introduce. The energies are depicted in Fig. 4.2. Obviously, the 'poor man's lanczos' scheme is superior, but not overwhelmingly so. Particularly disturbing is the observation, that it takes more than 10 iterations, which is the dimension of the matrix, to achieve convergence.
It is, however, straight forward, to generalized and improve the above ideas. Instead of taking only two vectors into account, we keep all vectors $|x_n\rangle$, generated during the iterations of the Power method. The set of vectors $|x_n\rangle$ spans the n-dimensional Krylov space. The minimization of the variational energy leads to the generalized eigenvalue problem depending on the matrix elements of the Hamiltonian and on the overlap matrix of the vectors $|x_n\rangle$. Linear dependencies of these basis states can lead to severe numerical problems. It is therefore better to transform the basis set $\{|x_n\rangle\}$ into an orthonormal set of vectors that still spans the Krylov space.

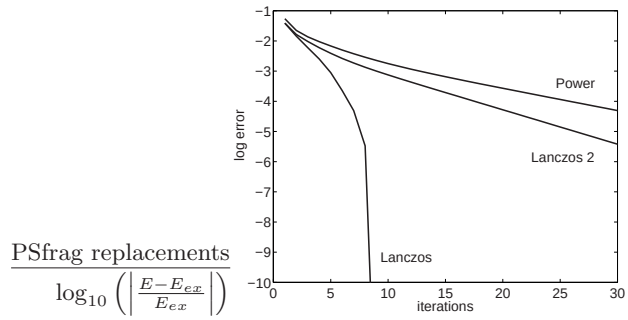

Fig. 4.2. Comparison of the speed of convergence to the exact ground-state energy of the Power method and the Lanczos method. Lanzcos 2 stands for the introductory example of only two vectors

4.2.2 Lanczos Method for Hermitean Matrices

The Lanczos procedure starts with an appropriate normalized initial vector $|x_0\rangle$, chosen along the lines outlined before. The corresponding energy-expectation value is

$$\varepsilon_0 = \langle x_0|\hat{H}|x_0\rangle\,.$$

Next we apply the Hamiltonian to $|x_0\rangle$ in order to determine the next basis vector

$$|\tilde{x}_1\rangle = \hat{H}|x_0\rangle - \varepsilon_0\,|x_0\rangle\ .$$

Apparently, the two vectors are orthogonal.

$$\langle x_0\,|\tilde{x}_1\,\rangle = 0$$

Again, the vector is normalized

$$|x_1\rangle = \frac{|\tilde{x}_1\rangle}{||\tilde{x}_1||}$$

and the energy-expectation value is computed

$$\varepsilon_1 = \langle x_1|\hat{H}|x_1\rangle\,.$$

The next basis vector is generated using the prescription

$$|\tilde{x}_2\rangle = H|x_1\rangle - \varepsilon_1\,|x_1\rangle - k_1|x_0\rangle$$

We choose the coefficients ε_2 and k_1 such that $|\tilde{x}_2\rangle$ is orthogonal to the previous basis vectors $\{|x_0\rangle, |x_1\rangle\}$:

$$\langle x_1 \,|\tilde{x}_2\,\rangle = \langle x_1|\hat{H}|x_1\rangle - \varepsilon_1 - k_1 \underbrace{\langle x_1 \,|x_0\,\rangle}_{=0} = 0$$
$$\langle x_0 \,|\tilde{x}_2\,\rangle = \langle x_0|\hat{H}|x_1\rangle - \varepsilon_1 \underbrace{\langle x_0 \,|x_1\,\rangle}_{=0} - k_1 = 0$$

Hence, ε_1 has again the interpretation of an expectation value,

$$\varepsilon_1 = \langle x_1|\hat{H}|x_1\rangle \;\text{ and }\; k_1 = \langle x_0|\hat{H}|x_1\rangle\,.$$

By construction, the quantity k_1 is real, since

$$k_1^* = \langle x_1|\hat{H}|x_0\rangle = \langle x_1 \,|\tilde{x}_1\,\rangle + \varepsilon_0 \underbrace{\langle x_1 \,|x_0\,\rangle}_{=0} = ||\tilde{x}_1|| \in \mathbb{R}\,.$$

We add the normalized vector $|\tilde{x}_2\rangle$ to the set of orthonormal basis states $\{|x_0\rangle, |x_1\rangle, |x_2\rangle\}$. Next we skip a several iterations steps and assume that we have already generated a set of $n+1$ mutually orthonormal vectors $\{|x_0\rangle, |x_1\rangle, \ldots |x_n\rangle\}$. The next vector $|x_{n+1}\rangle$ is determined as follows

$$\begin{aligned}
|\tilde{x}_{n+1}\rangle &= \hat{H}|x_n\rangle - \varepsilon_n\,|x_n\rangle - k_n\,|x_{n-1}\rangle \\
\varepsilon_n &= \langle x_n|\hat{H}|x_n\rangle \\
k_n &= \langle x_{n-1}|\hat{H}|x_n\rangle = ||\tilde{x}_n|| \\
|x_{n+1}\rangle &= \frac{|\tilde{x}_{n+1}\rangle}{||\tilde{x}_{n+1}||}\,.
\end{aligned}$$

We prove that $|x_{n+1}\rangle$ is orthogonal to all previous vectors.

$$\langle x_n \,|\tilde{x}_{n+1}\,\rangle = \underbrace{\langle x_n|\hat{H}|x_n\rangle}_{\varepsilon_n} - \varepsilon_n \underbrace{\langle x_n \,|x_n\,\rangle}_{=1} - k_n \underbrace{\langle x_n \,|x_{n-1}\,\rangle}_{=0} = 0$$
$$\langle x_{n-1} \,|\tilde{x}_{n+1}\,\rangle = \underbrace{\langle x_{n-1}|\hat{H}|x_n\rangle}_{k_n} - \varepsilon_n \underbrace{\langle x_{n-1} \,|x_n\,\rangle}_{=0} - k_n \underbrace{\langle x_{n-1} \,|x_{n-1}\,\rangle}_{=1} = 0$$

For $i = 1, \ldots, n-2$ we have

$$\langle x_i \,|\tilde{x}_{n+1}\,\rangle = \langle x_i|\hat{H}|x_n\rangle - \varepsilon_n \underbrace{\langle x_i \,|x_n\,\rangle}_{=0} - k_n \underbrace{\langle x_i \,|x_{n-1}\,\rangle}_{=0} = \langle x_i|\hat{H}|x_n\rangle\,.$$

The hermitecity of $\hat{H}$ yields

$$\begin{aligned}
\langle x_i|\hat{H}|x_n\rangle &= \Big(\langle x_n|\hat{H}|x_i\rangle\Big)^* \\
&= \Big(\langle x_n|(|\tilde{x}_{i+1}\rangle + \varepsilon_i\,|x_i\rangle + k_i\,|x_{i-1}\rangle)\Big)^* \\
&= \Big(\underbrace{\langle x_n \,|\tilde{x}_{i+1}\,\rangle}_{=0} + \varepsilon_i \underbrace{\langle x_n \,|x_i\,\rangle}_{=0} + k_i \underbrace{\langle x_n \,|x_{i-1}\,\rangle}_{=0}\Big)^* \\
&= 0\,,
\end{aligned}$$

which shows that the constructed set of $n+1$ vectors is indeed orthogonal. Moreover, it shows that the Hamilton matrix is tridiagonal in the Lanczos basis:

$$H_{ij}^t = \begin{pmatrix} \varepsilon_0 & k_1 & 0 & . & . \\ k_1 & \varepsilon_1 & k_2 & 0 & . \\ 0 & k_2 & \varepsilon_2 & k_3 & 0 \\ . & 0 & k_3 & \varepsilon_3 & k_4 \\ . & . & 0 & k_4 & \varepsilon_4 \end{pmatrix} \quad . \tag{4.5}$$

After L iterations the remaining task is the solution of the eigenvalue problem of the $(L+1) \times (L+1)$ tridiagonal matrix H^t

$$H^t \boldsymbol{c^\nu} = E_\nu \, \boldsymbol{c^\nu} \; .$$

The best approximation to the eigenvectors of the original Hamiltonian expanded in the the subspace $\mathcal{H}_k$ spanned by the Lanczos vectors $\{|x_0\rangle, \ldots, |x_L\rangle\}$ are therefore given by

$$|\psi_\nu\rangle = \sum_{i=0}^{L} c_i^\nu \; |x_i\rangle \; ,$$

where the components c_i^ν of the eigenvectors of the tridiagonal matrix H^t present the expansion coefficients in the Lanczos basis.

We summarize the Lanczos algorithm

Algorithm 4.2.1: LANCZOS ALGORITHM(.)

---

assign: $n_{\max}, N_{\text{diag}}, L, \delta$

initialize:
$|\tilde{x}_0\rangle$: appropriate initial vector
$|x_{-1}\rangle = 0$
$n = 0$
converged = **false**

while not *converged*
$k_n = \sqrt{\langle \tilde{x}_n | \tilde{x}_n \rangle}$
if $k_n < \delta$ **then** *converged* = **true**
$|x_n\rangle = |\tilde{x}_n\rangle / k_n$
$\varepsilon_n = \langle x_n | \hat{H} | x_n \rangle$
if MOD$(n, N_{\text{diag}}) = 0$ **then**
$H_t =$ TRIDIAGONALMATRIX$(\{\varepsilon_0, \ldots \varepsilon_n\}; \{k_1 \ldots k_n\})$
SOLVE EIGENVALUE-PROBLEM$(H_t; E_\nu, \boldsymbol{c}_\nu)$
if $E_1 \ldots E_L$ are converged **then** *converged* = **true**
endif
$|\tilde{x}_{n+1}\rangle = \hat{H}|x_n\rangle - \varepsilon_n |x_n\rangle - k_n |x_{n-1}\rangle$
$n = n + 1$
if $n \geq n_{\max}$ **then** *converged* = **true**
end while

In Fig. 4.2 the general performance of the Lanczos method is compared with that of the Power method and that of the simple Lanczos scheme. We observe a much faster convergence of the results of the Lanczos method and, as expected, exact convergence is achieved after 10 steps.
We will close this section by discussing a remarkable feature of the approximate eigenvectors. Let us define the projector $\hat{P}_L$ into the subspace $\mathcal{H}_L$

$$\hat{P}_L = \sum_{i=0}^{L} |x_i\rangle\langle x_i| \,. \tag{4.6}$$

The approximate eigenvector $|\psi_\nu\rangle$ is eigenvector of the projected Hamiltonian

$$\hat{H}_L := \hat{P}_L \hat{H} \hat{P}_L \,, \tag{4.7}$$

which is easily proven by

$$\begin{aligned}\hat{P}_L\hat{H}\hat{P}_L\,|\psi^\nu\rangle &= \sum_{i,j=0}^{L} |x_i\rangle H^t_{ij}\langle x_j| \sum_{l=0}^{L} c^\nu_l |x_l\rangle \\ &= \sum_{i,j=0}^{L} |x_i\rangle H^t_{ij}\; c^\nu_j = \sum_{i,j=0}^{L} |x_i\rangle E_\nu\; c^\nu_i \\ &= E_\nu\,|\psi^\nu\rangle\;.\end{aligned}$$

This implies that by virtue of the spectral theorem $\hat{H}_L$ can be expressed as

$$\hat{H}_L = \sum_{\nu=0}^{L} |\psi_\nu\rangle\; E_\nu\; \langle\psi_\nu|\;. \tag{4.8}$$

4.2.3 Dynamical Correlations

Dynamical correlations describe how a crystal reacts to weak external perturbations denoted by $E(t)$. Linear response theory expresses the reaction as

$$R(t) = \int_{-\infty}^{t} \chi(t,t')\, E(t')\, dt' \tag{4.9}$$

where χ is actually a function of the time-differences

$$\chi(t,t') = \chi(t-t') \; . \tag{4.10}$$

The response (4.9) has the form of a convolution and Fourier transformation yields a simple product

$$R(\omega) = \chi(\omega) E(\omega) \; . \tag{4.11}$$

The dynamical correlation function $\chi(\omega)$, or rather *susceptibility*, for zero temperature can be computed by the Lanczos procedure with little extra effort.

4.2.4 Dynamic Green's functions

To every dynamical correlation function corresponds a Green's function. For an operator $\hat{O}$ the retarded Green's function is defined by

$$\begin{aligned} \langle\langle \hat{O}(t)\,; \hat{O}^\dagger \rangle\rangle &\stackrel{\text{def}}{=} -\mathrm{i}\,\Theta(t) \left\langle [\hat{O}(t), \hat{O}^\dagger]_{\varepsilon=\pm 1} \right\rangle \\ &= -\mathrm{i}\,\Theta(t) \left(\left\langle \hat{O}(t)\, \hat{O}^\dagger \right\rangle + -\varepsilon \left\langle \hat{O}^\dagger\, \hat{O}(t) \right\rangle \right) \; , \end{aligned} \tag{4.12}$$

where in the second line the symbol $\langle\, \rangle$ denotes the thermodynamic average. Commutator ($\varepsilon = +1$) and anticommuator ($\varepsilon = -1$) Green's functions can be chosen at will. For a detailed introduction to the theory of Green's functions see e.g. [**?**]. At zero temperature, the average corresponds to the expectation value of the operators in the ground state $|\psi_0\rangle$ of the many-particle system. In this we focus on $T = 0$. Finite temperatures will be discussed later on. We proceed by inserting the Heisenberg time evolution of the operator $\hat{O}$

$$\hat{O}(t) = \mathrm{e}^{\mathrm{i}\hat{H}t}\, \hat{O}\, \mathrm{e}^{-\mathrm{i}\hat{H}t} \; , \qquad \hat{O} \stackrel{\text{def}}{=} \hat{O}(t=0) \tag{4.13}$$

into (4.12). Since $|\psi_0\rangle$ is the exact ground-state with energy E_0 we have

$$\mathrm{e}^{-\mathrm{i}\hat{H}t}\, |\psi_0\rangle = \mathrm{e}^{-\mathrm{i}E_0 t}\, |\psi_0\rangle \quad \text{and} \quad \langle\psi_0|\, \mathrm{e}^{\mathrm{i}\hat{H}t} = \langle\psi_0|\, \mathrm{e}^{\mathrm{i}E_0 t} \; , \tag{4.14}$$

and with $w^+ = w + \mathrm{i}\delta$, where δ is an infinitesimal positive quantity, we obtain

$$\begin{aligned}\left\langle\!\left\langle \hat{O};\hat{O}^\dagger\right\rangle\!\right\rangle_w &\stackrel{\text{def}}{=} \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}w^+t}\left\langle\!\left\langle \hat{O}(t),\hat{O}^\dagger\right\rangle\!\right\rangle dt \qquad (4.15)\\ &= -\mathrm{i}\int_0^\infty \mathrm{e}^{\mathrm{i}w^+t}\left(\left\langle \mathrm{e}^{\mathrm{i}\hat{H}t}\hat{O}\mathrm{e}^{-\mathrm{i}\hat{H}t}\hat{O}^\dagger\right\rangle - \varepsilon\left\langle \hat{O}^\dagger\mathrm{e}^{\mathrm{i}\hat{H}t}\hat{O}\mathrm{e}^{-\mathrm{i}\hat{H}t}\right\rangle\right) dt\\ &= -\mathrm{i}\int_0^\infty \mathrm{e}^{\mathrm{i}w^+t}\left(\left\langle \hat{O}\mathrm{e}^{-\mathrm{i}(\hat{H}-E_0)t}\hat{O}^\dagger\right\rangle - \varepsilon\left\langle \hat{O}^\dagger\mathrm{e}^{\mathrm{i}(\hat{H}-E_0)t}\hat{O}\right\rangle\right) dt\\ &= -\mathrm{i}\left(\left\langle \hat{O}\int_0^\infty \mathrm{e}^{\mathrm{i}w^+t}\mathrm{e}^{-\mathrm{i}(\hat{H}-E_0)t}dt\,\hat{O}^\dagger\right\rangle - \varepsilon\left\langle \hat{O}^\dagger\int_0^\infty \mathrm{e}^{\mathrm{i}w^+t}\mathrm{e}^{\mathrm{i}(\hat{H}-E_0)t}dt\,\hat{O}\right\rangle\right).\end{aligned}$$

With the aid of the spectral theorem the integral can now be evaluated. Now, taking into account the identity $-\mathrm{i}\,\mathrm{i}=1$ and recalling that we perform the average in the ground state $|\psi_0\rangle$, we obtain

$$\begin{aligned}\left\langle\!\left\langle \hat{O},\hat{O}^\dagger\right\rangle\!\right\rangle_w =& \left\langle \hat{O}\frac{1}{w^+-(\hat{H}-E_0)}\hat{O}^\dagger\right\rangle - \varepsilon\left\langle \hat{O}^\dagger\frac{1}{w^++(\hat{H}-E_0)}\hat{O}\right\rangle\\ =& \langle\psi_0|\hat{O}\hat{O}^\dagger|\psi_0\rangle\left\langle\varphi_0\right|\frac{1}{w^+-(\hat{H}-E_0)}\left|\varphi_0\right\rangle \qquad (4.16)\\ &-\varepsilon\,\langle\psi_0|\hat{O}^\dagger\hat{O}|\psi_0\rangle\left\langle\tilde{\varphi}_0\right|\frac{1}{w^++(\hat{H}-E_0)}\left|\tilde{\varphi}_0\right\rangle.\end{aligned}$$

The normalized state vectors $|\varphi_0\rangle$ and $|\tilde{\varphi}_0\rangle$, defined by,

$$|\varphi_0\rangle = \frac{\hat{O}^\dagger|\psi_0\rangle}{\sqrt{\langle\psi_0|\hat{O}\hat{O}^\dagger|\psi_0\rangle}} \qquad |\tilde{\varphi}_0\rangle = \frac{\hat{O}|\psi_0\rangle}{\sqrt{\langle\psi_0|\hat{O}^\dagger\hat{O}|\psi_0\rangle}} \qquad (4.17)$$

are used as initial vectors for two independent Lanczos sequences. The tridiagonal form of $\hat{H}$, and likewise of the energy denominators $\tilde{H}=w\pm(H-E_0)$, in the Lanczos basis can be exploited to determine the expectation value of the inverse of $\tilde{H}=w\pm(H-E_0)$ in (4.17). As for the ground state we calculate the matrix elements for the Lanczos vectors

$$\begin{aligned}\langle\varphi_i|\hat{H}-E_0|\varphi_i\rangle &= \Delta\varepsilon_i\\ \langle\varphi_i|\hat{H}-E_0|\varphi_{i+1}\rangle &= k_i\\ \langle\varphi_i|\hat{H}-E_0|\varphi_j\rangle &= 0\,\forall_{i,j},|i-j|>1 \qquad (4.18)\end{aligned}$$

Along with the orthonormality

$$\langle\varphi_i\,|\varphi_j\,\rangle = \delta_{i,j}\ ,$$

we obtain the tridiagonal form

$$(w^+\pm(\hat{H}-E_0)) = \begin{pmatrix} w^+\pm\Delta\varepsilon_0 & k_1 & 0 & . & .\\ k_1 & w^+\pm\Delta\varepsilon_1 & k_2 & 0 & .\\ 0 & k_2 & w^+\pm\Delta\varepsilon_2 & k_2 & 0\\ . & 0 & k_3 & w^+\pm\Delta\varepsilon_3 & k_3\\ . & . & 0 & k_4 & \ddots \end{pmatrix}.$$

We need the $(0,0)$–element of the inverse. The (ij)-element of the inverse matrix can be expressed by

$$A^{-1}_{ij} = (-1)^{i+j} \frac{\det \Delta_{ij}}{\det A} ,$$

where Δ_{ij} denotes the submatrix of A obtained upon eliminating from A the i-th row and the j-th column. Especially for the sought-for $(0,0)$-element of the inverse is

$$A^{-1}_{00} = \frac{\det \Delta_{00}}{\det A} , \tag{4.19}$$

Because of the tridiagonal structure of the above matrix, the formula simplifies as follows. Consider the matrix

$$A = \begin{pmatrix} A_{00} & A_{01} & 0 & . & . \\ A_{10} & A_{11} & A_{12} & 0. & \\ 0 & A_{21} & A_{22} & A_{23} & 0 \\ . & 0 & A_{32} & A_{33} & A_{34} \\ . & . & 0 & A_{43} & A_{44} \end{pmatrix}$$

The determinant can be expanded along the first row and column yielding

$$\det(A) = A_{00} \det \begin{pmatrix} A_{11} & A_{12} & 0 & . \\ A_{21} & A_{22} & A_{23} & 0 \\ 0 & A_{32} & A_{33} & A_{34} \\ . & 0 & A_{43} & A_{44} \end{pmatrix} - A_{01}A_{10} \det \begin{pmatrix} A_{22} & A_{23} & 0 & . \\ A_{32} & A_{33} & A_{34} & 0 \\ 0 & A_{43} & A_{44} & A_{45} \\ . & 0 & A_{54} & A_{55} \end{pmatrix} . \tag{4.20}$$

Upon defining the determinant of the submatrix of A beginning with the i-th column and row, i.e.

$$D_i \stackrel{\text{def}}{=} \det \begin{pmatrix} A_{i,i} & A_{i,i+1} & 0 & . \\ A_{i+1,i} & A_{i+1,i+1} & A_{i+1,i+2} & 0 \\ 0 & A_{i+2,i+1} & A_{i+2,i+2} & A_{i+2,i+3} \\ . & 0 & A_{i+3,i+2} & A_{i+3,i+3} \end{pmatrix} \tag{4.21}$$

we can express the sought-for element of the inverse matrix (4.19) by

$$(A^{-1})_{00} = \frac{1}{\frac{D_0}{D_1}} .$$

We can now use (4.20) to express $\frac{D_0}{D_1}$

$$\frac{D_0}{D_1} = \frac{A_{00}D_1 - |A_{01}|^2 D_2}{D_1} = A_{00} - \frac{|A_{01}|^2}{D_1/D_2}$$

by $\frac{D_1}{D_2}$. Iterating the above reasoning yields

$$\frac{D_l}{D_{l+1}} = A_{ll} - \frac{|A_{ll+1}|^2}{D_{l+1}/D_{l+2}} ,$$

which leads to a continued fraction for the desired quantity

$$(A^{-1})_{00} = \frac{1}{D_0/D_1} = \cfrac{1}{A_{00} - \cfrac{|A_{01}|^2}{A_{11} - \cfrac{|A_{12}|^2}{A_{22} - \cfrac{|A_{23}|^2}{A_{33} - \ddots}}}} \,. \tag{4.22}$$

For we original problem $(w^+ \pm \hat{H})^{-1}_{00}$ the continued fraction reads

$$(w^+ \pm (\hat{H} - E_0))^{-1}_{00} = \cfrac{1}{w^+ \pm \Delta\varepsilon_0 - \cfrac{|k_1|^2}{w^+ \pm \Delta\varepsilon_1 - \cfrac{|k_2|^2}{w^+ \pm \Delta\varepsilon_2 \ddots}}} \tag{4.23}$$

This expression is well suited for numerical treatment and can be iterated for arbitrary w.
To this end, we introduce the abbreviations

$$\begin{aligned} d_i &= \omega^+ \pm \Delta\varepsilon_i \qquad &&\text{for} \quad i = 0, 1, \ldots \\ e_i &= |k_i|^2 \qquad &&\text{for} \quad i = 1, 2, \ldots \end{aligned}$$

Beginning with the upper left 2×2 submatrix of A the continued fraction has the form

$$\frac{1}{d_0 - \frac{e_1}{d_1 - R_1}} = \frac{d_1 - R_1}{d_0 d_1 - e_1 - d_0 R_1} =: \frac{a_1 + a_0 R_1}{b_1 + b_0 R_1} \,. \tag{4.24}$$

In the last equation we anticipated the general form. The remainder R_1 has again the form of a continued fraction. In general the remainder reads

$$R_i = \frac{e_{i+1}}{d_{i+1} - R_{i+1}} \,. \tag{4.25}$$

Upon substituting this for $i = 1$ into (4.24) we obtain

$$\frac{a_1 + a_0 R_1}{b_1 + b_0 R_1} = \frac{\overbrace{a_1 d_2 + a_0 e_2}^{a_1} + \overbrace{(-a_1)}^{a_0} R_2}{\underbrace{b_1 d_2 + b_0 e_2}_{b_1} + \underbrace{(-b_1)}_{b_0} R_2} \tag{4.26}$$

which is again of the form.

$$\frac{a_1 + a_0 R}{b_1 + b_0 R} \,. \tag{4.27}$$

Thus the iteration formula for $i = 1, 2, \ldots$ deduced from the above considerations is given by

$$\begin{aligned} a_1 &\longrightarrow a_1 d_{i+1} + a_0\, e_{i+1} \\ a_0 &\longrightarrow -a_1 \\ b_1 &\longrightarrow b_1 d_{i+1} + b_0\, e_{i+1} \\ b_0 &\longrightarrow -b_1\ , \end{aligned}$$

with the initial values

$$a_1 = d_1, \quad a_0 = -1, \quad b_1 = d_0 d_1 - e_1, \quad b_0 = -d_0\ . \tag{4.28}$$

The sequence is iterated for each ω individually and ends if the Krylov space is exhausted or if a desired convergency of

$$g(\omega) = \frac{a_1}{b_1}$$

is achieved. In order to avoid numerical instabilities, it is recommendable to rescale all quantities a_0, a_1, b_0, b_1 e.g. by $b_1 = 1$ after each iteration.
In some cases it may happen that the Green's function of interest is not diagonal in the operators, e.g.

$$g_{AB} = \left\langle \hat{A}^\dagger \frac{1}{w^+ - (\hat{H} - E_0)} \hat{B} \right\rangle .$$

In this case we define two operators $\hat{O}_\alpha = \hat{A} + \alpha \hat{B}$ and determine the diagonal Green's functions

$$g_\alpha = \left\langle \hat{O}_\alpha^\dagger \frac{1}{w^+ - (\hat{H} - E_0)} \hat{O}_\alpha \right\rangle .$$

It is easily possible to separate g_{AB} by linearly combining the four Green's functions for $\alpha = \{\pm 1, \pm i\}$.

4.2.5 Lehmann – Representation

Before considering some simple examples, we want to present an alternative way of calculating Green's functions, the so *Lehmann representaion*. Again we consider the matrix elements of the form

$$\langle \psi_0 |\, \hat{O}^\dagger \, \frac{1}{\omega^+ \pm (\hat{H} - E_0)} \,\hat{=}\, |\psi_0\rangle\, , \tag{4.29}$$

where $\hat{O}$ is some appropriate operator and $|\psi_0\rangle$ represents the ground state. Like before we define $|\varphi_0\rangle$ as the normalized vector $\hat{O}\,|\psi_0\rangle$, which serves as initial vector of a Lanczos sequence. We insert a complete orthonormal set of eigenvectors of $\hat{H}$ given by

$$\mathbb{I} = \sum_{\nu} |\psi_\nu\rangle\langle\psi_\nu| \; .$$

Then (4.29) can be cast into the form

$$\langle\psi_0|\,\hat{O}^\dagger\,\frac{1}{\omega^+ \pm (\hat{H} - E_0)}\,\hat{O}\,|\psi_0\rangle = \sum_{\nu} \frac{\langle\psi_0|\,\hat{O}^\dagger\,|\psi_\nu\rangle\,\langle\psi_\nu|\,\hat{O}\,|\psi_0\rangle}{\omega^+ \pm (E_\nu - E_0)} \; .$$

Next we expand the eigenvectors $|\psi_\nu\rangle$ in the Lanczos basis $\{|\varphi_i\rangle\}$

$$|\psi_\nu\rangle = \sum_i c_i^{(\nu)}\,|\varphi_i\rangle\,, \quad \text{with} \;\; c_i^{(\nu)} = \langle\varphi_i\,|\psi_\nu\,\rangle$$

to obtain

$$\begin{aligned}\langle\psi_\nu|\,\hat{O}\,|\psi_0\rangle &= \sum_i c_i^{(\nu)*}\langle\varphi_i|\underbrace{\hat{O}\,|\psi_0\rangle}_{\sim|\varphi_0\rangle} = \sqrt{\langle\psi_0|O^\dagger O|\psi_0\rangle}\sum_i c_i^{(\nu)*}\underbrace{\langle\varphi_i\,|\varphi_0\,\rangle}_{\delta_{i,0}} \\ &= \sqrt{\langle\psi_0|O^\dagger O|\psi_0\rangle}\,c_0^{(\nu)*} \; .\end{aligned}$$

This means that except of the first terms all summands vanish. Thus (4.29) can be approximated by

$$\langle\psi_0|\,\hat{O}^\dagger\,\frac{1}{\omega^+ \pm (\hat{H} - E_0)}\,\hat{O}\,|\psi_0\rangle \;=\; \langle\psi_0|O^\dagger O|\psi_0\rangle\sum_{\nu=1}^{N_L}\frac{|c_0^{(\nu)}|^2}{\omega^+ \pm (\tilde{E}_\nu - \tilde{E}_0)} \; , \quad (4.30)$$

where only the first components $c_0^{(\nu)}$ of the expansion of the eigenvector $|\psi_\nu\rangle$ in the Lanczos basis are required. In general, the eigenstates $|\psi_\nu\rangle$ ($\nu = 1, \ldots, N_L$), computed by the Lanczos procedure, do not form a complete set of basis vectors, nor are the respective energies $\tilde{E}_\nu$ exact eigenvalues of $\hat{H}$. However, with increasing number of iterations, the Lanczos procedure converges towards the exact Green's function and the convergency can be monitored and stopped as soon as the desired accuracy is reached. The approximate Lehmann representation (**??**) is an explicit sum of simple poles. The same holds true for the continued fraction, less obviously though.

4.3 Finite Temperature Lanczos

In this section we present the finite-temperature Lanczos method (FTLM), developed by Jaklič and Prelovšek [**?**], which is a straight forward generalization of the Lanczos procedure to finite temperatures.

4.3.1 Static Observables

We consider a Hamiltonian $\hat{H}$ in a N_{st} dimensional vector space. In the canonical ensemble the expectation value of a static operator $\hat{A}$ can be written as

$$\langle \hat{A} \rangle = \frac{1}{Z} \operatorname{tr}\big(\hat{A}\, \mathrm{e}^{-\beta \hat{H}}\big) = \frac{1}{Z} \sum_{|\varphi\rangle} \big\langle \varphi \big| \hat{A}\, \mathrm{e}^{-\beta \hat{H}} \big| \varphi \big\rangle \tag{4.31}$$

with the partition function

$$Z = \sum_{|\varphi\rangle} \big\langle \varphi \big| \mathrm{e}^{-\beta \hat{H}} \big| \varphi \big\rangle \; . \tag{4.32}$$

The trace is carried out in any complete orthonormal set of N_{st} basis vectors $|\varphi\rangle$. Of course, if all the eigenvalues E_n and all the eigenstates $|\psi_n\rangle$ of the Hamiltonian are known, we immediately have

$$\langle \hat{A} \rangle = \frac{1}{Z} \sum_{n=1}^{N_{st}} \mathrm{e}^{-\beta E_n} \big\langle \psi_n \big| \hat{A} \big| \psi_n \big\rangle \tag{4.33}$$

and the partition function simplifies to

$$Z = \sum_{n=1}^{N_{st}} \mathrm{e}^{-\beta E_n} \; . \tag{4.34}$$

Since a complete solution of the eigenvalue problem can only be achieved for very small or very selected model systems one might be tempted to replace the eigenvalues and eigenvectors by the corresponding quantities obtained by the Lanczos procedure outlined in the previous section. It appears that the direct implementation of this idea does not work out well. Consider the limit $\beta = 0$, or rather $T \to \infty$. In this limit we have

$$Z \, \langle \hat{A} \rangle = \sum_{i=0}^{L} \big\langle \psi_i \big| \hat{A} \big| \psi_i \big\rangle$$

and

$$Z = \sum_{i=0}^{L} \big\langle \psi_i \big| \psi_i \big\rangle = L + 1 \; .$$

Obviously, the results depend heavily on the number of Lanczos iterations L and accurate results are only guaranteed for $L \to N_{\rm st}$, which is however beyond our reach. A moderate modification of this idea, however, leads to the FTLM that manages with $L \ll N_{\rm st}$.
To begin with, we replace the complete set of orthonormal vectors by random vectors $\big|\Phi^{(\nu)}\big\rangle$ as outlined in **??**. Next we expand the exponential of the Hamiltonian in (4.31) in a power series

$$\big\langle \hat{A} \big\rangle = \frac{1}{Z N_r} \sum_{\nu=1}^{N_r} \sum_{k=0}^{\infty} \frac{(-\beta)^k}{k!} \big\langle \Phi^{(\nu)} \big| \hat{A} \hat{H}^k \big| \Phi^{(\nu)} \big\rangle \,. \tag{4.35}$$

The resulting expectation values $\big\langle \Phi^{(\nu)} \big| \hat{A} \hat{H}^k \big| \Phi^{(\nu)} \big\rangle$ will be calculated in the frame of the Lanczos algorithm. To this end, $L \geq k$ Lanczos iterations are performed starting with $|x_0\rangle = \big|\Phi^{(\nu)}\big\rangle / \|\Phi^{(\nu)}\|$. Next we introduce the projection operators $\hat{P}_k$ defined by (4.6). Since the Hamiltonian is tridiagonal in the Lanczos basis, the application of the Hamiltonian on a vector in $\mathcal{H}_k$ yields a vector in $\mathcal{H}_{k+1}$, i.e.

$$\hat{H}\, \hat{P}_k = \hat{P}_{k+1}\, \hat{H}\, \hat{P}_k = \hat{P}_L\, \hat{H}\, \hat{P}_k \tag{4.36}$$

as long as $L > k$. The first vector of the basis is $\big|\Phi^{(\nu)}\big\rangle$ which implies $\big|\Phi^{(\nu)}\big\rangle = \hat{P}_0 \big|\Phi^{(\nu)}\big\rangle$ and we obtain along with (4.36)

$$\begin{aligned}
\big\langle \Phi^{(\nu)} \big| \hat{A}\, \hat{H}^k \big| \Phi^{(\nu)} \big\rangle &= \big\langle \Phi^{(\nu)} \big| \hat{A}\, \hat{H}^{k-1} \hat{H} \hat{P}_0 \big| \Phi^{(\nu)} \big\rangle = \big\langle \Phi^{(\nu)} \big| \hat{A}\, \hat{H}^{k-1} \hat{P}_1 \hat{H} \hat{P}_0 \big| \Phi^{(\nu)} \big\rangle \\
&= \big\langle \Phi^{(\nu)} \big| \hat{A}\, \hat{P}_k \hat{H} \hat{P}_{k-1} \ldots \hat{P}_2 \hat{H} \hat{P}_1 \hat{H} \hat{P}_0 \big| \Phi^{(\nu)} \big\rangle \\
&= \big\langle \Phi^{(\nu)} \big| \hat{A}\, \hat{P}_L \hat{H} \hat{P}_L \ldots \hat{P}_L \hat{H} \hat{P}_L \hat{H} \hat{P}_L \big| \Phi^{(\nu)} \big\rangle \\
&= \big\langle \Phi^{(\nu)} \big| \hat{A}\, \hat{H}_L^k \big| \Phi^{(\nu)} \big\rangle
\end{aligned}$$

In the last but one step we have substituted all projectors by $\hat{P}_L$ since $k \leq L$ has been assumed. In the last equation the definition (4.7) of the projected Hamiltonian is used. According to (4.8) we alternatively have

$$\big\langle \Phi^{(\nu)} \big| \hat{A}\, \hat{H}^k \big| \Phi^{(\nu)} \big\rangle = \sum_{i=0}^{L} (E_i^{(\nu)})^k \big\langle \Phi^{(\nu)} \big| \hat{A} \big| \psi_i^{(\nu)} \big\rangle \big\langle \psi_i^{(\nu)} \big| \Phi^{(\nu)} \big\rangle \,. \tag{4.37}$$

So far everything is exact as long as $k \leq L$. In order to get a grip on the higher order terms in the Taylor expansion we stick to (4.37) even for $k > L$, which brings (4.35) into the approximate form

$$\big\langle \hat{A} \big\rangle = \frac{1}{Z N_r} \sum_{\nu=1}^{N_r} \sum_{k=0}^{\infty} \frac{(-\beta)^k}{k!} \sum_{i=0}^{L} (E_i^{(\nu)})^k \big\langle \Phi^{(\nu)} \big| \hat{A} \big| \psi_i^{(\nu)} \big\rangle \big\langle \psi_i^{(\nu)} \big| \Phi^{(\nu)} \big\rangle \,. \tag{4.38}$$

The reliability of the approximation increases with increasing temperature, since for small β, high powers k are strongly suppressed by the factor β^k.

Intuitively, we expect the approximation to be even better for zero temperature, as the FTLM is build on the zero temperature Lanczos. We will see immediately than this speculation is erroneous. In (4.38) we can recombine the k-dependent terms to an exponential function

$$\langle \hat{A} \rangle = \frac{1}{Z N_r} \sum_{\nu} \sum_{i=0}^{L} \mathrm{e}^{-\beta E_i^{(\nu)}} \langle \Phi^{(\nu)} | \hat{A} | \psi_i^{(\nu)} \rangle \langle \psi_i^{(\nu)} | \Phi^{(\nu)} \rangle \tag{4.39}$$

Similarly, for the partition function we obtain

$$Z = \frac{1}{N_r} \sum_{\nu=1}^{N_r} \sum_{i=1}^{N_{st}} \mathrm{e}^{-\beta E_i^{(\nu)}} \, |\langle \Phi^{(\nu)} | \psi_i^{(\nu)} \rangle|^2 \, . \tag{4.40}$$

For $\beta \to 0$ the expressions simplify to $Z\langle \hat{A} \rangle = \frac{1}{N_r} \sum_{\nu} \langle \Phi^{(\nu)} | \hat{A} | \Phi^{(\nu)} \rangle$ and $Z = \frac{1}{N_r} \sum_{\nu} \langle \Phi^{(\nu)} | \Phi^{(\nu)} \rangle$. The mean values are identical to the exact infinite temperature results $\mathrm{tr}(A)$ and $\mathrm{tr}(\hat{1}) = N_{sp}$, respectively.
These expressions are slightly different to what we described in the introductory remarks. Of course, if we were able to use the eigenvectors $|\Phi_l\rangle$ of the Hamiltonian as orthonormal set $|\Phi^{(\nu)}\rangle$ everything would be perfect. The Lanczos iteration would stop right after the first iteration ($L = 0$) and both $|\psi_i^{(\nu)}\rangle$ and E_i would be exact and we recover (4.33). Unfortunately, since the Lanczos eigenvectors and eigenenergies depend upon the initial vector $|\Phi^{(\nu)}\rangle$, (4.39) is no longer a trace and the accuracy of (4.39) depends upon the choice of the vectors $|\Phi^{(\nu)}\rangle$. This fact is particularly obvious for $T = 0$

$$\langle \hat{A} \rangle_{T=0} = \lim_{\beta \to \infty} \frac{\sum_{\nu=1}^{N_r} e^{-\beta E_0^{(\nu)}} \langle \Phi^{(\nu)} | \hat{A} | \psi_0^{(\nu)} \rangle \langle \psi_0^{(\nu)} | \Phi^{(\nu)} \rangle}{\sum_{\nu=1}^{N_r} e^{-\beta E_0^{(\nu)}} \left| \langle \Phi^{(\nu)} | \psi_0^{(\nu)} \rangle \right|^2}$$

We assume that enough Lanczos iterations per random vector $|\varphi_\nu\rangle$ have been performed so that both, lowest eigenvalue and corresponding eigenvector are converged to the exact values leading to

$$\langle \hat{A} \rangle_{T=0} = \frac{\frac{1}{N_r} \sum_{\nu=1}^{N_r} \langle \Phi^{(\nu)} | \hat{A} | \psi_0 \rangle \langle \psi_0 | \Phi^{(\nu)} \rangle}{\frac{1}{N_r} \sum_{\nu=1}^{N_r} \langle \Phi^{(\nu)} | \psi_0 \rangle \langle \psi_0 | \Phi^{(\nu)} \rangle}$$

Numerator and denominator correspond to the stochastic evaluation of

$$\mathrm{tr}(\hat{A} |\psi_0\rangle\langle\psi_0|) = \langle \psi_0 | \hat{A} | \psi \rangle$$

and

$$\mathrm{tr}(|\psi_0\rangle\langle\psi_0|) = \langle \psi_0 | \psi_0 \rangle = 1 \, ,$$

respectively. The stochastic evaluation of numerator and denominator yields unbiased results for both quantities separately. The ratio, however, is biased.

On the one hand, because the mean of the inverse is different from the inverse of the mean and on the other hand, because numerator and denominator are estimated by the same set of random vectors.
According to (**??**) the variance of the numerator is $\frac{2}{N_r}\langle\psi_0|\hat{A}|\psi_0\rangle^2$ and that of the denominator reads $\frac{2}{N_r}$. In both cases, the relative statistical error is $\sqrt{\frac{2}{N_r}}$. I.e., although each Lanczos iteration is converged to the, as far as the ground state is concerned, and yields the exact ground state expectation value $\langle\psi_0|\hat{A}|\psi_0\rangle$ of the sought for observable, the stochastic evaluation via (4.39) introduces a considerable statistical uncertainty. At first glance, it appears to be expedient to switch to the original zero temperature for $T \to 0$ results. It is, however, possible to do better and to treat all temperatures on the same footing by combining the best of both limits $T \to \infty$ and $T \to 0$. To this end we go all the way back to the expression for the numerator $Z\left\langle\hat{A}\right\rangle = \mathrm{tr}\left(e^{-\beta\hat{H}}\hat{A}\right)$ and rewrite it symmetrically

$$Z\left\langle\hat{A}\right\rangle = \mathrm{tr}\left(e^{-\frac{\beta}{2}\hat{H}}\hat{A}e^{-\frac{\beta}{2}\hat{H}}\right) .$$

Next we proceed as before, but the Taylor expansion is employed separately for both exponentials. The same arguments as before lead to

$$Z\left\langle\hat{A}\right\rangle = \frac{1}{N_r}\sum_{\nu=1}^{N_r}\sum_{i,j=0}^{L} \mathrm{e}^{-\beta\frac{E_i^{(\nu)}+E_j^{(\nu)}}{2}}\langle\Phi^{(\nu)}|\psi_i^{(\nu)}\rangle\langle\psi_i^{(\nu)}|\hat{A}|\psi_j^{(\nu)}\rangle\langle\psi_j^{(\nu)}|\Phi^{(\nu)}\rangle .$$

Let us consider the low temperature limit. We assume again that enough Lanczos iterations have been performed and $E_0^{(\nu)}$ and $\left|\psi_0^{(\nu)}\right\rangle$ are converged to the exact ground state energy E_0 and eigen vector $|\psi_0\rangle$, respectively. Only the ground state contributes in the limit $T \to 0$ and we have

$$Z\left\langle\hat{A}\right\rangle \underset{T\to 0}{\longrightarrow} \langle\psi_0|\hat{A}|\psi_0\rangle\left(\mathrm{e}^{-\beta E_0}\ \frac{1}{N_r}\sum_{\nu=1}^{N_r}\sum_{i,j=0}^{L}\left|\langle\Phi^{(\nu)}|\psi_0\rangle\right|^2\right) .$$

Comparison with (4.40) reveals that the bracketed expression is identical to Z. Both contributions cancel and we and up with the exact result for $T = 0$ without any stochastical noise irrespective of the number N_r of random vectors. There is merely one drawback: when we perform the computation numerically, we don't know that the result has no statistical noise, since numerator and denominator considered separately suffer severely from noise. The reason for the discrepancy is the fact that both contributions are strongly correlated, since they are determined with the same set of random vectors. Correlations are often disadvantageous, but here they are highly desirable for the correct $T = 0$ result; we merely need a way to exploit this fact. A standard tool to estimate nonlinear functionals of random variables is the so

called *jackknife estimator*[**?**]. There is another shortcoming of the estimator presented thus far: it is biased, since the mean of the inverse is not the inverse of the mean. In other words, the expectation value of the ratio of the estimates (4.39) and (4.40), which are both random variables, is in general not the ratio of the expectation value of numerator and denominator. This bias can also be reduce by the jackknife approach.

4.3.2 The Jackknife estimator

In this section we describe a statistical approach to deal with biased estimators and which allows to infer the statistical error of the estimate. We follow closely the ideas of Kendall and Stuart[**?**]. Suppose we have a sample of N random variables $\{r\} := \{r_1, \ldots, r_N\}$ with which we evaluate an estimator $\theta(\{r\})$ for the true quantity θ^0. We assume that the estimator is biased for finite sample size N but asymptotically it becomes unbiased. Moreover we suppose the bias to be analytic in $1/N$, i.e. for large N we have the Taylor expansion

$$E\big(\theta(\{r\})\big) = \theta^0 + \frac{c_1}{N} + \frac{c_2}{N^2} + O(\frac{1}{N^3}) \; . \tag{4.41}$$

We will discuss the jackknife statistic guided by an example which is of particular interest to us: the ratio of two functionals

$$\theta(\{r_1, \ldots, r_N\}) = \frac{f(\{r\})}{g(\{r\})} \; .$$

Obviously, for finite N the estimator is biased but it is asymptotically exact. The estimate based on a particular sample is a random variable which possesses a distribution $p(\theta)$, which is however unaccessible in general. For our purposes it suffices to determine mean and variance of the distribution. The key idea of the Jackknife approach is to rewrite the estimator into an arithmetic mean

$$\theta^*(\{r_1, \ldots, r_N\}) = \frac{1}{N} \sum_{j=1}^{N} \theta_j^* \tag{4.42}$$

of suitable random variables θ_j^*, which depend on the sample $\{r\}$. If these random variables are iid then $\theta^*(\{r_1, \ldots, r_N\})$ has a normal distibution. The recipe of the Jackknife begins with the definition of an auxiliary random variable

$$\theta_{-j} := \theta(\{r_1, \ldots, r_{j-1}, r_{j+1}, \ldots, r_N\}) \; ,$$

which corresponds to the estimator θ, with the element r_j removed from the sample. We now consider the random variable

$$\theta_j^* := N\,\theta(\{r\}) - (N-1)\,\theta_{-j}\ , \tag{4.43}$$

which has a simple meaning in the special case

$$\theta(\{r\}) = \frac{1}{N}\sum_{i=1}^{N} r_i$$

of the sample mean. In this case, $\theta_j^* = r_j$ corresponds to the j-the element of the sample. Therefore the unbiased estimator for the mean is identical to the arithmetic mean of the random variables θ_i^*:

$$\overline{\theta^*} := \frac{1}{N}\sum_{j=1}^{N} \theta_j^*\ .$$

In the general nonlinear case, both estimators $\theta(\{r\})$ and $\overline{\theta^*}$ differ, and the latter has a reduced bias. This can be demonstrated as follows. We assume the bias can be expanded in powers of $1/N$

$$E\big(\theta(\{r\})\big) = \theta^0 + \frac{c_1}{N} + \frac{c_2}{N^2} + O(\frac{1}{N^3})\ ,$$

where θ^0 stands for the exact result to be estimated. Similarly we obtain

$$E\big(\theta_{-j}\big) = \theta^0 + \frac{c_1}{N-1} + \frac{c_2}{(N-1)^2} + O(\frac{1}{(N-1)^3})\ ,$$

as this estimator is based only upon $N-1$ elements. The expectation value of the modified random number θ_j^* is according to (4.43)

$$E\big(\theta_j^*\big) = N\theta^0 + c_1 + \frac{c_2}{N} - (N-1)\theta^0 - c_1 - \frac{c_2}{N-1} + O(\frac{1}{N^2}) = \theta^0 + O(\frac{1}{N^2})$$

We have reached the desired form (4.42) with the definition (4.43) for the random variables, which allows us to estimate the variance of the estimator $\overline{\theta^*}$ by the sample variance of the random variables θ_j^*

$$\mathrm{var}(\overline{\theta^*}) = \frac{\mathrm{var}(\theta_j^*)}{N}\ .$$

It can be shown that if the estimator $\theta(\{r\})$ has a bias of order $1/N$ as assumed before, then the variance of $\theta(\{r\})$ and θ^* are asymptotically the same[**?**].
Fortunately, the situation improves significantly for high temperatures. According to (**??**) the variance of the partition function $Z = \mathrm{tr}(e^{-\beta\hat{H}})$ determined via the stochastic evaluation of the trace is $\mathrm{var}(Z) = \frac{2}{N_r}\,\mathrm{tr}(e^{-2\beta\hat{H}})$. Hence the relative error is

$$\varepsilon_Z = \sqrt{\frac{2}{N_r}} \frac{\sqrt{\mathrm{tr}(e^{-2\beta\hat{H}})}}{\mathrm{tr}(e^{\beta\hat{H}})} \ .$$

For $\beta = 0$ the result is $\varepsilon_Z = \sqrt{\frac{2}{N_{st}N_r}}$ corroborating the general considerations in **??**. In summary, the little digression has illustrated that FTLM works well for high temperatures while for for $T \to 0$ the zero-temperature Lanczos procedure is preferable.

4.3.3 Dynamic Observables

For the evaluation of dynamic observables expectation values of the form

$$\left\langle \hat{B}(t)\, \hat{C} \right\rangle = \frac{1}{Z}\ \mathrm{tr}\left(\mathrm{e}^{-\beta\hat{H}} \mathrm{e}^{\mathrm{i}t\hat{H}} B\, \mathrm{e}^{-\mathrm{i}t\hat{H}} C \right) \tag{4.44}$$

have to be calculated. Here, the first two exponentials can be combined to a single one so that we actually have to treat two exponentials. We expand them in two Taylor series and calculate the trace in the basis $\{\left|\Phi^{(\nu)}\right\rangle\}$,

$$\left\langle \hat{B}(t)\, \hat{C} \right\rangle = \frac{1}{Z} \sum_{\left|\Phi^{(\nu)}\right\rangle} \sum_{k,l=0}^{\infty} \frac{(-\beta + \mathrm{i}t)^k}{k!} \frac{(-\mathrm{i}t)^l}{l!} \left\langle \Phi^{(\nu)} \middle| \hat{H}^k \hat{B} \hat{H}^l \hat{C} \middle| \Phi^{(\nu)} \right\rangle \ . \tag{4.45}$$

For the evaluation of the matrix elements, we insert the projectors $\hat{P}_k$ as we have done for static observables. An additional problem arises from the fact that $\hat{H}^l$ does not act directly on the state $\left|\Phi^{(\nu)}\right\rangle$. Therefore we have to perform a new Lanczos iteration with the start vector $\left|\tilde{\Phi}^{(\nu)}\right\rangle = \hat{C}\left|\Phi^{(\nu)}\right\rangle$. Quantities resulting from this second run will be denoted by tildes, e.g. $\left|\tilde{\psi}_j\right\rangle$ for the approximated eigenvector. We obtain for the matrix element

$$\left\langle \Phi^{(\nu)} \middle| \hat{H}^k \hat{B} \hat{H}^l \hat{C} \middle| \Phi^{(\nu)} \right\rangle = \sum_{i,j=0}^{n} (E_i^\nu)^k (\tilde{E}_j^\nu)^l \left\langle \Phi^{(\nu)} \middle| \psi_i^{(\nu)} \right\rangle \left\langle \psi_i^{(\nu)} \middle| \hat{B} \middle| \tilde{\psi}_j \right\rangle \left\langle \tilde{\psi}_j \middle| \tilde{\Phi}^{(\nu)} \right\rangle \ . \tag{4.46}$$

We emphasize that the approximated energy eigenvalues E_i^ν depend on the start vector $\left|\Phi^{(\nu)}\right\rangle$. By inserting this expression into (4.45) and exchanging the order of the sums we obtain

$$\left\langle \hat{B}(t)\, \hat{C} \right\rangle = \frac{1}{Z} \sum_{\left|\Phi^{(\nu)}\right\rangle} \sum_{i,j=0}^{n} \mathrm{e}^{-\beta E_i^\nu}\, \mathrm{e}^{-\mathrm{i}(\tilde{E}_j^\nu - E_i^\nu)t} \left\langle \Phi^{(\nu)} \middle| \psi_i^{(\nu)} \right\rangle \left\langle \psi_i^{(\nu)} \middle| \hat{B} \middle| \tilde{\psi}_j \right\rangle \left\langle \tilde{\psi}_j \middle| \tilde{\Phi}^{(\nu)} \right\rangle \ . \tag{4.47}$$

As before, the trace is actually calculated stochastically. The summation over a whole basis $\{\left|\Phi^{(\nu)}\right\rangle\}$ is replaced by the sum over N_r random vectors

$\{|\Phi^{(\nu)}\rangle\}$. Moreover, the Lanczos procedure is terminated after L iterations. This yields the approximation

$$\langle \hat{B}(t)\,\hat{C}\rangle = \frac{N_{st}}{MZ}\sum_{m=1}^{M}\sum_{i,j=0}^{L} \mathrm{e}^{-\beta E_i^{(m)}}\,\mathrm{e}^{-\mathrm{i}(\tilde{E}_j^{(m)}-E_i^{(m)})t}\langle\xi_m|\psi_i^{(\nu)}\rangle\langle\psi_i^{(\nu)}|\hat{B}|\tilde{\psi}_j\rangle\langle\tilde{\psi}_j|\tilde{\xi}_m\rangle\ .$$

In order to perform a Fourier transformation of the time variable we multiply this by $\mathrm{e}^{\mathrm{i}\omega t}/(2\pi)$ and integrate over all times. This yields

$$\begin{aligned}\langle \hat{B}(t)\,\hat{C}\rangle_\omega =& \frac{N_{st}}{MZ}\sum_{m=1}^{M}\sum_{i,j=0}^{L} \mathrm{e}^{-\beta E_i^{(m)}}\delta\Big(\omega-\big(\tilde{E}_j^{(m)}-E_i^{(m)}\big)\Big)\\ &\times\langle\xi_m|\psi_i^{(\nu)}\rangle\langle\psi_i^{(\nu)}|\hat{B}|\tilde{\psi}_j\rangle\langle\tilde{\psi}_j|\tilde{\xi}_m\rangle\ .\end{aligned}\tag{4.48}$$

In a simmilar way, the expectation value of the commuted operator $\langle\hat{C}\hat{B}(t)\rangle$ can be determined. By exploiting the cyclic invariance of the trace, we obtain

$$\langle\hat{C}\hat{B}(t)\rangle = \ \mathrm{tr}\,\mathrm{e}^{-\beta\hat{H}}\hat{C}\,\mathrm{e}^{\mathrm{i}t\hat{H}}\hat{B}\,\mathrm{e}^{-\mathrm{i}t\hat{H}} = \ \mathrm{tr}\,\mathrm{e}^{\mathrm{i}t\hat{H}}\hat{B}\,\mathrm{e}^{-\mathrm{i}t\hat{H}}\mathrm{e}^{-\beta\hat{H}}\hat{C}\tag{4.49}$$

By performing the same steps as above, we are led to

$$\langle \hat{C}(t)\,\hat{B}\rangle = \frac{N_{st}}{MZ}\sum_{m=1}^{M}\sum_{i,j=0}^{L} \mathrm{e}^{-\beta \tilde{E}_j^{(m)}}\,\mathrm{e}^{-\mathrm{i}(\tilde{E}_j^{(m)}-E_i^{(m)})t}\langle\xi_m|\psi_i^{(\nu)}\rangle\langle\psi_i^{(\nu)}|\hat{B}|\tilde{\psi}_j\rangle\langle\tilde{\psi}_j|\tilde{\xi}_m\rangle$$

whose Fourier transformed is given by

$$\begin{aligned}\langle \hat{C}\,\hat{B}(t)\rangle_\omega =& \frac{N_{st}}{MZ}\sum_{m=1}^{M}\sum_{i,j=0}^{L} \mathrm{e}^{-\beta \tilde{E}_j^{(m)}}\delta\big(\omega+\tilde{E}_j^{(m)}-E_i^{(m)}\big)\\ &\times\langle\xi_m|\psi_i^{(\nu)}\rangle\langle\psi_i^{(\nu)}|\hat{B}|\tilde{\psi}_j\rangle\langle\tilde{\psi}_j|\tilde{\xi}_m\rangle\ .\end{aligned}\tag{4.50}$$

Therefore, the spectral function of the two operators $\hat{B}$ and $\hat{C}$ is given by

$$\begin{aligned}S_{BC}(\omega) \overset{\mathrm{def}}{=}& \frac{1}{2\pi}\left\langle \hat{B}(t)\hat{C}-\epsilon\hat{C}\hat{B}(t)\right\rangle_\omega \qquad (4.51)\\ =& \frac{N_{st}}{2\pi MZ}\sum_{m=1}^{M}\sum_{i,j=0}^{L}\big(\mathrm{e}^{-\beta E_i^{(m)}}-\epsilon\mathrm{e}^{-\beta\tilde{E}_j^{(m)}}\big)\delta\Big(\omega-\big(\tilde{E}_j^{(m)}-E_i^{(m)}\big)\Big)\\ &\times\langle\xi_m|\psi_i^{(\nu)}\rangle\langle\psi_i^{(\nu)}|\hat{B}|\tilde{\psi}_j\rangle\langle\tilde{\psi}_j|\tilde{\xi}_m\rangle\ .\end{aligned}$$

The δ-distribution links the difference of the two energies $E_i^{(m)}$ and $\tilde{E}_j^{(m)}$ with ω. By exploiting this fact, we end up with the formula

$$\begin{aligned}S_{BC}(\omega) =& \frac{1-\epsilon\mathrm{e}^{-\beta\omega}}{2\pi}\frac{N_{st}}{MZ}\sum_{m=1}^{M}\sum_{i,j=0}^{L} \mathrm{e}^{-\beta E_i^{(m)}}\delta\Big(\omega-\big(\tilde{E}_j^{(m)}-E_i^{(m)}\big)\Big)\\ &\times\langle\xi_m|\psi_i^{(\nu)}\rangle\langle\psi_i^{(\nu)}|\hat{B}|\tilde{\psi}_j\rangle\langle\tilde{\psi}_j|\tilde{\xi}_m\rangle\ .\end{aligned}\tag{4.52}$$

5. Monte Carlo Methods

5.1 Probability Theory in a Nutshell

Let $A, B, C, \ldots$ be elementary propositions, e.g. statements that are either true or false. $P(A \,|\, C)$ denotes the probability that A is true under the condition that C is true. This is a so called *conditional probability*. Notice that there are no unconditional probabilities in the real world. There are two fundamental rules in probability theory that allow to tackle any problem in the realm of inductive logic: The *product rule* for joint probabilities

$$P(A \wedge B \,|\, C) = P(A \,|\, B \wedge C) \cdot P(B \,|\, C) = P(B \,|\, A \wedge C) \cdot P(A \,|\, C) \; . \quad (5.1)$$

One immediate consequence is *Bayes' Theorem*

$$P(A \,|\, B \wedge C) = \frac{P(B \,|\, A \wedge C) \cdot P(A \,|\, C)}{P(B \,|\, C)} \; . \quad (5.2)$$

It enables us to calculate backwards probabilities from forward probabilities and will be used exhaustively.
The *sum rule* to evaluate the logical OR of propositions

$$P(A \vee B \,|\, C) = P(A \,|\, C) + P(B \,|\, C) - P(A \wedge B \,|\, C) \; . \quad (5.3)$$

The last term cancels if A and B mutually exclude each other. If the propositions $\{B_i\}_{i=1}^N$ are mutually exclusive and $P(\vee_{i=1}^N B_i) = 1$ (normalization) we call the set $\{B_i\}$ complete. In this case we can express any other proposition A as

$$A = \vee_{i=1}^N (A \, B_i) \, . \quad (5.4)$$

The probability for A can therefore be expressed through the *marginalization rule*

$$P(A \,|\, C) = P(\vee_{i=1}^N (A \, B_i) \,|\, C) = \sum_{i=1}^{N} p(A \wedge B_i \,|\, C) \; . \quad (5.5)$$

For continuous quantities x we define $dB(x)$ as the proposition x *is from the the interval* $(x, x + dx)$. The corresponding probability is usually expressed via the the probability density

$$P(dB(x) \,|\, C) = p(x \,|\, C)\, dx \;. \tag{5.6}$$

The *marginalization rule* for a complete continuous set of propositions reads

$$P(A \,|\, C) = \int p(A, x \,|\, C)\, dx \;, \tag{5.7}$$

with the normalization condition

$$\int p(x \,|\, C)\, dx = 1 \;. \tag{5.8}$$

We will have ample opportunities to apply the rules of probability theory, so we note waste our precious time on mock examples here.

5.2 The Autocorrelation Function

The notion of the autocorrelation function is known in the following form: Suppose we have a real valued function $A(t)$, then the integral

$$C(\tau) = \int_{-\infty}^{\infty} A(t)\, A(t+\tau)\, d\tau \tag{5.9}$$

is called the autocorrelation of $A(t)$. Intuitively, $C(\tau)$ averages the correlation of values of A separated by the *lag* τ. If $A(t)$ is a periodic function with periodicity T, then $C(\tau)$ displays sharp peaks at $\tau = T, 2T, 3T, \ldots$.
In the context of Monte Carlo Simulations, we will be interested in the autocorrelation of the *fluctuations* of an observable A. Suppose we have N measurements of the observable A. The values are stored in the vector $\mathbf{A} = (A_0, A_1, \ldots A_{N-1})$. The mean value of A and the deviation of each trial are given by

$$\bar{A} = \frac{1}{N} \sum_{i=0}^{N-1} A_i \;, \quad \Delta\mathbf{A} = (A_0 - \bar{A}, A_1 - \bar{A}, \ldots A_{N-1} - \bar{A}) \;. \tag{5.10}$$

Analogously to Eq.(5.9), we define the *autocorrelation of the observable* A as the autocorrelation of its fluctuations about its mean $\bar{A}$. A discretized version of Eq.(5.9) has the form

$$C(\tau) = \frac{1}{N} \sum_{t=0}^{N-1} \Delta A(t)\, \Delta A(t+\tau) \;. \tag{5.11}$$

The definition (5.11) is problematic since $t+\tau$ is not necessarily smaller than N. There are several possibilities to overcome this problem. The simplest and straight forward one is to actually restrict the range of the sum from $t = 0$ to $t = N - \tau$, leading to

$$C'(\tau) = \frac{1}{N-L} \sum_{t=0}^{N-1-L} (A(t)-\bar{A}_0)(A(t+\tau)-\bar{A}_\tau) \ , \ \text{with } \tau \in \{0,1,\dots L\} \ , \ L \ll N \tag{5.12}$$

where the expectation value $\bar{A}_\tau$ with index τ stands for the average

$$\bar{A}_\tau \stackrel{\text{def}}{=} \frac{1}{N-L} \sum_{t=0}^{N-1-L} A(t+\tau) \ . \tag{5.13}$$

Expanding the product of Eq.(5.12) we find

$$C'(\tau) = \left(\frac{1}{N-L} \sum_{t=0}^{N-1-L} A(t)\, A(t+\tau) \right) - \bar{A}_\tau\, \bar{A}_0 \tag{5.14}$$

In the limit of uncorrelated data, the first sum of Eq.(5.14) tends to the product $\bar{A}_\tau\, \bar{A}_0$. Hence, the new definition $C'(\tau)$ is zero for uncorrelated data, as in the case of an infinite sample. In contrast to that, taking always the same average $\bar{A}$ instead of $\bar{A}_\tau$ in Eq. (5.12) does not result in $C'(\tau) = 0$ for uncorrelated data.

$$\begin{aligned} \tilde{C}(\tau) &= \frac{1}{N-L} \sum_{t=0}^{N-L-1} (A(t) - \bar{A})(A(t+\tau) - \bar{A}) \\ &= \frac{1}{N-L} \sum_{t=0}^{N-L-1} A(t)\, A(t+\tau) - \bar{A}(\bar{A}_\tau + \bar{A}_0) + \bar{A}^2 \\ &= \bar{A}_0\, \bar{A}_\tau - \bar{A}(\bar{A}_\tau + \bar{A}_0) + \bar{A}^2 \neq 0 \end{aligned} \tag{5.15}$$

This means that $C(\tau)$ erroneously indicates autocorrelations due to the finite data size.

5.3 Stochastic Evaluation of Sums and Integrals

We are interested in evaluating the sum or integral

$$\langle f \rangle = \int f(\mathbf{x})\, \rho(\mathbf{x})\, d\mu(\mathbf{x}) \ , \tag{5.16}$$

where μ is a measure and ρ denotes a probability density, $\rho(\mathbf{x}) \geq 0, \int \rho(\mathbf{x})\, d\mu(\mathbf{x}) = 1$. In order to simplify our life, we use $d\mu(\mathbf{x}) = d\mathbf{x}$. We estimate the integral $\langle f \rangle$ by

$$F = \frac{1}{N} \sum_{i=1}^{N} f(\mathbf{x}_i) \ , \tag{5.17}$$

where the states $\mathbf{x}_i$ are chosen in an appropriate random way, that has to be specified later on. The distribution of the random variable F is – according to the *marginalization rule* – given by

$$p(F|I) = \int \underbrace{p(F|\mathbf{x}_1, \ldots, \mathbf{x}_N, I)}_{\delta(F - \frac{1}{N}\sum_{i=1}^{N} f(\mathbf{x}_i))} p(\mathbf{x}_1, \ldots \mathbf{x}_N|I)\, d^N\mathbf{x}\,. \tag{5.18}$$

The probability density is normalized to one (0^{th} moment). Furthermore its mean value (1^{st} moment) reads

$$\begin{aligned} E(F\,|\,I) &= \int dF F p(F|I) = \frac{1}{N}\int \sum_i f(\mathbf{x}_i) p(\mathbf{x}_1, \ldots, \mathbf{x}_N|I)\, d^N x \\ &= \frac{1}{N}\sum_i \int_{\mathbf{x}_i} f(\mathbf{x}_i) \left[\int_{j\neq i} p(\mathbf{x}_1, \ldots, \mathbf{x}_N|I) \prod_{j\neq i} d\mathbf{x}_j\right] d\mathbf{x}_i \\ &= \frac{1}{N}\sum_i \int_{\mathbf{x}_i} f(\mathbf{x}_i)\, p(\mathbf{x}_i|I)\, d\mathbf{x}_i\,, \end{aligned} \tag{5.19}$$

where the *marginal distribution* $p_i = p(\mathbf{x}_i|I)$ has been introduced.

Warning! We are using a short hand notation for probabilities and probability densities in order to avoid overloading the notation. The price that we have to pay is that we have to be very careful with the correct interpretation. The expression $p(\mathbf{x}_i|I)$ actually mean $p(\mathbf{x}_i = x_i|I)$, that is: 1) the random variable $\mathbf{x}_i$ takes on the value x_i and 2) the conditional complex defines the context. Here I carries the information that we originally had N random variable and we have marginalized $N-1$ of them, leaving merely the variable with index i. The value that the random variable $\mathbf{x}_i$ has could also be noted by ξ and a more comprehensive notation could be $p_i(\xi|A_i, I)$, with the proposition A_i^N :*over all random variables* $(\mathbf{x}_1, \ldots \mathbf{x}_N)$ *apart form* $\mathbf{x}_i$ *has been marginalized.* We will nevertheless stick to the dangerous but short notation. We demand now that the random variables $\mathbf{x}_i$ are generated by a a so called *homogeneous stochastical process*, which means that $p(\mathbf{x}_i|I)$ does not depend on the index i, i.e. $p_i(\xi|A_i, I) = p_j(\xi|A_j^N, I)\forall j$ and we end up with the desired result

$$E(F|I) = \underbrace{\frac{1}{N}\sum_i}_{=1} \int f(\mathbf{x})\, p(\mathbf{x}\,|\,I)\, d\mathbf{x} \stackrel{!}{=} \langle f\rangle\,. \tag{5.20}$$

We have to ensure by the generation process of the values $\mathbf{x}_i$ that $p(\mathbf{x}\,|\,I) = \rho(x)$ The sample mean F is therefore *unbiased*. In order to scrutinize whether it is efficient we determine the variance (2^{nd} moment) of F

$$
\begin{aligned}
E(F^2 \,|\, I) &= \int dF F^2 p(F \,|\, I) \\
&= \int dF\, F^2\, \delta(F - \frac{1}{N}\sum_i f(\mathbf{x}_i)) \cdot p(\mathbf{x}_1, \ldots, \mathbf{x}_N|I)\; d^N\mathbf{x} \\
&= \frac{1}{N^2} \int \sum_{i,l} f(\mathbf{x}_i)\, f(\mathbf{x}_k)\, p(\mathbf{x}_1, \ldots, \mathbf{x}_N|I)\; d^N\mathbf{x} \\
&= \frac{1}{N^2} \sum_{i\neq k} \iint f(\mathbf{x}_i)\, f(\mathbf{x}_k) p(\mathbf{x}_i, \mathbf{x}_k|I) + \frac{1}{N^2}\sum_i \int f^2(\mathbf{x}_i)\, p(\mathbf{x}_i|I)\, d\mu(\mathbf{x}_i) \\
&= \frac{1}{N^2} \sum_{i\neq k} \overline{f(\mathbf{x}_i) f(\mathbf{x}_k)} + \frac{1}{N^2}\sum_i \overline{f(\mathbf{x}_i)^2}\;, \qquad (5.21)
\end{aligned}
$$

where we have introduced the marginal distribution $p(\mathbf{x}_i, \mathbf{x}_k|I)$ of two variables. We can combine the result

$$
\sum_{i,k} \overline{f(\mathbf{x}_i) f(\mathbf{x}_k)} = \sum_{i\neq k} \overline{f(\mathbf{x}_i) f(\mathbf{x}_k)} + \sum_i \overline{f(\mathbf{x}_i)^2}\;. \qquad (5.22)
$$

and the variance is

$$
E(\Delta F^2|I) = \frac{1}{N^2}\sum_{i,k} \overline{f(\mathbf{x}_i) f(\mathbf{x}_k)} - \left(\frac{1}{N}\sum_i \overline{f(\mathbf{x}_i)}\right)^2 = \frac{1}{N^2}\sum_{i,k} \underbrace{\overline{\Delta f(\mathbf{x}_i)\Delta f(\mathbf{x}_k)}}_{\sim a_{ik}}\;. \qquad (5.23)
$$

It is expedient to introduce the (normalized) autocorrelation a_{ik}

$$
a_{ik} = \frac{\overline{\Delta f(\mathbf{x}_i)\Delta f(\mathbf{x}_k)}}{\overline{\Delta^2 f(\mathbf{x}_i)}}\;, \quad \Delta f(\mathbf{x}) = f(\mathbf{x}) - \bar{f}\;. \qquad (5.24)
$$

Along with the definition $\sigma_f^2 = \overline{(\Delta f(\mathbf{x}))^2}$ we have

$$
E(\Delta F^2|I) = \frac{\sigma_f^2}{N^2}\sum_{i,k} a_{ik} \;=\; \frac{\sigma_f^2}{N}\sum_l a(l)\;. \qquad (5.25)
$$

where we used the fact that for homogeneous stochastical processes $a_{ik} = a(i-k)$. For small values of l, the autocorrelation is superposition of exponential decays. For sufficiently large l, the slowest exponential decay dominates the behavior, which defines a typical correlation length ξ

$$
a_l = e^{-|l|/\xi} \qquad \text{for sufficiently large } l\;. \qquad (5.26)
$$

For a quick and dirty estimate, we assume that (5.26) is true for all l. Then the variance simplifies to

$$E(\Delta F^2|I) = \frac{\sigma_f^2}{N}\left(\frac{2}{1-e^{-1/\xi}} - 1\right) . \tag{5.27}$$

We can distinguish two extreme cases:

$$\xi \to 0 : E(\Delta F^2|I) = \frac{\sigma_f^2}{N} \qquad \text{(uncorrelated data)} \tag{5.28}$$

$$\xi \gg 1,\ \xi < N : E(\Delta F^2|I) = \frac{\sigma_f^2}{N/(2\xi)} . \tag{5.29}$$

These limiting cases are actually always valid if we identify ξ by as an effective correlation length. Let's summarize the results: In both cases the dependence on N goes like $1/N$. That means that the uncertainty in F is proportional to $1/\sqrt{N}$ and independent of the dimension of the problem. Using other methods like rejection sampling, the error usually increases exponentially with the dimension. Furthermore ΔF depends on the variance σ_f^2 and on the autocorrelation length ξ. The requirements to the process generating the random variable ξ are thus

- $p(\mathbf{x}\,|\,I) = \rho(x)$
- homogeneous process
- ξ as small as possible

5.4 Markov Chain Monte Carlo (MCMC)

5.4.1 Markov Events

To fix ideas we consider a sequence of L random variables $\{x_1, \ldots, x_L\}$ which can take on discrete values from a set of N mutually exclusive discrete states $\{\xi_1, \ldots, \xi_N\}$. We denote the realization i of the sequence as

$$\{\xi_{i_1}, \ldots, \xi_{i_L}\} \qquad \text{with } i_\alpha \in \{1, \ldots, N\} \; . \tag{5.30}$$

Suppose we can calculate the probability of the event $L+1$ according to some law

$$P(x_{L+1} = \xi_j \,|\, x_L, x_{L-1}, \ldots x_1) \; . \tag{5.31}$$

The sequence is called a *Markov – chain* if the above probability actually depends only on x_L, i.e.

$$P(x_{L+1} = \xi_j \,|\, x_L = \xi_i) =: M_{ji}^{(L)} \; . \tag{5.32}$$

The quantities $M_{ji}^{(L)}$ are called *Stochastic matrices* of the Markov chain of *Markov matrices*. The parameter L, labeling the random variable $\mathbf{x}$, can be viewed as a *time*. The matrices $M_{ji}^{(L)}$ fulfill the following obvious relations of positivity and normalization

$$M_{ji}^{(L)} \geq 0 \qquad \text{and} \qquad \sum_{j=1}^{N} M_{ji}^{(L)} = 1 \; . \tag{5.33}$$

A Markov chain is called *homogeneous* if the probabilities $M_{ji}^{(L)}$ do *not* depend on L. In the following we focus on homogeneous markov chains. The marginalization rule allows to calculate the probabilities for transitions from time 1 to m leading to

$$P(x_m = \xi_j \,|\, x_1 = \xi_i) = (M^m)_{ji} \; . \tag{5.34}$$

Suppose that for a given time n the probability that the system is in state ξ_i is given by the distribution

$$P(x_n = \xi_i) =: \rho^{(n)}(\xi_i) \; , \tag{5.35}$$

how does the distribution look like in the next step (at time $n+1$).

$$P(x_{n+1} = \xi_i) = \rho^{(n+1)}(\xi_i) = \sum_{j=1}^{N} \underbrace{P(x_{n+1} = \xi_i \,|\, x_n = \xi_j)}_{M_{ij}} \, P(x_n = \xi_j)$$

Consequently, the *evolution* is given by

$$\rho^{(n+1)}(\xi_i) = \sum_{j=1}^{N} M_{ij}\, \rho^{(n)}(\xi_j) \; . \tag{5.36}$$

Obviously the norm is a conserved quantity

$$\sum_{i=1}^{N} \rho^{(n+1)}(\xi_i) = \sum_{i=1}^{N} \sum_{j=1}^{N} M_{ij}\, \rho^{(n)}(\xi_j) = \sum_{j=1}^{N} \underbrace{\sum_{i=1}^{N} M_{ij}}_{=1}\, \rho^{(n)}(\xi_j) = 1 \; . \tag{5.37}$$

A distribution is called the *invariant distribution* if it does not change by application of the stochastic matrix. It is denoted by $\rho^{(\infty)}(\xi_i) \equiv \rho^{(inv)}(\xi_i)$ and satisfies at the same time the eigenvalue equation

$$\rho^{(\infty)}(\xi_i) = \sum_{j=1}^{N} M_{ij}\, \rho^{(\infty)}(\xi_j) \tag{5.38}$$

with eigenvalue $\lambda = 1$. According to what we learned from the vector iteration scheme, the procedure will converge towards the invariant distribution if the eigenvalue 1 is the dominant eigenvalue of the stochastic matrix M_{ji} and if the initial state is not orthogonal to invariant distribution. Starting from the general eigenvalue equation

$$\sum_{j=1}^{N} M_{ij}\, \tilde{\rho}(\xi_j) = \lambda\, \tilde{\rho}(\xi_i) \tag{5.39}$$

and summing over i and exchanging the order of summation yields

$$\sum_{i=1}^{N} \sum_{j=1}^{N} M_{ij}\, \tilde{\rho}(\xi_j) = \sum_{j=1}^{N} \sum_{i=1}^{N} M_{ij}\, \tilde{\rho}(\xi_j) = \lambda \sum_{i=1}^{N} \tilde{\rho}(\xi_i) \; , \tag{5.40}$$

resulting in

$$\sum_{j=1}^{N} \tilde{\rho}(\xi_j) = \lambda \sum_{i=1}^{N} \tilde{\rho}(\xi_i) \; . \tag{5.41}$$

The eigensolutions are

- $\sum_{j=1}^{N} \tilde{\rho}_1(\xi_j) \neq 0 \quad \Rightarrow \quad \lambda_1 = 1$
- $\sum_{j=1}^{N} \tilde{\rho}_\nu(\xi_j) = 0 \quad \Rightarrow \quad \lambda_\nu = \text{arbitrary} \qquad \forall \nu > 1$

We start the iteration with an – to some extend – arbitrary density $\rho^{(0)}(\xi_i)$, that is normalized to one. This is compatible with any linear combination of eigenvectors of the form

$$\rho^{(0)}(\xi_i) = \tilde{\rho}_1(\xi_i) + \sum_{\nu=2}^{N} c_\nu \tilde{\rho}_\nu(\xi_i) \ ,$$

with arbitrary coefficients c_ν. But obviously, a normalized initial distribution can never be orthogonal the invariant distribution. We merely have to make sure that the eigenvalue one is not degenerate and that it is largest eigenvalue of the Markov matrix. The proof can be found in standard text books on Markov processes, such as the book of William Feller. The proof shows that one is the dominating eigenvalue for all Markov matrices, i.e. $|\lambda_\nu| \leq 1$. However, in order to guarantee that there is only one eigenvector, the process has to be ergodic, i.e. starting from any state ξ_i it is possible to reach any other state ξ_j within finite time, or rather for all j there is an integer m for which $(M^m)_{ij} > 0$. In the MCMC algorithms we have to make sure that we if we start from any state i, we can reach any other state by repeated moves.

5.4.2 The Metropolis Hastings choice of the Matrix M_{ij}

We have seen that the Markov process will ultimately converge towards the invariant distribution. We can exploit this fact if we construct the Markov matrix such that the invariant distribution is identical to the probability density $\rho(x)$ of the underlying physical problem for which we want to compute $\int f(x)\rho(x)d^N x$. A widely used approach stems from Metropolis.

Metropolis – Hastings Algorithm:.

- Start with an initial state $\mathbf{x}_0$
- Set the MC time to $n = 0$
- Create a trial state $\mathbf{x}^T$ for time $n+1$ from the actual state $\mathbf{x}_n$ according to the proposal distribution $q(\mathbf{x}^T|\mathbf{x}_n)$. This proposal distribution q is typically a normal deviate

$$q(\mathbf{x}^T|\mathbf{x}) \sim \exp\left(-\frac{1}{2}\left(\mathbf{x}^T - \mathbf{x}\right) C^{-1} \left(\mathbf{x}^T - \mathbf{x}\right)\right) \ . \tag{5.42}$$

  The best choice for the matrix C is the covariance matrix of the desired distribution $p(\mathbf{x})$. Since the covariance matrix will presumably not be known, a rough estimation usually does a good job. Otherwise, uniform densities restricted to a cube or a sphere about $\mathbf{x}$ are also commonly used to create the trial state $\mathbf{x}^T$ in the neighborhood of the reference state x.
- The trial state $\mathbf{x}^T$ is accepted with probability $\alpha(\mathbf{x}^T, \mathbf{x})$ given by

$$\alpha(\mathbf{x}^T, \mathbf{x}) = \min\left(1, \frac{p(\mathbf{x}^T)\, q(\mathbf{x}|\mathbf{x}^T)}{p(\mathbf{x})\, q(\mathbf{x}^T|\mathbf{x})}\right) \ . \tag{5.43}$$

  The second factor in the numerator and in the denominator is due to Hastings. He improved the original idea of Metropolis. This correction assures *detailed balance* also in the case $q(\mathbf{x}|\mathbf{x}^T) \neq q(\mathbf{x}^T|\mathbf{x})$.

We illustrate the importance of the Hastings factor on the basis of a four site Ising chain with open boundary conditions. We suppose that the updating procedure flips two adjacent spins if they are unequal. This keeps the magnetization constant. Consider the updating of the state

$$| \uparrow, \downarrow, \uparrow, \downarrow | \overset{p=1/3}{\longrightarrow} \begin{cases} | \downarrow, \uparrow, \uparrow, \downarrow | \\ | \uparrow, \uparrow, \downarrow, \downarrow | \\ | \uparrow, \downarrow, \downarrow, \uparrow | \end{cases} \overset{p=1}{\longrightarrow} | \uparrow, \downarrow, \uparrow, \downarrow | \, .$$

We see that from the state $| \uparrow, \downarrow, \uparrow, \downarrow |$ three different states can be reached with probability $p = 1/3$. However, from one of the the resulting states, namely $| \uparrow, \uparrow, \downarrow, \downarrow |$, only one state can be obtained. I.e. the probabilities back and forth are different and without the Hastings term the result would be biased.

5.4.3 The invariant distribution of the Metropolis Hastings MC

In this section we study the convergence and autocorrelation properties of a Markov-Chain $\{x_1, x_2, \ldots, x_N\}$. The chain is governed by the homogeneous Markov process

$$M_{ji} := P(\hat{x}_{\nu+1} = \xi_j | \hat{x}_\nu = i, \mathcal{B}) \, , \tag{5.44}$$

which is independent of the 'time' ν. The background information $\mathcal{B}$ contains the details of the Markov process, e.g. whether Metropolis-Hastings or Glauber dynamics is used and which proposal distribution is employed. The Markov matrix element M_{ji} consists of two parts, the proposal distribution $q(\xi_k|\xi_i)$ to propose the state ξ_k starting from state ξ_i and the acceptance or rejection according to the probability $\alpha(\xi_k|\xi_i)$ to accept state ξ_k coming from state ξ_i. We introduce the trial state $\mathbf{x}^T$ via the marginalization rule

$$\begin{aligned} P(\hat{x}_{\nu+1} = \xi_j | \hat{x}_\nu = \xi_i, \mathcal{B}) & \qquad (5.45) \\ &= \sum_{k=1}^{\mathcal{N}} P(\hat{x}_{\nu+1} = \xi_j | x^T = \xi_k, \hat{x}_\nu = \xi_i, \mathcal{B}) \; P(x^T = \xi_k | \hat{x}_\nu = \xi_i, \mathcal{B}) \\ &= \sum_{k=1}^{\mathcal{N}} P(\hat{x}_{\nu+1} = \xi_j | x^T = \xi_k, \hat{x}_\nu = \xi_i, \mathcal{B}) \; q(\xi_k|\xi_i) \, . \end{aligned}$$

According to the rules, by which the Markov process is generated, we have two alternatives: either the state is accepted or rejected, which is described by the respective propositions A or $\overline{A}$. The repeated use of the marginalization rule yields

$$
\begin{aligned}
M_{ji} &= P(\hat{x}_{\nu+1} = \xi_j | \hat{x}_\nu = \xi_i, \mathcal{B}) \\
&= \sum_{k=1}^{\mathcal{N}} \overbrace{P(\hat{x}_{\nu+1} = \xi_j | A, x^T = \xi_k, \hat{x}_\nu = \xi_i, \mathcal{B})}^{\delta_{jk}} \; \alpha(\xi_k|\xi_i) \; q(\xi_k|\xi_i) \\
&+ \sum_{k=1}^{\mathcal{N}} \overbrace{P(\hat{x}_{\nu+1} = \xi_j | \overline{A}, x^T = \xi_k, \hat{x}_\nu = \xi_i, \mathcal{B})}^{\delta_{ji}} \; \Big(1 - \alpha(\xi_k|\xi_i)\Big) \; q(\xi_k|\xi_i) \\
&= \alpha(\xi_j|\xi_i) \; q(\xi_j|\xi_i) + \delta_{ji} \sum_{k=1}^{\mathcal{N}} \Big(1 - \alpha(\xi_k|\xi_i)\Big) \; q(\xi_k|\xi_i) \, . \qquad (5.46)
\end{aligned}
$$

We now multiply with $\rho(\xi_i)$ and obtain

$$
\begin{aligned}
M_{ji}\rho(\xi_i) &= \alpha(\xi_j|\xi_i) \; q(\xi_j|\xi_i)\rho(\xi_i)) \\
&\quad + \delta_{ji} \sum_{k=1}^{\mathcal{N}} \Big(\rho(\xi_i) q(\xi_k|\xi_i) - \alpha(\xi_k|\xi_i)\rho(\xi_i) q(\xi_k|\xi_i)\Big) \; . \qquad (5.47)
\end{aligned}
$$

We immediately realize that the second term of the rhs is symmetric in i and j. Next we invoke the definition of the acceptance probability α to proof the the same symmetry for the first term

$$
\alpha(\xi_j|\xi_i)\rho(\xi_i) q(\xi_j|\xi_i) = \min\Big(q(\xi_j|\xi_i)\rho(\xi_i), q(\xi_i|\xi_j)\rho(\xi_j)\Big) \; .
$$

Hence the rhs of (5.47) (and therefore also the lhs) is invariant under exchange of the indices i and j resulting in the detailed balance condition

$$
M_{ji}\rho(\xi_i) = M_{ij}\rho(\xi_j) \; . \qquad (5.48)
$$

If we next sum over the index i we have

$$
\sum_i M_{ji}\rho_i = \rho_j \, . \qquad (5.49)
$$

I.e., the invariant distribution of the Metropolis-Hastings Markov matrix is indeed identical to that of the physical problem.

5.4.4 Properties of the Markov matrix

We know already that

$$
\sum_{j=1}^{\mathcal{N}} M_{ji} = 1 \, . \qquad (5.50)
$$

This has two consequences. First, if we introduce the vector $\mathbf{1}$ whose components are all one, $(\mathbf{1})_i = 1$ we have

$$\mathbf{1}^T M = \mathbf{1}^T \,, \tag{5.51}$$

i.e. $\mathbf{1}$ is the left-eigenvector of M with eigenvalue 1. The corresponding right-eigenvector is according to (**??**) the vector $\boldsymbol{\rho}$ with components ρ_i.
Multiplication of both sides of (5.49) with $(\rho_i \rho_j)^{-1/2}$ yields

$$\rho_j^{-1/2} M_{ji} \rho_i^{1/2} = \rho_i^{-1/2} M_{ij} \rho_j^{1/2} \,.$$

We introduce the real symmetric matrix

$$A_{ij} := \rho_i^{-1/2} M_{ij} \rho_j^{1/2} \tag{5.52}$$

and the diagonal matrix

$$\Delta_{ij} := \delta_{ij}\ \rho_i^{1/2} \tag{5.53}$$

and express the Markov matrix in these quantities

$$M = \Delta A \Delta^{-1} \,. \tag{5.54}$$

If the spectral representation of A is written as

$$A = U D U^T$$

then the singular-value decomposition of M reads

$$M = \Delta U D U^T \Delta^{-1} = \Delta U D (\Delta^{-1} U)^T \,,$$

which we define as

$$M = X D Y^T \,. \tag{5.55}$$

Obviously, the matrix of right-eigenvalues is

$$X = \Delta\, U \tag{5.56}$$

and the matrix of left-eigenvalues is

$$Y = \Delta^{-1}\, U \,. \tag{5.57}$$

It should be stressed that the column vectors of X and Y respectively need not to be normalized to 1 if derived this way. They can, however, easily be normalized:

$$\begin{aligned} M &= \sum_l\ \boldsymbol{x}_l\ d_l\ \boldsymbol{y}_l^T \\ &= \sum_l\ \frac{1}{\|x_l\|}\ \boldsymbol{x}_l\ d_l\ \|x_l\| \boldsymbol{y}_l^T \,. \end{aligned}$$

Since $\|x_l\| = 1/\|y_l\|$ the left and right eigenvectors are now normalized. An immediate consequence of (5.56) and (5.56) is the generally valid property

$$X^T\, Y = Y^T\, X = \hat{1}\,; \tag{5.58}$$

left- and right-eigenvectors are mutually orthogonal. Moreover, combining (5.56) and (5.57), we derive

$$X = \Delta^2\, Y \qquad \text{and} \qquad Y = \Delta^{-2} X\,, \tag{5.59}$$

which is obviously fulfilled for the dominant eigenvalue $\lambda_1 = 1$, where

$$x_{i1} = \rho_i \tag{5.60a}$$
$$y_{i1} = 1\,. \tag{5.60b}$$

The corresponding eigenvector of A is

$$u_{i1} = \sqrt{\rho_i}\,. \tag{5.61}$$

The eigenvectors of M do not form an orthogonal set of eigenvectors, the relation is rather according to (5.58) and (5.59)

$$\hat{1} = Y^T \Delta^2 Y = X^T \Delta^{-2} X\,. \tag{5.62}$$

Due to the mutual orthogonality of left- and right-eigenvectors (5.58) the extension of the spectral representation to powers of M applies

$$M^\nu = X\; D^\nu\; Y^T\,. \tag{5.63}$$

If we assume an ergodic Markov process then

$$\lambda_\nu < 1\; \forall \nu > 1\,. \tag{5.64}$$

We therefore have again

$$(M^\nu)_{ji} \underset{\nu\to\infty}{\longrightarrow} X(j,1)\; d_1^\nu\; Y(i,1) = \rho_j \tag{5.65}$$

that the Markov process converges irrespective of the initial state to the invariant distribution. For the following it is expedient to extract the dominant eigenvalue from the spectral representation of M and to define the matrix

$$M'_{ji} := M_{ji} - X(j,1)\; d_1\; Y(i,1) = \sum_{l=2}^{\mathcal{N}} X(j,l)\; d_l\; Y(i,l) \tag{5.66}$$

$$M_{ji} = M'_{ji} + \rho_j\,, \tag{5.67}$$

which is equivalent to the substitution of the eigenvalues of M

$$d_1 \to d'_1 = 0 \quad , \quad d_\nu \to d'_\nu = d_\nu \, \forall \nu > 2 \tag{5.68}$$

$$M' = X D' Y^T \, . \tag{5.69}$$

From (5.66) we readily see that

$$M'^{\nu}_{ji} := M^{\nu}_{ji} - X(j,1) \; d^{\nu}_1 \; Y(i,1) = \sum_{l=2}^{\mathcal{N}} X(j,l) \; d^{\nu}_l \; Y(i,l) \tag{5.70}$$

$$M^{\nu}_{ji} = M'^{\nu}_{ji} + \rho_j \, , \tag{5.71}$$

5.4.5 MCM Sample Mean

The sought-for mean

$$\Big\langle f \Big\rangle = \sum_{i=1}^{\mathcal{N}} f(\xi_i) \; \rho(\xi_i) \tag{5.72}$$

is estimated by the MC mean

$$S = \frac{1}{N} \sum_{\nu=1}^{N} f(\hat{x}_\nu) \, . \tag{5.73}$$

In the following text we will simplify the notation by the abbreviations $f_i = f(\xi_i)$ and $\rho_i = \rho(\xi_i)$. Instead of investigating the probability density of the sample mean S, in analogy with the central limit theorem, we are merely interested in the lowest moments, namely mean and variance. We start out with the expectation value of the sample/MC mean

$$\Big\langle S \Big\rangle = \frac{1}{N} \sum_{\nu=1}^{N} \Big\langle f(\hat{x}_\nu) \Big\rangle \tag{5.74}$$

$$= \frac{1}{N} \sum_{\nu=1}^{N} \sum_{j=1}^{\mathcal{N}} f(\xi_j) \; P(\hat{x}_\nu = \xi_j | p_0, \mathcal{B}) \, . \tag{5.75}$$

The Markov chain is started in the initial state $\hat{x}_0$, which is drawn from a distribution p^0, with $p^0_i = p^0(\xi_i)$. As a special case, the chain could always start with the same state, say $\hat{x}_0 = \xi_{i_0}$. The argument p_0 in the conditioning part of the probability specifies which initial distribution is being used. We invoke the marginalization rule of probability theory

$$\Big\langle S \Big\rangle = \frac{1}{N} \sum_{\nu=1}^{N} \sum_{j=1}^{\mathcal{N}} \sum_{i=1}^{\mathcal{N}} f(\xi_j)\; P(\hat{x}_\nu = \xi_j | \hat{x}_0 = x_i, \mathcal{B})\; P(\hat{x}_0 = \xi_i | p_0, \mathcal{B}) \tag{5.76}$$

$$= \frac{1}{N} \sum_{\nu=1}^{N} \sum_{j=1}^{\mathcal{N}} \sum_{i=1}^{\mathcal{N}} f(\xi_j)\; P(\hat{x}_\nu = \xi_j | \hat{x}_0 = x_i, \mathcal{B})\; p_i^0 \tag{5.77}$$

$$= \frac{1}{N} \sum_{\nu=1}^{N} \sum_{j=1}^{\mathcal{N}} \sum_{i=1}^{\mathcal{N}} f(\xi_j)\; (M^\nu)_{ji}\; p_i^0 \,. \tag{5.78}$$

In the extremely unlikely situation that the initial distribution p^0 is equivalent to the distribution of the underlying physical problem ρ we have

$$\sum_j M_{ji}^\nu\, p_j^0 = p_j^0 = \rho_j \,,$$

independent of the 'Markov-time' ν, and expectation value of the sample mean is identical to the true mean

$$\Big\langle S \Big\rangle = \sum_{j=1}^{\mathcal{N}} f_j\, \rho_j = \Big\langle f \Big\rangle \,.$$

For a general initial state the expectation of the sample mean (5.76) is

$$\Big\langle S \Big\rangle = \frac{1}{N} \sum_{\nu=1}^{N} \sum_{j=1}^{\mathcal{N}} \sum_{i=1}^{\mathcal{N}} f(\xi_j)\; (M^\nu)_{ji}\; p_i^0 \tag{5.79}$$

$$= \frac{1}{N} \sum_{\nu=1}^{N} \sum_{j=1}^{\mathcal{N}} \sum_{i=1}^{\mathcal{N}} f(\xi_j) \left({M'}_{ji}^{\nu} + \rho_j \right) p_i^0 \tag{5.80}$$

$$= \frac{1}{N} \sum_{\nu=1}^{N} \sum_{j=1}^{\mathcal{N}} \sum_{i=1}^{\mathcal{N}} f(\xi_j)\; {M'}_{ji}^{\nu}\; p_i^0 + \sum_{j=1}^{\mathcal{N}} f(\xi_j)\; \rho_j \tag{5.81}$$

$$= \Big\langle f \Big\rangle + \frac{1}{N} \sum_{\nu=1}^{N} \sum_{j=1}^{\mathcal{N}} \sum_{i=1}^{\mathcal{N}} f(\xi_j)\; {M'}_{ji}^{\nu}\; p_i^0 \,. \tag{5.82}$$

Due to the initial distribution there is a bias

$$B := \frac{1}{N} \sum_{\nu=1}^{N} \sum_{j=1}^{\mathcal{N}} \sum_{i=1}^{\mathcal{N}} f_j \; {M'}^{\nu}_{ji} \; p_i^0 \tag{5.83}$$

$$= \frac{1}{N} \sum_{l=2}^{\mathcal{N}} \underbrace{\left(\sum_{i=1}^{\mathcal{N}} f_j \; x_{j,l} \right)}_{\tilde{f}_l} \left(\sum_{\nu=1}^{N} \; d_l^{\nu} \right) \underbrace{\left(\sum_i \; p_i^0 \; y_{il} \right)}_{\bar{p}_l^0} \tag{5.84}$$

$$= \frac{1}{N} \sum_{l=2}^{\mathcal{N}} \tilde{f}_l \left(d_l \frac{1 - d_l^N}{1 - d_l} \right) \tilde{p}_l^0 \, . \tag{5.85}$$

Since d_l^N declines exponentially, the leading term for large sample size N is

$$B = \frac{1}{N} \sum_{l=2}^{\mathcal{N}} \tilde{f}_l \left(\frac{d_l}{1 - d_l} \right) \tilde{p}_l^0$$

proportional to $1/N$, with

$$\tilde{f}_l = \sum_j f_j x_{jl} = \sum_j f_j \sqrt{p_j} U_{jl} = \sum_j f_j U_{j1} U_{jl} \, .$$

5.4.6 Equilibration

The meaning of equilibration is to ignore the first K steps of the Markov chain in the sample mean, in other words, $\boldsymbol{p}^0$ is replaced by

$$\bar{\boldsymbol{p}}^0 = M^K \; \boldsymbol{p}^0 \, .$$

Hence, with

$$\tilde{\bar{\boldsymbol{p}}}^0 = Y^T \; \bar{\boldsymbol{p}}^{\boldsymbol{0}} = Y^T \; M^K \; \boldsymbol{p}^0 = Y^T \; X \; D^K \; Y^T \; \boldsymbol{p}^0 = D^K \; Y^T \; \boldsymbol{p}^0 = D^K \; \tilde{\boldsymbol{p}}^0 \, . \tag{5.86}$$

the bias reads now

$$B = \frac{1}{N} \sum_{l=2}^{\mathcal{N}} \tilde{f}_l \left(d_l^{1+K} \frac{1 - d_l^N}{1 - d_l} \right) \tilde{p}_l^0 \, , \tag{5.87}$$

so to leading order the bias is now given by

$$B = \frac{1}{N} \sum_{l=2}^{\mathcal{N}} \tilde{f}_l \left(\frac{d_l^{1+K}}{1 - d_l} \right) \tilde{p}_l^0$$

and decays exponentially with K, since $d_l < 1$. The convergence is dictated by the d_2, the largest remaining eigenvalue. If the number of Markov steps is limited, and that is naturally the case, it is therefore expedient to use a certain fraction of them for equilibration, since the bias is exponentially rather then by a $1/N$ behavior suppressed. On the other hand, the variance of the sample mean increases, if the sample size is reduced, There is a tread-off between bias reduction and variance reduction.

5.4.7 Variance of sample mean

$$\begin{aligned}
\left\langle S^2 \right\rangle =& \frac{1}{N^2} \sum_{\nu,\nu'} \left\langle f(\hat{x}_\nu) f(\hat{x}_{\nu'}) \right\rangle \\
=& \frac{1}{N^2} \sum_{\nu} \left\langle f(\hat{x}_\nu)^2 \right\rangle + \frac{2}{N^2} \sum_{\nu'>\nu} \left\langle f(\hat{x}_\nu) f(\hat{x}_{\nu'}) \right\rangle \\
=& \underbrace{\frac{1}{N^2} \sum_i f_i^2 \sum_\nu P(\hat{x}_\nu = \xi_i | p^0, \mathcal{B})}_{=:T_1} \\
&+ \underbrace{\frac{2}{N^2} \sum_{i,j} f_i f_j \sum_{\nu'>\nu} P(\hat{x}_{\nu'} = \xi_j, \hat{x}_\nu = \xi_i | p^0, \mathcal{B})}_{=:T_2} .
\end{aligned}$$

We evaluate the two terms $T_{1/2}$ separately.

$$\begin{aligned}
T_1 &= \frac{1}{N^2} \sum_i f_i^2 \sum_\nu \left(\rho_i + (M^\nu \boldsymbol{p}^0)_i \right) \\
&= \frac{1}{N} \sum_i f_i^2 \rho_i + \frac{1}{N^2} \sum_i f_i^2 \left(\sum_\nu M^\nu \boldsymbol{p}^0)_i \right) \\
&= \frac{1}{N} \left\langle f^2 \right\rangle + \frac{1}{N^2} \sum_{l=2}^{\mathcal{N}} \underbrace{\left(\sum_i f_i^2 \, x_{il} \right)}_{=:\widetilde{f_l^2}} \left(\sum_{\nu=1}^{N} d_l^\nu \right) \left(\sum_j y_{jl} \, p_j^0 \right) \\
&= \frac{1}{N} \left\langle f^2 \right\rangle + \frac{1}{N^2} \sum_{l=2}^{\mathcal{N}} \widetilde{f_l^2} \left(d_l \frac{1 - d_l^N}{1 - d_l} \right) \tilde{p}_l^0
\end{aligned}$$

$$
\begin{aligned}
T_2 &= \frac{2}{N^2} \sum_{i,j} f_i f_j \sum_{\nu=1}^{N-1} \sum_{\nu'=\nu+1}^{N} P(\hat{x}_{\nu'} = \xi_j | \hat{x}_\nu = \xi_i, \mathcal{B})\ P(\hat{x}_\nu = \xi_i | p^0, \mathcal{B}) \\
&= \frac{2}{N^2} \sum_{i,j} f_i f_j \sum_{\nu=1}^{N-1} \sum_{\mu=1}^{N-\nu} P(\hat{x}_\mu = \xi_j | \hat{x}_0 = \xi_i, \mathcal{B})\ P(\hat{x}_\nu = \xi_i | p^0, \mathcal{B}) \\
&= \frac{2}{N^2} \sum_{i,j} f_i f_j \sum_{\nu=1}^{N-1} \sum_{\mu=1}^{N-\nu} \left(\rho_j + M^\mu_{ji} \right) \left(\rho_i + (M^\nu p^0)_i \right) \\
&= \frac{2}{N^2} \left(\sum_i f_i \rho_i \right)^2 \sum_{\nu=1}^{N-1} \sum_{\mu=1}^{N-\nu} 1 \\
&\quad + \frac{2}{N^2} \sum_j f_j\ \rho_j \sum_i f_i \sum_{\nu=1}^{N-1} (M^\nu p^0)_i \sum_{\mu=1}^{N-\nu} 1 \\
&\quad + \frac{2}{N^2} \sum_{i,j} f_i f_j \sum_{\nu=1}^{N-1} \sum_{\mu=1}^{N-\nu} M^\mu_{ji}\ \rho_i \\
&\quad + \frac{2}{N^2} \sum_{i,j} f_i f_j \sum_{\nu=1}^{N-1} \sum_{\mu=1}^{N-\nu} M^\mu_{ji}\ M^\nu p^0)_i \\
T_2 &= \frac{N-1}{N} \left\langle f \right\rangle^2 && (:= T_{21}) \\
&\quad + \frac{2}{N^2} \left\langle f \right\rangle \sum_i f_i \sum_{\nu=1}^{N-1} (M^\nu p^0)_i\ (N - \nu) && (:= T_{22}) \\
&\quad + \frac{2}{N^2} \sum_{i,j} f_i f_j \sum_{\nu=1}^{N-1} \sum_{\mu=1}^{N-1} \theta(\nu \le N - \mu) M^\mu_{ji}\ \rho_i && (:= T_{23}) \\
&\quad + \frac{2}{N^2} \sum_{i,j} f_i f_j \sum_{\nu=1}^{N-1} \sum_{\mu=1}^{N-\nu} M^\mu_{ji}\ (M^\nu p^0)_i && (:= T_{24})
\end{aligned}
$$

The first term needs no further consideration. We proceed with term

$$
\begin{aligned}
T_{22} &= \frac{2}{N^2} \left\langle f \right\rangle \sum_i f_i \sum_{\kappa=1}^{N-1} (\kappa\ M^{N-\kappa} p^0)_i \\
&= \frac{2}{N^2} \left\langle f \right\rangle \sum_l \left(\sum_i f_i\ x_{il} \right) \left(\sum_{\kappa=1}^{N-1} \kappa\ d_l^{N-\kappa} \right) \left(\sum_j y_{jl}\ p_j^0 \right) \\
&= \frac{2}{N^2} \left\langle f \right\rangle \sum_l \tilde{f}_l \left(\sum_{\kappa=1}^{N-1} \kappa\ d_l^{N-\kappa} \right) \tilde{p}_l^0
\end{aligned}
$$

$$\begin{aligned}
\sum_{\kappa=1}^{N-1} \kappa\, d_l^{N-\kappa} &= d_l^N \sum_{\kappa=1}^{N-1} \kappa\, q^\kappa \Big|_{q=d_l^{-1}} = d_l^N\, q \frac{\partial}{\partial q} \sum_{\kappa=1}^{N-1} q^\kappa \Big|_{q=d_l^{-1}} \\
&= d_l^N\, q \frac{\partial}{\partial q} \left(\frac{1-q^N}{1-q} - 1 \right) \Big|_{q=d_l^{-1}} \\
&= d_l^N\, q \left(\frac{-N q^{N-1}}{1-q} + \frac{1-q^N}{(1-q)^2} \right) \Big|_{q=d_l^{-1}} \\
&= d_l^{N-1} \left(\frac{-N d_l^{-(N-1)}}{1-1/d_l} + \frac{1-d_l^{-N}}{(1-1/d_l)^2} \right) \\
&= \frac{N d_l}{1-d_l} \left(1 - \frac{1}{N} \frac{1-d_l^N}{1-d_l} \right) \qquad (5.88)
\end{aligned}$$

Hence we have

$$T_{22} = \frac{2\,\langle f \rangle}{N} \sum_l \tilde{f}_l\, \frac{d_l}{1-d_l} \left(1 - \frac{1}{N} \frac{1-d_l^N}{1-d_l}\right) \tilde{p}_l^0 \qquad (5.89)$$

Next we compute T_{23}

$$\begin{aligned}
T_{23} &= \frac{2}{N^2} \sum_{i,j} f_j \sum_{\mu=1}^{N-1} (N-\mu)\, M_{ji}^\mu\, \rho_i\, f_i \\
&= \frac{2}{N^2} \sum_{l=2}^{\mathcal{N}} \left(\sum_j f_j\, x_{jl} \right) \left(\sum_{\mu=1}^{N-1} (N-\mu)\, d_l^\mu \right) \left(\sum_i \rho_i\, f_i\, y_{il} \right)
\end{aligned}$$

According to (5.59) ($Y = \Delta^{-} 2X$) the last factor can be expressed in terms of X as $\sum_i\ \rho_i\, f_i\, \rho_i^{-1} x_{il} = \tilde{f}_l$. Along with (5.88) we obtain

$$T_{23} = \frac{2}{N} \sum_{l=2}^{\mathcal{N}} \tilde{f}_l^2\, \frac{d_l}{1-d_l} \left(1 - \frac{1}{N} \frac{1-d_l^N}{1-d_l}\right). \qquad (5.90)$$

Finally, we determine

$$\begin{aligned}
T_{24} &= \frac{2}{N^2} \sum_{i,j} f_i f_j \sum_{\nu=1}^{N-1} \sum_{\mu=1}^{N-\nu} M_{ji}^\mu\, (M^\nu p^0)_i \\
&= \frac{2}{N^2} \sum_{l,l'=2}^{N} \sum_{\nu=1}^{N-1} \sum_{\mu=1}^{N-\nu} \left(\sum_j f_j\, x_{jl} \right) d_l^\mu \underbrace{\left(\sum_i y_{il}\, f_i\, x_{il'} \right)}_{=:F_{ll'}} d_{l'}^\nu \left(\sum_k y_{kl'} p_k^0 \right) \\
&= \frac{2}{N^2} \sum_{l,l'=2}^{N} \tilde{f}_l\, F_{ll'}\, \tilde{p}_{l'}^0 \sum_{\nu=1}^{N-1} d_{l'}^\nu \sum_{\mu=1}^{N-\nu} d_l^\mu
\end{aligned}$$

We need

$$\sum_{\nu=1}^{N-1} d_{l'}^{\nu} \sum_{\mu=1}^{N-\nu} d_l^{\mu} = \sum_{\nu=1}^{N-1} d_{l'}^{\nu} \left(\frac{d_l}{1-d_l} - \frac{d_l^{N-\nu+1}}{1-d_l} \right)$$

$$= d_{l'} \frac{1-d_{l'}^{N-1}}{1-d_{l'}} \frac{d_l}{1-d_l} - \frac{d_l^{N+1}}{1-d_l} \sum_{\nu=1}^{N-1} (d_{l'}/d_l)^{\nu}$$

$$= \frac{d_l d_{l'}}{1-d_l} \begin{cases} \frac{1-d_{l'}^{N-1}}{1-d_{l'}} - d_l^{N-1}\,(N-1) & \text{for } d_l = d_{l'} \\ \frac{1-d_{l'}^{N-1}}{1-d_{l'}} - d_l^{N-1}\,\frac{1-(d_{l'}/d_l)^{N-1}}{1-d_{l'}/d_l} & \text{otherwise} \end{cases} .$$

With the definition

$$Q_{ll'} := \frac{d_l d_{l'}}{1-d_l} \begin{cases} \frac{1-d_{l'}^{N-1}}{1-d_{l'}} - d_l^{N-1}\,(N-1) & \text{for } d_l = d_{l'} \\ \frac{1-d_{l'}^{N-1}}{1-d_{l'}} - d_l^{N-1}\,\frac{1-(d_{l'}/d_l)^{N-1}}{1-d_{l'}/d_l} & \text{otherwise} \end{cases} \tag{5.91}$$

we have

$$T_{24} = \frac{2}{N^2} \sum_{l,l'=2}^{N} \tilde{f}_l \, F_{ll'} \, \tilde{p}_{l'}^{0} \, Q_{ll'} \, . \tag{5.92}$$

Eventually, we have for $\langle S^2 \rangle$

$$\begin{aligned}
\left\langle S^2 \right\rangle &= \frac{1}{N}\left\langle f^2 \right\rangle + \frac{1}{N^2}\sum_{l=2}^{\mathcal{N}} \widetilde{f_l^2}\left(d_l \frac{1-d_l^N}{1-d_l}\right)\tilde{p}_l^0 \\
&+ \frac{N-1}{N}\left\langle f \right\rangle^2 + \frac{2\left\langle f \right\rangle}{N}\sum_{l} \tilde{f}_l \frac{d_l}{1-d_l}\left(1 - \frac{1}{N}\frac{1-d_l^N}{1-d_l}\right)\tilde{p}_l^0 \\
&+ \frac{2}{N}\sum_{l=2}^{\mathcal{N}} \tilde{f}_l^2 \frac{d_l}{1-d_l}\left(1 - \frac{1}{N}\frac{1-d_l^N}{1-d_l}\right) \\
&+ \frac{2}{N^2}\sum_{l,l'=2}^{N} \tilde{f}_l\, F_{ll'}\, \tilde{p}_{l'}^0\, Q_{ll'} \\
\left\langle S^2 \right\rangle &= \frac{1}{N}\left\langle (\Delta f)^2 \right\rangle + \left\langle f \right\rangle^2 + \frac{1}{N^2}\sum_{l=2}^{\mathcal{N}} \widetilde{f_l^2}\left(d_l \frac{1-d_l^N}{1-d_l}\right)\tilde{p}_l^0 \\
&+ \frac{2\left\langle f \right\rangle}{N}\sum_{l} \tilde{f}_l \frac{d_l}{1-d_l}\tilde{p}_l^0 - \frac{2\left\langle f \right\rangle}{N^2}\sum_{l} \tilde{f}_l \frac{d_l}{1-d_l}\frac{1-d_l^N}{1-d_l}\tilde{p}_l^0 \\
&+ \frac{2}{N}\sum_{l=2}^{\mathcal{N}} \tilde{f}_l^2 \frac{d_l}{1-d_l}\left(1 - \frac{1}{N}\frac{1-d_l^N}{1-d_l}\right) \\
&+ \frac{2}{N^2}\sum_{l,l'=2}^{N} \tilde{f}_l\, F_{ll'}\, \tilde{p}_{l'}^0\, Q_{ll'}
\end{aligned}$$

In order to compute the variance we subtract

$$\begin{aligned}
\left\langle S \right\rangle^2 &= \left(\left\langle f \right\rangle + \frac{1}{N}\sum_{l=2}^{\mathcal{N}} \tilde{f}_l \left(d_l \frac{1-d_l^N}{1-d_l}\right)\tilde{p}_l^0\right)^2 \\
&= \left\langle f \right\rangle^2 + \frac{2\langle f \rangle}{N}\sum_{l=2}^{\mathcal{N}} \tilde{f}_l \left(d_l \frac{1-d_l^N}{1-d_l}\right)\tilde{p}_l^0 + \left(\frac{1}{N}\sum_{l=2}^{\mathcal{N}} \tilde{f}_l \left(d_l \frac{1-d_l^N}{1-d_l}\right)\tilde{p}_l^0\right)^2
\end{aligned}$$

So the variance reads

VARIANCE OF SAMPLE MEAN

$$\left\langle (\Delta S)^2 \right\rangle = \frac{1}{N} \left\langle (\Delta f)^2 \right\rangle + \frac{1}{N^2} \sum_{l=2}^{\mathcal{N}} \widetilde{f_l^2} \left(d_l \frac{1-d_l^N}{1-d_l} \right) \tilde{p}_l^0 + \frac{2}{N} \sum_{l=2}^{\mathcal{N}} \tilde{f}_l^2 \, \frac{d_l}{1-d_l} \left(1 - \frac{1}{N} \frac{1-d_l^N}{1-d_l} \right) + \frac{2}{N^2} \sum_{l,l'=2}^{N} \tilde{f}_l \, F_{ll'} \, \tilde{p}_{l'}^0 \, Q_{ll'} + \frac{2\langle f \rangle}{N} \sum_{l=2}^{\mathcal{N}} \tilde{f}_l \, \frac{d_l}{1-d_l} \left(d_l^N - \frac{1}{N} \, \frac{1-d_l^N}{1-d_l} \right) \tilde{p}_l^0 - \left(\frac{1}{N} \sum_{l=2}^{\mathcal{N}} \tilde{f}_l \left(d_l \frac{1-d_l^N}{1-d_l} \right) \tilde{p}_l^0 \right)^2 .$$

The terms independent of p^0 are

VARIANCE OF SAMPLE MEAN (LEADING TERMS)

$$\begin{aligned} \left\langle (\Delta S)^2 \right\rangle &= \frac{1}{N} \left\langle (\Delta f)^2 \right\rangle + \frac{2}{N} \sum_{l=2}^{\mathcal{N}} \tilde{f}_l^2 \, \frac{d_l}{1-d_l} \left(1 - \frac{1}{N} \frac{1-d_l^N}{1-d_l} \right) \\ &= \frac{1}{N} \left\langle (\Delta f)^2 \right\rangle \left[1 + 2 \sum_{l=2}^{\mathcal{N}} \frac{\tilde{f}_l^2}{\langle (\Delta f)^2 \rangle} \, \frac{d_l}{1-d_l} \left(1 - \frac{1}{N} \frac{1-d_l^N}{1-d_l} \right) \right] . \end{aligned} \tag{5.93}$$

Apart form the $O(1/N)$ term in the last factor, these are also the leading order terms. The result is equivalent to the approximation

$$P(\hat{x}_\nu = \xi_i | p^0, \mathcal{B}) \simeq \rho_i \, ,$$

because in this case all p^0-dependent terms vanish, as the dominant eigenvalue is separated off. So if the MCMC run is properly equilibrated the variance is given by (5.93). We see that also the variance gets worse, if $d_2 \to 1$.

Influence of equilibration on the variance. According to (5.86) we merely have to replace $\tilde{p}_l^0$ by $d_l^K \, \tilde{p}_l^0$.

VARIANCE OF SAMPLE MEAN AFTER EQUILIBRATION

$$\begin{aligned}\left\langle (\Delta S)^2 \right\rangle = \frac{1}{N}\left\langle (\Delta f)^2 \right\rangle &+ \frac{1}{N^2}\sum_{l=2}^{\mathcal{N}} \widetilde{f_l^2}\left(d_l^{K+1}\frac{1-d_l^N}{1-d_l}\right)\tilde{p}_l^0 \\ &+ \frac{2}{N}\sum_{l=2}^{\mathcal{N}} \tilde{f}_l^2\,\frac{d_l}{1-d_l}\left(1-\frac{1}{N}\frac{1-d_l^N}{1-d_l}\right) + \frac{2}{N^2}\sum_{l,l'=2}^{N} \tilde{f}_l\,F_{ll'}\,d_l^K\,\tilde{p}_{l'}^0\,Q_{ll'} \\ &+ \frac{2\langle f\rangle}{N}\sum_{l=2}^{\mathcal{N}} \tilde{f}_l\,\frac{d_l^{K+1}}{1-d_l}\left(d_l^N - \frac{1}{N}\,\frac{1-d_l^N}{1-d_l}\right)\tilde{p}_l^0 - \left(\frac{1}{N}\sum_{l=2}^{\mathcal{N}} \tilde{f}_l\left(d_l^{K+1}\frac{1-d_l^N}{1-d_l}\right)\tilde{p}_l^0\right)^2 .\end{aligned}$$

Without equilibration, the next to leading terms where of order $1/N$ smaller. Now they are exponentially suppressed and the correction to (5.93) is now exponentially small.

5.4.8 Dominant terms

We consider the case, that additional eigenvalues approach One, i.e. $d_l = 1-\varepsilon$.

$$\begin{aligned} d_l^N &= (1-\varepsilon)^N = 1 - \varepsilon N + \frac{(\varepsilon N)^2}{2} - \frac{(\varepsilon N)^3}{6} + O(\varepsilon N)^4 \\ \frac{1}{N}\frac{1-d_l^N}{1-d_l} &= 1 - \frac{(\varepsilon N)}{2} + \frac{(\varepsilon N)^2}{6} + O(\varepsilon N)^3) \\ &\Rightarrow \\ 1 - \frac{1}{N}\frac{1-d_l^N}{1-d_l} &= \frac{(\varepsilon N)}{2}\left(1 - \frac{\varepsilon N}{3} + O(\varepsilon N)^2)\right) \\ &\Rightarrow \\ d_l^N - \frac{1}{N}\frac{1-d_l^N}{1-d_l} &= -\frac{(\varepsilon N)}{2}\left(1 - \frac{2\varepsilon N}{3} + O(\varepsilon N)^2\right) \end{aligned}$$

CONTRIBUTION TO VARIANCE OF SAMPLE MEAN FROM DOMINANT TERMS FOR $\varepsilon N < 1$ AND $N \gg 1$

$$
\begin{aligned}
\Delta\Big\langle (\Delta S)^2 \Big\rangle = \frac{1}{N} \sum_{l=2}^{\mathcal{N}} \widetilde{f_l^2}\, d_l^{K+1} \left(1 - \frac{\varepsilon N}{2}\right) \tilde{p}_l^0 \\
+ \sum_{l=2}^{\mathcal{N}} \tilde{f}_l^2 \left(1 - \frac{\varepsilon N}{3}\right) + \frac{2}{N^2} \sum_{l,l'=2}^{N} \tilde{f}_l\, F_{ll'}\, d_l^K\, \tilde{p}_{l'}^0\, Q_{ll'} \\
- \langle f \rangle \sum_{l=2}^{\mathcal{N}} \tilde{f}_l\, d_l^{K+1} \left(1 - \frac{2\varepsilon N}{3}\right) \tilde{p}_l^0 \\
- \left(\sum_{l=2}^{\mathcal{N}} \tilde{f}_l\, d_l^{K+1} \left(1 - \frac{\varepsilon N}{2}\right) \right)^2 .
\end{aligned}
$$

$$
Q_{ll'} \begin{cases} \frac{N^2}{2}(1 + \frac{2\varepsilon N}{3}) & d_l = d_l' = 1 - \varepsilon \\ O(N) & \text{otherwise} \end{cases}
$$

Ignoring terms of order $O(\frac{1}{N})$,$O(\varepsilon N)$ and $O(\varepsilon K)$ and assuming there is one dominant term, we obtain

$$
\begin{aligned}
\Delta\Big\langle (\Delta S)^2 \Big\rangle &= \tilde{f}_l^2 + \tilde{f}_l\, F_{ll'}\, d_l^K\, \tilde{p}_{l'}^0 - \langle f \rangle \sum_{l=2}^{\mathcal{N}} \tilde{f}_l\, \tilde{p}_l^0 - \left(\tilde{f}_l\right)^2 \\
&= \tilde{f}_l\, F_{ll'}\, d_l^K\, \tilde{p}_{l'}^0 - \langle f \rangle \sum_{l=2}^{\mathcal{N}} \tilde{f}_l\, \tilde{p}_l^0 .
\end{aligned}
$$

If on the other hand $\tilde{p}_l^0 = 0$, which might be achieved by symmetry considerations, the entire variance simplifies to

VARIANCE OF SAMPLE MEAN FOR $\tilde{p}_l^0 = 0$
$\varepsilon N < 1$ AND $N \gg 1$

$$\begin{aligned}\left\langle (\Delta S)^2 \right\rangle &= \frac{1}{N} \left\langle (\Delta f)^2 \right\rangle + \frac{2}{N} \sum_{l=2}^{\mathcal{N}} \tilde{f}_l^2 \, \frac{d_l}{1-d_l} \left(1 - \frac{1}{N} \frac{1-d_l^N}{1-d_l} \right) \\ &= \frac{1}{N} \left\langle (\Delta f)^2 \right\rangle + \sum_{l}^{\text{dom. terms}} \tilde{f}_l^2 \left(1 - O(\varepsilon N) \right) \\ &\simeq \sum_{l}^{\text{dom. terms}} \tilde{f}_l^2 \, .\end{aligned}$$

Hence the variance is for sufficiently large N independent of N. There is no $1/N$ reduction. The meaning is that given an appropriate p^0 which does not couple to the next-dominant eigenvalue [1] yields the correct mean, in the sense as mean value over several independent MCMC runs whose initial state is distributed according to p^0. But the mean variance is finite and independent of N.
The mean over several independent bins, i.e.

$$S^{Mb} = \frac{1}{NM} \sum_{\nu=1}^{N} \sum_{b=1}^{M} \hat{x}_\nu^b$$

yields

$$\langle S^{\mathrm{M\ b}} \rangle = \langle S^{1\ \mathrm{b}} \rangle$$

and

$$\langle (\Delta S^{\mathrm{M\ b}})^2 \rangle = \frac{1}{M} \langle (\Delta S^{1\ \mathrm{b}})^2 \rangle \, .$$

5.4.9 Behavior of autocorrelation

We start out with the autocorrelation without normalization

$$A(\tau) = \frac{1}{N} \sum_{\nu} f(\hat{x}_{\nu+\tau}) f(\hat{x}_\nu)$$

The mean value is

[1] not the once with eigenvalue p_i

$$
\begin{aligned}
\Big\langle A(\tau)\Big\rangle &= \frac{1}{N}\sum_{\nu}\Big\langle \Delta f(\hat{x}_{\nu+\tau})\Delta f(\hat{x}_{\nu})\Big\rangle \\
&= \frac{1}{N}\sum_{i,j}\Delta f_i\Delta f_j\sum_{\nu} P(\hat{x}_{\nu+\tau}=\xi_j|\hat{x}_{\nu}=\xi_i,p^0,\mathcal{B})\;P(\hat{x}_{\nu}=\xi_i|\hat{x}_0=\xi_k,p^0,\mathcal{B})\;p^0(\xi_k) \\
&= \frac{1}{N}\sum_{i,j}\Delta f_i\Delta f_j\sum_{\nu}(M^{\tau})_{ji}\sum_{k}(M^{\nu})_{ik}\,p^0_k \\
&= \frac{1}{N}\sum_{i,j}\Delta f_i\Delta f_j\sum_{\nu}\Big((M'^{\tau})_{ji}+\rho_j\Big)\Big(\sum_{k}(M'^{\nu})_{ik}\,p^0_k+\rho_i\sum_{k}p^0_k\Big) \\
&= \frac{1}{N}\sum_{i,j}\Delta f_i\Delta f_j\sum_{\nu}\Big((M'^{\tau})_{ji}+\rho_j\Big)\Big((M'^{\nu}\,p^0)_i+\rho_i\Big) \\
&= \frac{1}{N}\sum_{i,j}\Delta f_i\Delta f_j\sum_{\nu}\Big((M'^{\tau})_{ji}(M'^{\nu}\,p^0)_i+(M'^{\tau})_{ji}\rho_i+\rho_j(M'^{\nu}\,p^0)_i+\rho_j\rho_i\Big) \\
&= \frac{1}{N}\sum_{i,j}\Delta f_i\Delta f_j\,(M'^{\tau})_{ji}\Big(\sum_{\nu}M'^{\nu}\,p^0\Big)_i \\
&+ \frac{N}{N}\sum_{j,i}\Delta f_j\,(M'^{\tau})_{ji}\rho_i\,\Delta f_i \\
&+ \frac{1}{N}\underbrace{\Big(\sum_{j}\Delta f_j\rho_j\Big)}_{=0}\sum_{i}\Delta f_i\Big(\sum_{\nu}M'^{\nu}\,p^0\Big)_i \\
&+ \frac{N}{N}\underbrace{\Big(\sum_{i}\Delta f_i\rho_i\Big)\Big(\sum_{j}\Delta f_j\,\rho_j\Big)}_{=0}
\end{aligned}
$$

Leading to

$$
\Big\langle A(\tau)\Big\rangle = \underbrace{\sum_{j,i}\Delta f_j\,(M'^{\tau})_{ji}\rho_i\,\Delta f_i}_{T_1} + \underbrace{\tfrac{1}{N}\sum_{i,j}\Delta f_i\Delta f_j\,(M'^{\tau})_{ji}\Big(\sum_{\nu}M'^{\nu}\,p^0\Big)_i}_{T_2}\,.
$$

$$
\begin{aligned}
T_1 &= \sum_{j,i}\Delta f_j\,(M'^{\tau})_{ji}\rho_i\,\Delta f_i \\
&= \sum_{l=2}^{N} d_l^{\tau}\Big[\big(\sum_{j}\Delta f_j X_{jl}\big)\big(\sum_{i}\rho_i\Delta f_i Y_{il}\big)\Big]
\end{aligned}
$$

$$
\begin{aligned}
T_2 &= \tfrac{1}{N} \sum_{i,j} \Delta f_i \Delta f_j \, (M'^{\tau})_{ji} \Big(\sum_{\nu} M'^{\nu} \, p^0 \Big)_i \\
&= \tfrac{1}{N} \sum_{i,j} \Delta f_j \, (M'^{\tau})_{ji} \underbrace{\Big(X \frac{1 - D'^N}{1 - D'} \, Y^T \, p^0 \Big)_i \, \Delta f_i}_{g_i} \\
&= \sum_{l=2}^{N} d_l^{\tau} \Big[\big(\sum_j \Delta f_j X_{jl} \big) \big(\tfrac{1}{N} \sum_i g_i Y_{il} \big) \Big]
\end{aligned}
$$

So the final result has the form

$$
\Big\langle A(\tau) \Big\rangle = \sum_{l=2}^{N} e^{-l/\xi_l} \, c_l
$$

with

$$
\xi_l = |1/\ln(d_l)| \tag{5.94}
$$

5.4.10 Example

The presumably most simple example is given by an electron moving along 1d lattice of length N. The possible states are the positions $i \in \{1, 2, \ldots, N\}$ with probability ρ_i. The current state be $x_n = i$. As proposal distribution we choose left right moves, i.e. $x^T = i \pm 1$ with pbc, or more precisely

$$
q(i|i) = \frac{1}{2} \big(\delta_{j,[i+1,N]} + \delta_{j,[i-1,N]} \big) \, .
$$

The symbol $[i, N]$ indicates pbc

$$
[i, N] = \begin{cases} 1 & \text{if } i > N \\ N & \text{if } i < 1 \\ i & \text{otherwise} \end{cases}
$$

According to (5.46) we generally have

$$
M_{ji} = \alpha(j|i) q(j, i) + \delta_{ji} (1 - \sum_k \alpha(k|i) q(k, i)) \, ,
$$

which in the present case becomes

$$
\begin{aligned}
M_{ji} &= \frac{1}{2} \min \Big(1, \frac{\rho_j}{\rho_i} \Big) \Big(\delta_{j,[i+1,N]} + \delta_{j,[i-1,N]} \Big) \; + \delta_{ji} Z_i \\
&= \frac{1}{2} \Big[\min \Big(1, \frac{\rho_{[i+1,N]}}{\rho_i} \Big) \delta_{j,[i+1,N]} + \min \Big(1, \frac{\rho_{[i-1,N]}}{\rho_i} \Big) \delta_{j,[i-1,N]} \Big] \; + \delta_{ji} Z_i \, ,
\end{aligned}
$$

where Z_i ensures the proper normalization. To keep things simple we consider a flat distribution $\rho_i = 1/N$, which leads to

$$M_{ji} = \frac{1}{2}\left[\delta_{j,[i+1,N]} + \delta_{j,[i-1,N]}\right] .$$

Here, $Z_i = 0$, which implies that moves are always accepted because $\alpha(i \pm 1|i) = \min(1,1) = 1$. This is simply the 1d tight-binding matrix with pbd. It is symmetric, i.e. left eigenvectors and right eigenvectors are identical, i.e. $X = Y$. The well-known eigenvalues are $\epsilon_k = \cos((k-1)2\pi/N)$, with $(k = 1, \ldots, N)$. The corresponding eigenvectors are

$$X_{jk} = \frac{1}{\sqrt{N}}\, e^{i(k-1)j} \qquad , \; j = 1, 2, \ldots, N .$$

The dominant eigenvalue is $\epsilon_{k=1} = 1$. The next dominant eigenvalues are given for $k = 2$ and $k = N$ with

$$\epsilon = \cos(2\pi/N) \approx 1 - \tfrac{1}{2}(2\pi/N)^2 .$$

The corresponding correlation length given by (5.94) is $\xi = N^2/(2\pi^2)$. The result is very reasonable, as we are studying a random walk for which the mean distance, moved in t steps, is $\sqrt{t}$. In order to traverse the lattice once, i.e. to cover a mean distance N it takes N^2 steps (time units).

6. Quantum Monte Carlo Methods (QMC)

If the exact diagonalization of the Hamiltonian is possible, a MCMC method can be applied brut force and no further considerations are necessary. The thermodynamic expectation of an observable O is then calculated as a trace in the complete eigenbasis of the Hamiltonian, denoted by $|n\rangle$. It is given by

$$< O >_T = \frac{1}{Z}\ \mathrm{tr}(\hat{O}\mathrm{e}^{-\beta\hat{H}}) = \frac{1}{Z}\sum\!\!\!\!\!\!\int_n \langle n|\hat{O}|n\rangle \exp(-\beta H_n) \tag{6.1}$$

with the canonical partition function

$$Z = \sum\!\!\!\!\!\!\int_n \exp(-\beta H_n)\ . \tag{6.2}$$

In the general case where no exact diagonalization of the Hamiltonian is possible, the trace has to be evaluated in a different basis. Then the expectation value reads

$$< O >_T = \frac{1}{Z}\ \mathrm{tr}(\hat{O}\mathrm{e}^{-\beta\hat{H}}) = \frac{1}{Z}\sum\!\!\!\!\!\!\int_{n,m} \langle n|\hat{O}|m\rangle\langle m|\exp(-\beta\hat{H})|n\rangle\ , \tag{6.3}$$

where we have inserted a complete set $|m\rangle$. The term $\langle m|\exp(-\beta\hat{H})|n\rangle$ in the above formula causes several difficulties

- its evaluation is not simple,
- it can change sign depending on the vectors $|n\rangle, |m\rangle$,
- it is not normalized to one, i.e. does not represent a probability distribution.

The reason for all these shortcomings is found in the appearance of *non-vanishing commutators*. We try to eliminate them by mapping the quantum mechanical problem on a classical problem. This mapping is achieved by the *Suzuki–Trotter decomposition* presented in what follows.

6.1 Suzuki–Trotter–Decomposition

In principle, the Suzuki–Trotter decomposition maps a d dimensional quantum mechanical problem on a $d+1$ dimensional classical problem. The additional dimension introduced by the mapping is called an *artificial time* or

Trotter–time. We present the decomposition for a sum of only two operators A and B. Extension to the case of n operators is straight forward. Thus, suppose that the Hamiltonian is given by the sum

$$\hat{H} = \hat{A} + \hat{B} \ , \quad \text{with} \ \ [\hat{A}, \hat{B}] \neq 0 \ . \tag{6.4}$$

The operators $\hat{A}$ and $\hat{B}$ do *not* commute and we assume that their individual diagonalization is possible. If the commutator of $\hat{A}$ and $\hat{B}$ vanished, we could use the formula

$$\mathrm{e}^{-\beta(\hat{A}+\hat{B})} = \mathrm{e}^{-\beta\hat{A}}\,\mathrm{e}^{-\beta\hat{B}} \ , \quad \text{for} \ \ [\hat{A}, \hat{B}] = 0 \tag{6.5}$$

and insert a common complete set of eigenstates. However, in our case of non-vanishing commutators, the exponential function does not simply decompose into a product. We introduce an error R writing

$$\mathrm{e}^{-\beta(\hat{A}+\hat{B})} = \mathrm{e}^{-\beta\hat{A}}\,\mathrm{e}^{-\beta\hat{B}} + R \ , \quad \text{with} \ \ R = -\frac{\beta^2}{2}\,[\hat{A}, \hat{B}] + O(\beta^3) \ . \tag{6.6}$$

Proof: We expand both, LHS and RHS of (6.6) in Taylor series retaining only the leading three terms. This yields

$$\begin{aligned}
\mathrm{e}^{-\beta(\hat{A}+\hat{B})} &= 1 - \beta(\hat{A}+\hat{B}) + \frac{\beta^2}{2}\,(\hat{A}^2 + \hat{B}^2 + 2\hat{A}\hat{B} + [\hat{B}, \hat{A}]) + O(\beta^3), \\
\mathrm{e}^{-\beta\hat{A}}\,\mathrm{e}^{-\beta\hat{B}} &= (1 - \beta\hat{A} + \frac{\beta^2}{2}\hat{A}^2)(1 - \beta\hat{B} + \frac{\beta^2}{2}\hat{B}^2) \\
&= 1 - \beta(\hat{A}+\hat{B}) + \frac{\beta^2}{2}\,(\hat{A}^2 + \hat{B}^2 + 2\hat{A}\hat{B}) + O(\beta^3) \ .
\end{aligned}$$

Comparing the RHS's of the above equations, we obtain the estimate for the error R in (6.6) with the accuracy of $O(\beta^3)$. □

Thus, the error has the form of a product of the two operators $\hat{A}$ and $\hat{B}$ multiplied by $\beta^2/2$. If t_A, t_B denote the order of magnitude of the operator $\hat{A}$ and $\hat{B}$, respectively, the error is of the order

$$R \approx \frac{\beta^2}{2}\,O(t_A\,t_B) \ . \tag{6.7}$$

In the case of the Hubbard model with its Hamiltonian

$$\hat{H} = -t \sum_{<i,j>} c_i^\dagger c_j + h.c. + U \sum_i n_{i\uparrow} n_{i\downarrow} \tag{6.8}$$

the quantity t_A corresponds to t whereas t_B corresponds to U. Therefore, one cannot argue that t_A and t_B have really small values. As a result, when applying (6.6), the error R will be of order unity. An improved decomposition is given by the symmetrized form

$$\mathrm{e}^{-\beta(\hat{A}+\hat{B})} = \mathrm{e}^{-\frac{\beta}{2}\hat{A}}\,\mathrm{e}^{-\beta\hat{B}}\,\mathrm{e}^{-\frac{\beta}{2}\hat{A}} + \frac{\beta^3}{24} O(t_A\,t_B\ \max(t_A, t_B)) \ . \tag{6.9}$$

But even here, for the same reason, the error will be of order unity.
The *Suzuki–Trotter decomposition* proceeds with a trick. It takes advantage of the formula

$$\mathrm{e}^{-\beta\hat{H}} = \left(\mathrm{e}^{\frac{\beta}{m}\hat{H}}\right)^m , \quad \text{for any } m \in \mathbb{N} . \tag{6.10}$$

The quantity $\frac{\beta}{m}$ in (6.10) can be made as small as desired by increasing the number m. And this same quantity $\frac{\beta}{m}$ appears in the error estimate. Thus

$$\begin{aligned} \mathrm{e}^{-\beta\hat{H}} &= \Big(\underbrace{\mathrm{e}^{\frac{\beta}{2m}\hat{A}}\mathrm{e}^{\frac{\beta}{m}\hat{B}}\mathrm{e}^{\frac{\beta}{2m}\hat{A}}}_{C}+R\Big)^m \\ &= C^m + mC^{m-1}R + \frac{m(m-1)}{2}C^{m-2}R^2 + \dots \\ &= C^m + mC^{m-1}O\Big(\Big(\frac{\beta}{m}\Big)^3\Big) + m^2C^{m-2}O\Big(\Big(\frac{\beta}{m}\Big)^6\Big) \end{aligned} \tag{6.11}$$

The leading correction is of the order $\beta O((\frac{\beta}{m})^3)$ and rewriting the power m as a product we obtain

$$\mathrm{e}^{-\beta\hat{H}} = \prod_{\tau=1}^{m} \mathrm{e}^{\frac{\beta}{2m}\hat{A}}\,\mathrm{e}^{\frac{\beta}{m}\hat{B}}\mathrm{e}^{\frac{\beta}{2m}\hat{A}} + O\Big(\Big(\frac{\beta}{m}\Big)^2 \beta\,\frac{t_A t_B}{24}\max(t_A,t_B)\Big) . \tag{6.12}$$

The new quantity τ is called the *Trotter time* or *imaginary time*. The integer m must be made big enough to assure that the correction term in (6.12) is small.
Since the trace is invariant against cyclic permutation, the partition function Z is approximately given by

$$Z = \mathrm{tr}\mathrm{e}^{-\beta\hat{H}} = \mathrm{tr}\prod_{\tau=1}^{m} \mathrm{e}^{\frac{\beta}{m}\hat{A}}\,\mathrm{e}^{\frac{\beta}{m}\hat{B}} . \tag{6.13}$$

The decomposition of the exponential function is now achieved. However, the price to be paid is an additional coordinate τ that apears as imaginary time. There is a variety of methods using higher order decompositions for the exponential function $\mathrm{e}^{-\beta\hat{H}}$. Unfortunaltely, they contain commutators $[\hat{A},\hat{B}]$ that are not always cheaply obtained. Suzuki himself suggested to choose a *fractal decomposition*, i.e. a decomposition with fractal coefficients to mitigate the sign problem of fermionic systems. A variant of the Suzuki–Trotter decomposition is the basis of most of the QMC algorithms.

6.2 World Lines Monte Carlo

The underlying idea of the *World Lines Monte Carlo method* is to decompose a model Hamiltonian, say of Hubbard or Heisenberg type, into commuting

pieces. We illustrate this strategy by means of a one-dimensional Hamiltonian with nearest neighbour interaction. This operator can be split as

$$H = \sum_i H_{i,i+1} = H_o + H_e = \sum_{i=\text{odd}} H_{i,i+1} + \sum_{i=\text{even}} H_{i,i+1} \; . \tag{6.14}$$

It is easily checked that all commutators constituting the operators H_o and H_e vanish:

$$[H_{i,i+1}, H_{j,j+1}] = 0 \qquad \text{for } i,j \text{ even, or } i,j \text{ odd} \; . \tag{6.15}$$

The Hamiltonian matrix thus decomposes in small blocks. The size L of these blocks depends on the model. In the case of the spin–$\frac{1}{2}$ Heisenberg model, as well as for the Hubbard model, $L = 2$ in one spatial dimension.

6.2.1 Heisenberg Model in One Dimension

We investigate a generalized Heisenberg model including far–ranging interactions. The Hamiltonian reads

$$H = -J_z \sum_i S_i^z S_{i+1}^z - \frac{J}{2} \sum_i \left(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+ \right) - \sum_{i,j} J_{ij} S_i^z \, S_j^z \; . \tag{6.16}$$

The generalization of the Heisenberg model, i.e. the third term on the RHS of the above equation, causes no complications because it is diagonal in a the basis of the z–component of the spins. We decompose the Hamiltonian H into

$$H = H_e + \frac{1}{2}H' + H_o + \frac{1}{2}H' \; , \tag{6.17}$$

where H_e and H_o refer to terms with even/odd index of the first two terms of (6.16). The symbol H' denotes the third term of (6.16), i.e. it represents the introduced generalization. Now we apply the Trotter decomposition of the canonical partition function Z

$$\begin{aligned} Z = \; \operatorname{tr} \mathrm{e}^{-\beta H} &= \operatorname{tr} \prod_{\tau=1}^{m} \exp\{-\frac{\beta}{m}(H_o + \frac{1}{2}H')\} \exp\{-\frac{\beta}{m}(H_e + \frac{1}{2}H')\} \\ &= \operatorname{tr} \prod_{\tau=1}^{m} \exp\{-\frac{\beta}{4m}H'\} \exp\{-\frac{\beta}{m}H_o\} \exp\{-\frac{\beta}{4m}H'\} \\ &\quad \times \exp\{-\frac{\beta}{4m}H'\} \exp\{-\frac{\beta}{m}H_e\} \exp\{-\frac{\beta}{4m}H'\} \; . \end{aligned} \tag{6.18}$$

It is obvious that the third and the fourth exponential function can be summarized to one factor. Furthermore, exchanging the factors cyclically does not change the trace. Therefore, we combine the first and the last factor writing

$$Z = \ \mathrm{tr} \prod_{\tau=1}^{m} \exp\{-\frac{\beta}{2m} H'\} \exp\{-\frac{\beta}{m} H_o\} \exp\{-\frac{\beta}{2m} H'\} \exp\{-\frac{\beta}{m} H_e\} \ . \quad (6.19)$$

To calculate the trace we insert $2m$ complete sets of eigenfunctions

$$\sum_{\sigma_1^{(i)} \ldots \sigma_N^{(i)}} \left| \underline{\sigma}^{(i)} \right\rangle \left\langle \underline{\sigma}^{(i)} \right| , \qquad i = 1 \ldots 2m \quad (6.20)$$

of the operators S_i^z. The partition function Z reads

$$\begin{aligned} Z = \sum_{\underline{\sigma}} & \left\langle \underline{\sigma}^{(1)} \right| \mathrm{e}^{-\frac{\beta}{m} H_o} \mathrm{e}^{-\frac{\beta}{2m} H'} \left| \underline{\sigma}^{(2)} \right\rangle \left\langle \underline{\sigma}^{(2)} \right| \mathrm{e}^{-\frac{\beta}{m} H_e} \mathrm{e}^{-\frac{\beta}{2m} H'} \left| \underline{\sigma}^{(3)} \right\rangle \\ & \left\langle \underline{\sigma}^{(3)} \right| \mathrm{e}^{-\frac{\beta}{m} H_o} \mathrm{e}^{-\frac{\beta}{2m} H'} \left| \underline{\sigma}^{(4)} \right\rangle \left\langle \underline{\sigma}^{(4)} \right| \mathrm{e}^{-\frac{\beta}{m} H_e} \mathrm{e}^{-\frac{\beta}{2m} H'} \left| \underline{\sigma}^{(5)} \right\rangle \\ & \ \vdots \qquad\quad \vdots \qquad\quad \vdots \qquad\quad \vdots \qquad\quad \vdots \\ & \left\langle \underline{\sigma}^{(2m-1)} \right| \mathrm{e}^{-\frac{\beta}{m} H_o} \mathrm{e}^{-\frac{\beta}{2m} H'} \left| \underline{\sigma}^{(2m)} \right\rangle \left\langle \underline{\sigma}^{(2m)} \right| \mathrm{e}^{-\frac{\beta}{m} H_e} \mathrm{e}^{-\frac{\beta}{2m} H'} \left| \underline{\sigma}^{(1)} \right\rangle . \end{aligned} \quad (6.21)$$

We can now explicitly calculate the exponentials of H' because this operator is diagonal. Terms with superscript k yield

$$\mathrm{e}^{-\frac{\beta}{2m} H'} \left| \underline{\sigma}^{(k)} \right\rangle = \mathrm{e}^{-\frac{\beta}{2m} \left(-\sum_{i,j} J_{ij} \frac{1}{4} \sigma_i^{(k)} \sigma_j^{(k)} \right)} \left| \underline{\sigma}^{(k)} \right\rangle = \mathrm{e}^{\frac{\beta}{8m} V(\underline{\sigma}^{(k)})} \left| \underline{\sigma}^{(k)} \right\rangle \quad (6.22)$$

with the abbreviation $V(\underline{\sigma}^{(k)}) = \sum_{i,j} J_{ij} \, \sigma_i^{(k)} \sigma_j^{(k)}$. Thus, the partition function reads

$$\begin{aligned} Z = & \sum \exp \left\{ \frac{\beta}{8m} \sum_{\tau=1}^{2m} V(\underline{\sigma}^{(\tau)}) \right\} \\ & \times \prod_{\tau=1}^{m} \left\langle \underline{\sigma}^{(2\tau-1)} \right| \mathrm{e}^{-\frac{\beta}{m} H_o} \left| \underline{\sigma}^{(2\tau)} \right\rangle \left\langle \underline{\sigma}^{(2\tau)} \right| \mathrm{e}^{-\frac{\beta}{m} H_e} \left| \underline{\sigma}^{(2\tau+1)} \right\rangle . \end{aligned} \quad (6.23)$$

The trace induces periodic boundary conditions in the Trotter time implying the relation $\left| \underline{\sigma}^{(2m+1)} \right\rangle = \left| \underline{\sigma}^{(1)} \right\rangle$. Therefore, in order to proceed, we have to calculate the matrix elements containing the exponentials of the even/odd part of the Hamiltonian.

$$\langle \underline{\sigma} | \mathrm{e}^{-\frac{\beta}{m} H_{e/o}} | \underline{\sigma}' \rangle = \langle \sigma_N \ldots \sigma_1 | \prod_{i}^{e/o} \mathrm{e}^{-\frac{\beta}{m} H_{i,i+1}} | \sigma_1' \ldots \sigma_N' \rangle \quad (6.24)$$

The operator $H_{i,i+1}$ affects only the spins i and $i+1$. Thus it can be written in the two-spin basis $|s_i, s_{i+1}\rangle$. To this end, only the 2×2 matrix elements

$$A_{i,i+1}(s_{i+1}, s_i, s_i', s_{i+1}') \stackrel{\mathrm{def}}{=} \left\langle s_{i+1} s_i \right| \mathrm{e}^{-\frac{\beta}{m} H_{i,i+1}} \left| s_i' s_{i+1}' \right\rangle \quad (6.25)$$

have to be evaluated and, conversely, yield

$$\mathrm{e}^{-\frac{\beta}{m}H_{i,i+1}} = \sum_{s_{i+1},s_i,s'_i,s'_{i+1}} \big|s_i, s_{i+1}\big\rangle A_{i,i+1}(s_{i+1}, s_i, s'_i, s'_{i+1})\big\langle s'_{i+1}, s'_i\big| \,. \quad (6.26)$$

By inserting this representation into (6.24), we obtain

$$\begin{aligned}&\Big\langle \underline{\sigma}\Big|\mathrm{e}^{-\frac{\beta}{m}H_{e/o}}\Big|\underline{\sigma}'\Big\rangle \qquad (6.27)\\ &= \Big\langle \sigma_N \ldots \sigma_1\Big|\prod_{i}^{e/o}\sum_{\substack{s_{i+1},s_i\\ s'_i,s'_{i+1}}} \big|s_i, s_{i+1}\big\rangle A_{i,i+1}(s_{i+1}, s_i, s'_i, s'_{i+1})\big\langle s'_{i+1}, s'_i\big|\Big|\sigma'_1 \ldots \sigma'_N\Big\rangle.\end{aligned}$$

Since each index appears only once at each side, for nonvanishing matrix elements we have to satisfy the condition

$$s_i = \sigma_i \qquad \text{and} \qquad s'_i = \sigma'_i$$

for all i. Therefore, the sum simplifies to

$$\begin{aligned}&\Big\langle \underline{\sigma}\Big|\mathrm{e}^{-\frac{\beta}{m}H_{e/o}}\Big|\underline{\sigma}'\Big\rangle \qquad (6.28)\\ &= \Big\langle \sigma_N \ldots \sigma_1\Big|\prod_{i}^{e/o} |\sigma_i, \sigma_{i+1}\rangle A_{i,i+1}(\sigma_{i+1}, \sigma_i, \sigma'_i, \sigma'_{i+1})\big\langle \sigma'_{i+1}, \sigma'_i\big|\Big|\sigma'_1 \ldots \sigma'_N\Big\rangle\end{aligned}$$

or equivalently

$$\begin{aligned}&= \prod_{i}^{e/o} A_{i,i+1}(\sigma_{i+1}, \sigma_i, \sigma'_i, \sigma'_{i+1})\\ &\quad\times \underbrace{\Big\langle \sigma_N \ldots \sigma_1\Big|\prod_{i}^{e/o} |\sigma_i, \sigma_{i+1}\rangle\big\langle \sigma'_{i+1}, \sigma'_i\big|\Big|\sigma'_1 \ldots \sigma'_N\Big\rangle}_{S(\underline{\sigma},\underline{\sigma}')} \,.\end{aligned}$$

By re-inserting the definition of A (6.25), we obtain

$$\Big\langle \underline{\sigma}\Big|\mathrm{e}^{-\frac{\beta}{m}H_{e/o}}\Big|\underline{\sigma}'\Big\rangle = S(\underline{\sigma},\underline{\sigma}')\prod_{i}^{e/o}\langle\sigma_{i+1}\sigma_i|\mathrm{e}^{-\frac{\beta}{m}H_{i,i+1}}\big|\sigma'_i\sigma'_{i+1}\big\rangle \,. \quad (6.29)$$

In general, the quantity S can either be $S = +1$ or $S = -1$ depending on the number of permutations necessary to pair corresponding creation and annihilition operators. The case $S = -1$ causes non-local sign problems that typically complicate WLMC simulations for fermionic systems. In our case of the Heisenberg model, we only have to deal with spin operators. Fortunately, spin operators at different sites commute. Therefore permutations do not yield minus signs and $S \equiv 1$.

We continue by evaluating the 2×2 matrix elements (6.25). Upon introducing the abbreviation

$$M \stackrel{\text{def}}{=} -\frac{\beta}{m} H_{i,i+1} = \frac{\beta}{m} J_z S_i^z S_{i+1}^z + \frac{\beta}{m}\frac{J}{2} F_i \tag{6.30}$$

with the Flip operator F_i, they are calculated in a straight forward manner. The results are summarized in Table 6.1. We want to evaluate the exponential

Table 6.1. Matrix elements of the one-dimensional Heisenberg model

$\sigma_i\sigma_{i+1}/\sigma_i'\sigma_{i+1}'$	$(\uparrow\downarrow)$	$(\downarrow\uparrow)$	$(\uparrow\uparrow)$	$(\downarrow\downarrow)$
$(\uparrow\downarrow)$	$-\frac{\beta J_z}{4m}$	$\frac{\beta J}{2m}$	0	0
$(\downarrow\uparrow)$	$\frac{\beta J}{2m}$	$-\frac{\beta J_z}{4m}$	0	0
$(\uparrow\uparrow)$	0	0	$\frac{\beta J_z}{4m}$	0
$(\downarrow\downarrow)$	0	0	0	$\frac{\beta J_z}{4m}$

of M, i.e. e^M. For this end it is convenient to apply the spectral theorem. Thus, we need the eigenvalues λ_i and eigenvectors $\mathbf{x}_i$. They are given by

$$\begin{aligned}
\mathbf{x}_1 &= \begin{pmatrix} 0\\0\\0\\1 \end{pmatrix}, \lambda_1 = \frac{\beta J_z}{4m} \qquad \mathbf{x}_2 = \begin{pmatrix} 0\\0\\1\\0 \end{pmatrix}, \lambda_2 = \frac{\beta J_z}{4m} \\
\mathbf{x}_3 &= \frac{1}{\sqrt{2}}\begin{pmatrix} 1\\1\\0\\0 \end{pmatrix}, \lambda_3 = -\frac{\beta J_z}{4m} + \frac{\beta J}{2m} \\
\mathbf{x}_4 &= \frac{1}{\sqrt{2}}\begin{pmatrix} 1\\-1\\0\\0 \end{pmatrix}, \lambda_4 = -\frac{\beta J_z}{4m} - \frac{\beta J}{2m}\ .
\end{aligned} \tag{6.31}$$

Thus using the spectral theorem, we obtain

$$\mathrm{e}^M = \sum_{i=1}^{4} \mathrm{e}^{\lambda_i} \mathbf{x}_i \mathbf{x}_i^\dagger = \begin{pmatrix} \mathrm{e}^{-\frac{\beta J_z}{4m}}\,\mathrm{ch} & \mathrm{e}^{-\frac{\beta J_z}{4m}}\,\mathrm{sh} & 0 & 0 \\ \mathrm{e}^{-\frac{\beta J_z}{4m}}\,\mathrm{sh} & \mathrm{e}^{-\frac{\beta J_z}{4m}}\,\mathrm{ch} & 0 & 0 \\ 0 & 0 & \mathrm{e}^{\frac{\beta J_z}{4m}} & 0 \\ 0 & 0 & 0 & \mathrm{e}^{\frac{\beta J_z}{4m}} \end{pmatrix}. \tag{6.32}$$

The new symbols ch and sh represent

$$\mathrm{ch} = \cosh\big(\frac{\beta J}{2m}\big)\ , \quad \mathrm{sh} = \sinh\big(\frac{\beta J}{2m}\big)\ . \tag{6.33}$$

We can simplify the above expressions by splitting off an exponential factor and reducing it to a 2×2 block matrix. This matrix will be denoted by w.

$$\begin{aligned} \mathrm{e}^{M} &= \mathrm{e}^{\frac{\beta J_z}{4m}} \begin{pmatrix} \mathrm{e}^{-\frac{\beta J_z}{2m}} \begin{pmatrix} \mathrm{ch} & \mathrm{sh} \\ \mathrm{sh} & \mathrm{ch} \end{pmatrix} & \mathbb{O}_2 \\ \mathbb{O}_2 & \mathbb{I}_2 \end{pmatrix} \\ &= \mathrm{e}^{\frac{\beta J_z}{4m}}\ w\big(\sigma_i, \sigma_{i+1}, \sigma_i', \sigma_{i+1}'\big)\ . \end{aligned} \tag{6.34}$$

We conclude that, for N spins, the matrix elements are products of the form

$$\begin{aligned} \big\langle\, \underline{\sigma} \big| \mathrm{e}^{-\frac{\beta}{m} H_{e/o}} \big| \underline{\sigma}' \,\big\rangle &= \prod_i^{e/o} \mathrm{e}^{\frac{\beta J_z}{4m}}\, w\big(\sigma_i, \sigma_{i+1}, \sigma_i', \sigma_{i+1}'\big) \\ &= \mathrm{e}^{\frac{\beta J_z}{4m}\frac{N}{2}} \prod_i^{e/o} w\big(\sigma_i, \sigma_{i+1}, \sigma_i', \sigma_{i+1}'\big)\ . \end{aligned} \tag{6.35}$$

Inserting the obtained result into (6.23), the partition function Z becomes

$$\begin{aligned} Z &= \sum_{\sigma_i} \mathrm{e}^{\frac{\beta}{8m}\sum_j V\left(\underline{\sigma}^{(j)}\right)} \prod_{\tau=1}^{m} \big\langle \underline{\sigma}^{(2\tau-1)} \big| \mathrm{e}^{-\frac{\beta}{m} H_o} \big| \underline{\sigma}^{(2\tau)} \big\rangle \big\langle \underline{\sigma}^{(2\tau)} \big| \mathrm{e}^{-\frac{\beta}{m} H_e} \big| \underline{\sigma}^{(2\tau+1)} \big\rangle \\ &= \sum_{\sigma_i} \mathrm{e}^{\frac{\beta}{8m}\sum_j V\left(\underline{\sigma}^{(j)}\right)} \mathrm{e}^{\frac{\beta J_z}{8m} 2mN} \prod_{\tau=1}^{m} \prod_i^{\mathrm{odd}} w\big(\sigma_i^{(2\tau-1)}, \sigma_{i+1}^{(2\tau-1)}, \sigma_i'^{(2\tau)}, \sigma_{i+1}'^{(2\tau)}\big) \\ &\quad \times \prod_i^{\mathrm{even}} w\big(\sigma_i^{(2\tau)}, \sigma_{i+1}^{(2\tau)}, \sigma_i'^{(2\tau+1)}, \sigma_{i+1}'^{(2\tau+1)}\big)\ . \end{aligned}$$

We observe that most of the elements of the matrix w, namely 10 out of 16 are zero. This is a consequence of form of the Flip operator and of the preservation of the z–component of the integral spin. If both spins i and $i+1$ point in the same direction, F_i reduces the state to zero. Therefore it is convenient to introduce the notion of *active plaquettes*. Imagine a spin $\uparrow$ at the site i=odd and Trotter–time τ=odd. Where will this spin $\uparrow$ be found at time $\tau + 1$? The answer depends on the matrix w and thus on the state of the spin $i+1$ at time τ. If spin $i+1$ is also a $\uparrow$ state, the only possibility is that at time $\tau + 1$ the same state occurs. This is due to the $w_{33} = 1$ (third column and third row of the matrix w). If, however, spin $i+1$ is in the $\downarrow$ state at time τ, the two spins can either be flipped ($w_{12} \neq 0$) or keep their orientations ($w_{11} \neq 0$). In general the two possibilities have different weight. Notice that the fate of spin i is independent of spin $i-1$. The same is true for an even Trotter–time τ and an even site i. Conversely, if τ is odd and i is even or if τ is even and i is odd, the "evolution" of this spin depends on the

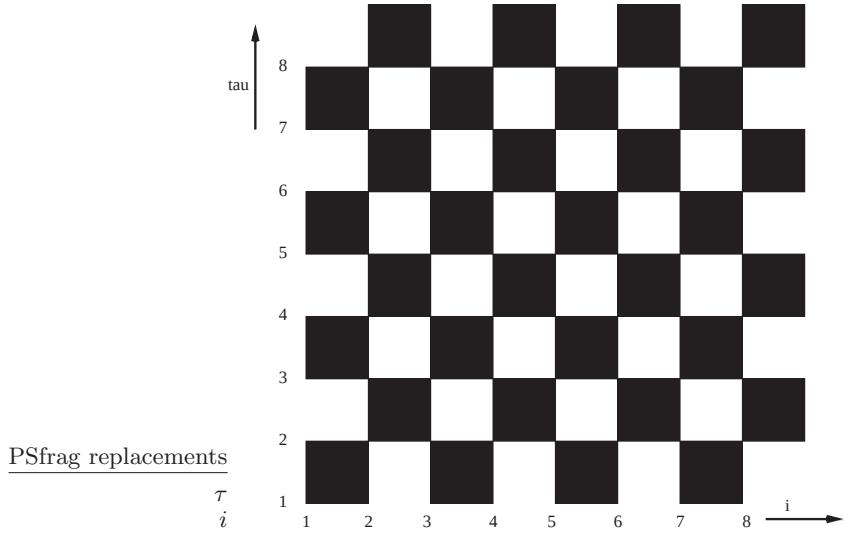

Fig. 6.1. The Checker Board for the Suzuki-Trotter decomposition of the Canonical Partition function of eight spins in the Heisenberg model

orientation of spin $i-1$. This situation can be visualized with the *checker board* of black and white fields. A spin is located at each corner of a field. Black fields are called *active plaquettes* because spins that are coupled via black fields influence each other.
We introduce an intermediate notation depicting sites of spin $\uparrow$ with filled circles and sites with spin $\downarrow$ with open circles. The discussion can be reduced to investigating one active plaquette. There are several possible configurations shown in Fig. 6.2. The weights for each configuration are inferred from

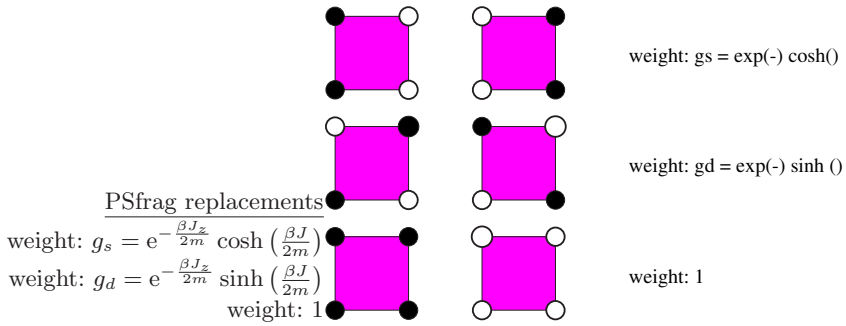

Fig. 6.2. Weights of the six different configurations of an active plaquette

the matrix w. Since the z–component of the spin is a conserved quantity,

the number of filled circles at the base line of the active plaquette must be the same as at the top. A more common visualization is to join spin ↑ sites with lines. These are the so called *world lines*. Spin ↓ sites are not mentioned any more. As can be deduced from Fig. 6.2, world lines can run in diagonal

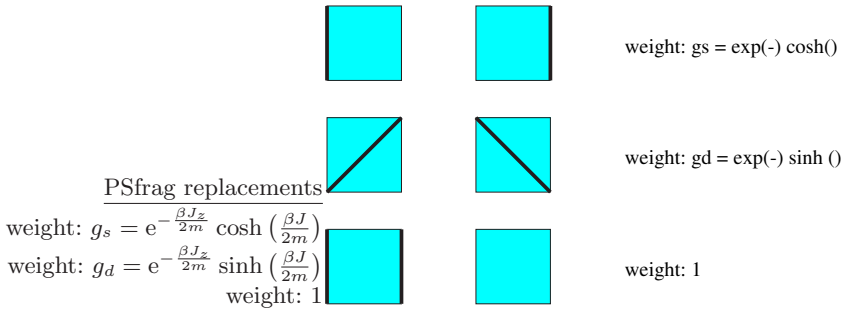

Fig. 6.3. World line visualization of the six different configurations of an active plaquette

direction only on active plaquettes. Furthermore, it is common to join spin ↑ sites with straight lines whenever this is possible. Thus, active plaquettes with four spin ↑ sites are visualized with two straight world lines. Due to the conservation of S_z, world lines cannot be interrupted anywhere. As a consequence of the trace in the partition function, periodic boundary conditions in the Trotter time have to be applied. Additionally, we can choose periodic boundary conditions in real space. The canonical partition function Z can be written as a *sum over all world–line configurations* W. One such world–line configurations W contributes with the statistical weight $\rho(W)$ given by

$$\rho(W) = g_s^{n_s}\, g_d^{n_d} \ , \tag{6.36}$$

where the integers n_s and n_d count the numbers of active plaquettes occupied by one straight / diagonal piece of a world line, respectively. The preservation of S_z on each active plaquette implies that the number of the world lines remains constant. The partition function thus reads

$$\begin{aligned} Z =& \mathrm{e}^{\frac{\beta J_z N}{4}} \sum_W \exp\left\{\frac{\beta}{8m} \sum_{i,j} J_{ij} \sum_\tau \sigma_i^{(\tau)} \sigma_j^{(\tau)}\right\} g_s^{n_s} g_d^{n_d} \\ =& \mathrm{e}^{\frac{\beta J_z N}{4}} \sum_W \exp\left\{\frac{\beta}{8m} \sum_{i,j} J_{ij} \sum_\tau \sigma_i^{(\tau)} \sigma_j^{(\tau)}\right\} \rho(W) \ . \end{aligned} \tag{6.37}$$

The thermodynamical expectation of the energy E can be inferred from the partition function through differentiation. This is outlined for the general case in Sec. 6.2.3. In the one–dimensional case the thermal energy is given by

$$
\begin{aligned}
E = < H > &= \frac{1}{\mathrm{tr}(\mathrm{e}^{-\beta H})}\ \mathrm{tr}\big(H\,\mathrm{e}^{-\beta H}\big) = -\frac{\partial}{\partial\beta}\log Z \\
&= -J_z\Big(\frac{N}{4} - \frac{1}{2m}\big(< n_s > + < n_d > \big)\Big) \\
&\quad -J\frac{1}{2m}\Big(\tanh\big(\frac{\beta J_z}{2m}\big) < n_s > + \coth\big(\frac{\beta J_z}{2m}\big) < n_d > \Big)
\end{aligned}
\tag{6.38}
$$

where $< n_s >$ and $< n_d >$ denote the average number of straight and diagonal plaquettes, respectively. The long ranging *spin–spin correlations* can be evaluated through differentiation

$$
< S_i^z\, S_j^z > = \frac{1}{\beta}\frac{\partial}{\partial J_{ij}}\log Z\Big|_{H'=0} = \frac{1}{8m}\sum_W \rho(W)\sum_{\tau=1}^{2m}\sigma_i^{(\tau)}\sigma_j^{(\tau)} \tag{6.39}
$$

This formula is valid even for the case $H' = 0$ and can thus also be applied to the original Heisenberg model without long-rangin interactions.

6.2.2 Higher Spatial Dimensions

In higher dimensions ($d = 2$ or 3), the Trotter decomposition has to be carried out for each direction separately. Instead of the one–dimensional chain, we consider a cubic lattice of N sites. We have to take into account the contributions of the nearest neighbour interaction in each spatial direction (H_x, H_y, H_z). In the two-dimensional case, for instance, a possible breakup of the Hamiltonian reads

$$
H = H_x + H_y = H_{ex} + H_{ox} + H_{ey} + H_{oy}\ , \tag{6.40}
$$

with $H_{e/ox}, H_{e/oy}$ denoting the even and odd part of the interaction in $x-$ and $y-$ direction, respectively. Often, a more symmetric decomposition like

$$
H = \frac{1}{2}\,H_{ex} + H_{ox} + \frac{1}{2}\,H_{ex} + \frac{1}{2}\,H_{ey} + H_{oy} + \frac{1}{2}\,H_{ey} \tag{6.41}
$$

can be convenient. To cover the general case, we introduce the symbol N_b denoting the number of components of the decomposition. The Suzuki–Trotter approximation of one Trotter slice is then given by the product

$$
\mathrm{e}^{-\frac{\beta}{m}H} \approx \prod_{b=1}^{N_b}\mathrm{e}^{-\Delta\tau_b H_b}\ , \tag{6.42}
$$

with time intervals $\Delta\tau_b$. When using the decomposition stated in (6.40), we find $N_b = 4$ and all $\Delta\tau_b = \beta/m$. The operators H_b are given by $H_1 = H_{xe}, H_2 = H_{xo}, H_3 = H_{ye}$ and $H_4 = H_{yo}$, respectively. On the other hand, choosing the symmetric form of (6.41), we have $N_b = 6$ and $\Delta\tau_2 = \Delta\tau_5 = \beta/m$ whereas $\Delta\tau_1 = \Delta\tau_3 = \Delta\tau_4 = \Delta\tau_6 = \beta/(2m)$. In this case,

the operators H_b are given by $H_1 = H_3 = H_{xe}, H_2 = H_{xo}, H_4 = H_6 = H_{ye}$ and $H_5 = H_{yo}$. The sum over all $\Delta\tau_b$ equals

$$\sum_{b=1}^{N_b} \Delta\tau_b = \frac{\beta}{m} \sum_{b=1}^{N_b} f_b = 2\,\frac{\beta}{m}\,d\,. \tag{6.43}$$

The new symbols f_b are defined as $\Delta\tau_b \stackrel{\text{def}}{=} f_b\,\beta/m$. Therefore, the partition function Z reads in Suzuki–Trotter approximation

$$Z \approx \ \mathrm{tr} \prod_{\tau=1}^{m} \prod_{b=1}^{N_b} \mathrm{e}^{-\Delta\tau_b H_b}\ . \tag{6.44}$$

To evaluate the trace, we use a collection of $m \times N_b$ sets of complete bases S labelled by l. When using cyclic boundary conditions, $S^{(mN_b+1)} = S^{(1)}$, and the function $l(\tau, b) = \tau\, N_b + b$ we obtain

$$Z \approx \sum_{S^{(1)} \ldots S^{(mN_b)}} \prod_{\tau=1}^{m} \prod_{b=1}^{N_b} \left\langle S^{(l)} \left| \mathrm{e}^{-\Delta\tau_b H_b} \right| S^{(l+1)} \right\rangle\,. \tag{6.45}$$

Now we can evaluate each matrix element in the same way as outlined for the one-dimensional case. Since the Hamiltonians H_b consist of sums of commuting operators, the exponential $\exp(-\Delta\tau_b H_b)$ factorizes. As in the one–dimensional case, each H_b consists of $N/2$ terms. The resulting factors can be cast in the form

$$\mathrm{e}^{\frac{\Delta\tau_b}{4}\,J_z} \begin{pmatrix} \mathrm{e}^{-\frac{J_z \Delta\tau_b}{2}} \begin{pmatrix} \cosh(\Delta\tau_b J/2) & \sinh(\Delta\tau_b J/2) \\ \sinh(\Delta\tau_b J/2) & \cosh(\Delta\tau_b J/2) \end{pmatrix} & \mathbb{O}_2 \\ \mathbb{O}_2 & \mathbb{I}_2 \end{pmatrix}\,. \tag{6.46}$$

When inserting this matrix into the matrix element of (6.45), we obtain the structure of active plaquettes. Since H_b consists of $N/2$ terms, each Trotter slice comprises $N/2$ active plaquettes per direction b. From (6.46) we see that we can split off the common factor $\exp(\Delta\tau_b J_z/4)$. Upon introducing the b dependent plaquette weights

$$\begin{aligned} g_{s,b} &= \mathrm{e}^{-\Delta\tau_b J_z/2}\ \cosh\left(|\Delta\tau_b J/2|\right) \\ g_{d,b} &= \mathrm{e}^{-\Delta\tau_b J_z/2}\ \sinh\left(|\Delta\tau_b J/2|\right)\,, \end{aligned} \tag{6.47}$$

as well as the numbers $n_s(b,\tau)$ and $n_d(b,\tau)$ of straight and diagonal plaquettes of one direction b within one Trotter slice τ we obtain

$$\begin{aligned} Z &\approx \sum_{S^{(1)} \ldots S^{(mN_b)}} \prod_{\tau=1}^{m} \prod_{b=1}^{N_b} \mathrm{e}^{\frac{J_z}{4}\,\frac{N}{2}\,\Delta\tau_b}\, g_{s,b}^{n_s(b,\tau)}\, g_{d,b}^{n_d(b,\tau)} \\ &= \mathrm{e}^{\frac{J_z}{4}\,\frac{N}{2}\,\sum_\tau \sum_b \Delta\tau_b} \sum_{S^{(1)} \ldots S^{(mN_b)}} \prod_{b=1}^{N_b} g_{s,b}^{\sum_\tau n_s(b,\tau)}\, g_{d,b}^{\sum_\tau n_d(b,\tau)}\,. \end{aligned} \tag{6.48}$$

By using (6.43) we simplify the two sums of the first exponential. By abbreviating the sums occurring in the other exponentials by $n_s(b) = \sum_\tau n_s(b,\tau)$ and $n_d(b) = \sum_\tau n_d(b,\tau)$, respectively, we obtain the final result

$$Z \;=\; \mathrm{e}^{\frac{\beta J_z}{4} Nd} \sum_W \prod_{b=1}^{N_b} g_{s,b}^{n_s(b)}\, g_{d,b}^{n_d(b)} \;. \tag{6.49}$$

Instead of extending the sum over all spin configurations, we now sum over all possible world-line configurations W. The two summations are equivalent, because each spin configuration maps uniquely to one world line configuration. From (6.49) we infer that the statistical weight of a world–line configuration W is given by

$$\rho(W) = \prod_{b=1}^{N_b} g_{s,b}^{n_s(b)}\, g_{d,b}^{n_d(b)} \;. \tag{6.50}$$

As we have seen, in higher spatial dimensions the trace of the partition function Z cannot be simplified with cyclic permutations to the same extent as in one dimension. The weights g_s and g_d become *time–dependent* as they vary periodically with the Trotter time τ. Additionally, the Trotter slices become more extended. The same phenomena occur for long ranging interactions.

6.2.3 Correlations, Energy

In the field of statistical mechanics, many expectation values can be derived from the partition function by means of differentiation. Among these observables we find the thermal (internal) energy and – for spin systems – correlation functions. Therefore, we now discuss the differentiation of the logarithm of (6.49) with respect to J_z and J. This logarithm is given by

$$\log Z = \frac{\beta J_z}{4} Nd + \log\left(\sum_W \prod_b g_{s,b}^{n_s(b)}\, g_{d,b}^{n_d(b)} \right) \;. \tag{6.51}$$

Let's start with the simpler case, namely with the differentiation with respect to J_z. By exploiting the identity $(\log f)' = f'/f$ and exchanging the order of summation and differentiation, we obtain

$$\frac{\partial \log Z}{\partial J_z} = \frac{\beta}{2} Nd + \frac{\sum_W \frac{\partial}{\partial J_z} \prod_b g_{s,b}^{n_s(b)}\, g_{d,b}^{n_d(b)}}{\sum_W \prod_b g_{s,b}^{n_s(b)}\, g_{d,b}^{n_d(b)}} \;. \tag{6.52}$$

From the definition of the plaquette weights (6.47) we derive that the product over b can be cast into the form

$$\begin{aligned}
&\prod_b g_{s,b}^{n_s(b)}\, g_{d,b}^{n_d(b)} \qquad (6.53)\\
&= \prod_b \left(\mathrm{e}^{-\frac{\Delta\tau_b J_z}{2}}\right)^{n_s(b)+n_d(b)} \cosh^{n_s(b)}\left(|\frac{\Delta\tau_b J}{2}|\right)\, \sinh^{n_d(b)}\left(|\frac{\Delta\tau_b J}{2}|\right)\\
&= \mathrm{e}^{-\frac{J_z}{2}\sum_b \Delta\tau_b(n_s(b)+n_d(b))} \prod_b \cosh^{n_s(b)}\left(|\frac{\Delta\tau_b J}{2}|\right) \sinh^{n_d(b)}\left(|\frac{\Delta\tau_b J}{2}|\right) .
\end{aligned}$$

The arguments of the hyperbolic functions do not depend on J_z. Thus, differentiation with respect to J_z affects only the exponential part of the above expression and yields

$$\frac{\partial}{\partial J_z}\prod_b g_{s,b}^{n_s(b)}\, g_{d,b}^{n_d(b)} = -\frac{1}{2}\left(\sum_b \Delta\tau_b(n_s(b)+n_d(b))\right)\prod_b g_{s,b}^{n_s(b)}\, g_{d,b}^{n_d(b)} \ . \quad (6.54)$$

We find that the statistical weight is of the world-line configuration is reproduced by the differentiation. By inserting the above expression into (6.52) and using the definition of (6.50) we finally find

$$\begin{aligned}
\frac{\partial \log Z}{\partial J_z} &= \frac{\beta}{4}Nd - \frac{1}{2}\frac{\sum_W \rho(W)\left(\sum_b \Delta\tau_b(n_s(b)+n_d(b))\right)}{\sum_W \rho(W)}\\
&= \frac{\beta}{4}Nd - \frac{1}{2}\sum_b \Delta\tau_b\left(< n_s(b) > + < n_d(b) >\right)\\
&= \frac{\beta}{4}Nd - \frac{\beta}{2m}\sum_b f_b\left(< n_s(b) > + < n_d(b) >\right) . \qquad (6.55)
\end{aligned}$$

Now let's consider the differentiation of (6.51) with respect to J. Obviously, the first term cancels because it does not depend on J. Remains the product

$$\frac{\partial \log Z}{\partial J} = \frac{\sum_W \frac{\partial}{\partial J}\prod_b g_{s,b}^{n_s(b)}\, g_{d,b}^{n_d(b)}}{\sum_W \prod_b g_{s,b}^{n_s(b)}\, g_{d,b}^{n_d(b)}} \qquad (6.56)$$

whose evaluation involves the derivatives of the plaquette weights g with respect to J. By using (6.47) we find

$$\frac{\partial g_{s,b}}{\partial J} = \frac{\Delta\tau_b}{2}\, g_{d,b} \qquad \text{and} \qquad \frac{\partial g_{d,b}}{\partial J} = \frac{\Delta\tau_b}{2}\, g_{s,b} \ , \qquad (6.57)$$

and, therefore, the derivatives of the powers of g can be written as

$$\frac{\partial g_{s,b}^{n_s(b)}}{\partial J} = \frac{\Delta\tau_b}{2}\, n_s(b)\, \frac{g_{d,b}}{g_{s_b}}\, g_{s_b}^{n_s(b)}\, \frac{\partial g_{d,b}^{n_d(b)}}{\partial J} \quad = \frac{\Delta\tau_b}{2}\, n_d(b)\, \frac{g_{s,b}}{g_{d_b}}\, g_{d_b}^{n_d(b)} \ . \quad (6.58)$$

By application of the product rule of calculus, each term in the sum in the numerator of (6.56) can be written as

$$\frac{\partial}{\partial J}\prod_b g_{s,b}^{n_s(b)}\, g_{d,b}^{n_d(b)} = \frac{\partial}{\partial J}\left[\left(\prod_b g_{s,b}^{n_s(b)}\right)\left(\prod_b g_{d,b}^{n_d(b)}\right)\right] \tag{6.59}$$
$$= \left(\frac{\partial}{\partial J}\prod_b g_{s,b}^{n_s(b)}\right)\left(\prod_b g_{d,b}^{n_d(b)}\right) + \left(\prod_b g_{s,b}^{n_s(b)}\right)\left(\frac{\partial}{\partial J}\prod_b g_{d,b}^{n_d(b)}\right) .$$

The differentiation of the products over b is achieved by using (6.58) and the generalized product rule. This yields sums of the form

$$\frac{\partial}{\partial J}\prod_b g_{s,b}^{n_s(b)} = \frac{1}{2}\sum_b \Delta\tau_b\, n_s(b)\,\frac{g_{d,b}}{g_{s,b}}\prod_{b'} g_{s,b'}^{n_s(b')} \tag{6.60}$$
$$\frac{\partial}{\partial J}\prod_b g_{d,b}^{n_d(b)} = \frac{1}{2}\sum_b \Delta\tau_b\, n_d(b)\,\frac{g_{s,b}}{g_{d,b}}\prod_{b'} g_{d,b'}^{n_d(b')} . \tag{6.61}$$

Again, by inserting these identities into (6.59), we find that the weight of the world line configuration reappears. The fractions of plaquette weights are given by hyperbolic tangent and co–tangent functions:

$$\frac{\partial}{\partial J}\prod_b g_{s,b}^{n_s(b)}\, g_{d,b}^{n_d(b)} = \frac{1}{2}\sum_b \Delta\tau_b\left(n_s(b)\frac{g_{d,b}}{g_{s,b}} + n_d(b)\,\frac{g_{s,b}}{g_{d,b}}\right)\prod_b g_{s,b}^{n_s(b)} g_{d,b}^{n_d(b)} \tag{6.62}$$
$$= \frac{1}{2}\sum_b \Delta\tau_b\left(n_s(b)\underbrace{\tanh\left(\frac{\Delta\tau_b J}{2}\right)}_{\stackrel{\text{def}}{=}\mathrm{th}(b)} + n_d(b)\underbrace{\coth\left(\frac{\Delta\tau_b J}{2}\right)}_{\stackrel{\text{def}}{=}\mathrm{cth}(b)}\right)\rho(W) .$$

When inserting this relation into (6.56), we find

$$\frac{\partial \log Z}{\partial J} = \frac{\sum_W \frac{1}{2}\sum_b \Delta\tau_b\left(n_s(b)\tanh\left(\frac{\Delta\tau_b J}{2}\right) + n_d(b)\coth\left(\frac{\Delta\tau_b J}{2}\right)\right)\rho(W)}{\sum_W \rho(W)} \tag{6.63}$$

By exchanging the order of summation and abbreviating the weighted sum over all world line configurations W by the symbol $<>$ we finally obtain

$$\frac{\partial \log Z}{\partial J} = \frac{1}{2}\sum_b \Delta\tau_b\left(< n_s(b) > \tanh\left(\frac{\Delta\tau_b J}{2}\right) + < n_d(b) > \coth\left(\frac{\Delta\tau_b J}{2}\right)\right)$$
$$= \frac{\beta}{2m}\sum_b f_b\,(< n_s(b) > \mathrm{th}(b) + < n_d(b) > \mathrm{cth}(b)) . \tag{6.64}$$

We now have the main ingredients to evaluate the spin–spin correlation functions C^{zz} and C^{xy} and the thermal energy E. The former are defined as

$$C^{zz} \stackrel{\text{def}}{=} \left\langle \sum_{<i,j>} S_i^z S_j^z \right\rangle = \frac{1}{\beta} \frac{\partial}{\partial J_z} \log Z \tag{6.65}$$

$$C^{xy} \stackrel{\text{def}}{=} \left\langle \sum_{<i,j>} \frac{1}{2}(S_i^+ S_j^- + S_i^- S_j^+) \right\rangle = \frac{1}{\beta} \frac{\partial}{\partial J} \log Z \tag{6.66}$$

and follow immediately from the above calculations of the derivatives of the partition function. In fact, by inserting (6.55) and (6.64) into these definitions and cancelling the factor β/β we obtain

$$C^{zz} = \frac{1}{4} Nd - \frac{1}{2m} \sum_b f_b \left(< n_s(b) > + < n_d(b) > \right) , \tag{6.67}$$

$$C^{xy} = \frac{1}{2m} \sum_b f_b \left(< n_s(b) > \, \mathrm{th}(b) + < n_d(b) > \, \mathrm{cth}(b) \right) . \tag{6.68}$$

In case of the Heisenberg model, the thermal energy E is a weighted sum of the correlation functions.

$$\begin{aligned} E = < H > &= \Big\langle - J_z \sum_{<i,j>} S_i^z S_j^z - \frac{J}{2} \sum_{<i,j>} \left(S_i^+ S_j^- + S_i^- S_j^+ \right) \Big\rangle \\ &= -J_z \, C^{zz} - J \, C^{xy} . \end{aligned} \tag{6.69}$$

Inserting the explicit expressions for the correlations functions and collecting terms with $< n_s(b) >$ and $< n_d(b) >$, respectively, yields

$$\begin{aligned} E = & - \frac{J_z}{4} Nd + \sum_b < n_s(b) > \frac{f_b}{2m} (J_z - J \, \mathrm{th}(b)) \\ & + \sum_b < n_d(b) > \frac{f_b}{2m} (J_z - J \, \mathrm{cth}(b)) \\ = & - \frac{J_z}{4} Nd + \sum_b < n_s(b) > \, f_s(b) + < n_d(b) > f_d(b) . \end{aligned} \tag{6.70}$$

The vectors $f_s(b)$ and $f_d(b)$ are given by

$$f_s(b) = \frac{f_b}{2m} (J_z - J \, \mathrm{th}(b)) \tag{6.71}$$

$$f_d(b) = \frac{f_b}{2m} (J_z - J \, \mathrm{cth}(b)) . \tag{6.72}$$

6.2.4 Local moves, Metropolis

In this subsection we describe a concrete algorithm to simulate the canonical averages of a Heisenberg Hamiltonian. We restrict ourselves to local changes

on the checker board (local moves) to trace though the whole phase space. The Metropolis algorithm shall be employed to create world–line configurations according to the distribution $\rho(W)$ given by $\rho(W) = g_d^{n_d} g_s^{n_s}$.
To proceed from one configuration to the next, a world line number n and a Trotter–Time τ have to be chosen at random. Figure 6.4 shows the local moves that are possible if the white field happens to be at the right-hand side of a locally straight (at time τ) world line n.

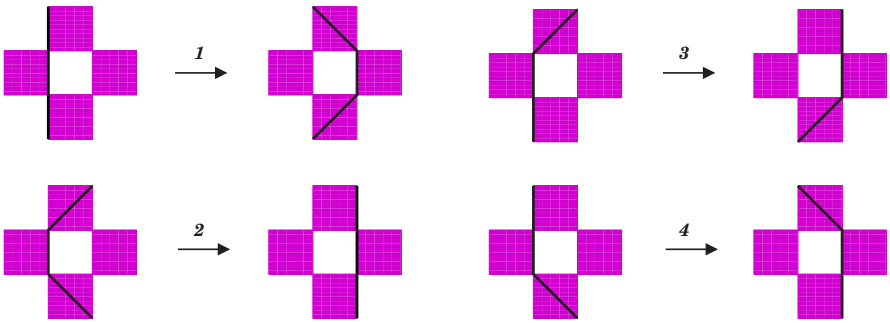

Fig. 6.4. Possible moves consistent with the rules of the Checker board

Each possibility changes the weight of the world line configuration in a different way. In case 1, for instance, two more diagonal lines appear increasing the number n_d by two: $n'_d = n_d + 2$. The two disappeared straight lines decrease the number n_s by two: $n'_s = n_s - 2$.
Does the move of the straight piece of a world line from the left-hand side of a white field to the right-hand side of the same field affect the weight of the configuration? Since only active plaquettes with one single line contribute to n_s, this depends on the state of the active plaquettes at either side of the white field. If the active plaquettes at the left-hand side of the white field is occupied by an additional straight piece of a world line and the other is not, then the number n_s increases by two: $n'_d = n_d + 2$. Conversely, if the opposite is true, it decreases by two: $n'_d = n_d - 2$. If both plaquettes have the same state, nothing changes. The other three possibilities are treated in a similar way, and one remarks that all changes of the weights are calculated *locally*. Thus the efficiency of the local algorithm in evaluating the weight of the new configuration.
According to Metropolis' rule, however, the altered configuration is only accepted with the probability

$$q = \frac{p(n'_d, n'_s)}{p(n_d, n_s)} = \frac{g_d^{n'_d} g_s^{n'_s}}{g_d^{n_d} g_s^{n_s}} = g_d^{n'_d - n_d} g_s^{n'_s - n_s} \tag{6.73}$$

or 1, if $q > 1$. Generally speaking, it takes about 1.000 to 10.000 local moves to change the configuration globally. Therefore, measurements can only be

performed after a huge number of moves. This is an obvious drawback of the adopted algorithm. Additionally, a low acceptance ($< 5\%$) adds to the inefficiency of this local approach.

6.2.5 Outlook

The above presented formalism of World Lines Quantum Monte Carlo can also be applied to the Hubbard model with the kinetic term

$$\hat{H}_0 = -t \sum_{ij,\sigma} a^\dagger_{i,\sigma} a_{j,\sigma} \ . \tag{6.74}$$

Only the meaning of the various terms in the formalism changes. For each spin orientation $\sigma = \uparrow, \downarrow$ a separate checker board has to be introduced. If only $\hat{H}_0$ is considered, the world lines of the two checker boards evolve independently. The Hubbard model, however, also includes on-site interaction of the form

$$\hat{H}_1 = U \sum_i \hat{n}_{i\uparrow} \, \hat{n}_{i\downarrow} \ .$$

This interaction term links the two checker boards: If a $\uparrow$ world line at time τ goes through site i_0, the presence of a $\downarrow$ world line at the same site and time is suppressed by the interaction energy U.
The Hubbard model is considered to be a good candidate to describe High Temperature Superconductors. However, for WLMC simulations the inverse temperature β must be bigger than the parameter t of the Hamiltonian. This yields to temperatures of about 10.000 K, that are much too high for real superconductivity.
A drawback of the WLMC algorithm must also be mentioned: This algorithm is always an approximation and has no exact limit. (??? Due to the Trotter decomposition ????) Even in the particular Hubbard model with $U = 0$ WLMC doesn't yield exact results.

6.3 Projector–Quantum–Monte Carlo

As we explained in the last section, World Lines Monte Carlo fails for low temperatures. The method presented next is designed to fill this gap.
The basic idea of the Projector method is to take a trial state $|\psi_T\rangle$ and evaluate expectation values of operators $\hat{O}$ in a state generated as *low temperature limit* of the trial state $|\psi_T\rangle$. By low temperature limit we mean the state

$$|\psi\rangle = \lim_{\beta\to\infty} \mathrm{e}^{-\beta\hat{H}}|\psi_T\rangle \ . \tag{6.75}$$

The quantity β does not actually correspond to a real inverse thermodynamic temperature. Nevertheless, it displays some analogies to it: If $|\psi_T\rangle$ contains a component in the direction of the non–degenerate ground state of the system, the operator $\mathrm{e}^{-\beta H}$ amplifies this component. This is seen by inserting a complete set of eigenfunctions $|\eta_n\rangle$ of the Hamiltonian $\hat{H}$ with energies E_n.

$$\begin{aligned} |\psi_\beta\rangle =& \mathrm{e}^{-\beta\hat{H}} \sum_{n\geq 0} |\eta_n\rangle\langle\eta_n\,|\psi_T\,\rangle \\ =& \sum_{n\geq 0} \mathrm{e}^{-\beta E_n}\, |\eta_n\rangle\langle\eta_n\,|\psi_T\,\rangle \\ =& \mathrm{e}^{-\beta E_0}\Big(\langle\eta_0\,|\psi_T\,\rangle|\eta_0\rangle + \mathrm{e}^{-\beta(E_1-E_0)}\langle\eta_1\,|\psi_T\,\rangle|\eta_1\rangle + \dots\Big) \end{aligned} \tag{6.76}$$

We can choose the ground-state energy $E_0 = 0$ and see that the for an increasing β, the the contribution of excited states becomes exponentially smaller. We can say that the artificial inverse temperature β controls a *window* in the energy room. States within this window contribute to $|\psi_\beta\rangle$, the others don't. This is illustrated in Fig. 6.5. We observe that the weight of an excited state $|\eta_n\rangle$ depends on the gap between E_0 and E_n and on the inverse temperature β.
Since we are interested in the physical properties of systems in the ground state, we have the tendency to take β as large as possible. On the other hand, due to non-commuting operators in the Hamiltonian, we will have to carry out a Trotter decomposition. In this context a large β implies that we have to take a big number m of Trotter times in order to keep the fraction β/m (and thus the error) small. Therefore, it depends on our computational capacity how large a β we can choose. Furthermore, the quality of the simulation depends on our skill to choose the trial function $|\psi_T\rangle$. If $|\psi_T\rangle = |\eta_0\rangle$, we see the exact correlations of the ground state for any β. It should be noted that, in contrast to statistical mechanics, the state $|\psi_T\rangle$ is a pure state, i.e. a vector in the Hilbert space of the system. This implies that we can measure correlations whose thermodynamical mixture cancels.
We will introduce the Projector Quantum Monte Carlo (PQMC) on the basis of the Hubbard model

$$\hat{H} = \hat{H}_0 + \hat{H}_1 \ , \tag{6.77}$$

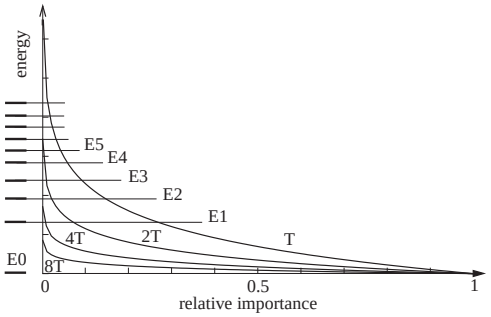

Fig. 6.5. relative importance of the lowest few eigenvalues of the Hamiltonian for different temperatures T

where $\hat{H}_0$ is the hopping operatore and $\hat{H}_1$ the on-site interaction of the particles. The *band structure* of the hopping operator can be exploited by using the dispersion relation $\varepsilon(k)$ of the lattice. This approach is possible, because the band structure is modeled as an external potential with a one-particle operator. Therefore, we write the contributions to the many-particle Hamiltonian as

$$\hat{H}_0 = \sum_{k,\sigma} \varepsilon(k) \hat{a}^\dagger_{k\sigma} \hat{a}_{k\sigma} = -\sum_{i,j,\sigma} t_{ij} \hat{a}^\dagger_{i\sigma} \hat{a}_{j\sigma} \ , \quad \hat{H}_1 = U \sum_i \hat{n}_{i\downarrow} \hat{n}_{i\uparrow} \tag{6.78}$$

The expectation value of an observable $\hat{O}$ in the pure state $|\psi\rangle$ is given by the fraction

$$< \hat{O} >= \frac{\langle\psi|\hat{O}|\psi\rangle}{\langle\psi\,|\psi\,\rangle} = \frac{\langle\psi_T|\mathrm{e}^{-\beta\hat{H}}\hat{O}\,\mathrm{e}^{-\beta\hat{H}}|\psi_T\rangle}{\langle\psi_T|\mathrm{e}^{-2\,\beta H}|\psi_T\rangle} \tag{6.79}$$

In contrast to a grand canonical approach presented in Sec. 6.4, this expectation value contains no sum over a mixture of states. We expand the expression $\mathrm{e}^{-\beta H}|\psi_T\rangle$ in a product of m Trotter times and absorb the last factor in a new trial state $\left|\tilde{\psi}_T\right\rangle$

$$\mathrm{e}^{-\beta\hat{H}}|\psi_T\rangle = \mathrm{e}^{-\frac{\beta\hat{H}_0}{2m}}\mathrm{e}^{-\frac{\beta\hat{H}_1}{m}}\mathrm{e}^{-\frac{\beta\hat{H}_0}{m}}\ldots\underbrace{\mathrm{e}^{-\frac{\beta\hat{H}_0}{2m}}|\psi_T\rangle}_{|\tilde{\psi}_T\rangle} = \prod_{\tau=1}^{m}\hat{K}^{(\tau)}\hat{V}^{(\tau)}|\tilde{\psi}_T\rangle\ . \quad (6.80)$$

The new symbols $\hat{K}^{(\tau)}$ and $\hat{V}^{(\tau)}$ correspond to the operators of kinetic and potential energy. They are defined as

$$\hat{K}^{(\tau)} = \exp\Big(-\frac{\beta\hat{H}_0}{(\delta_{1\tau}+1)m}\Big)\,, \qquad \hat{V}^{(\tau)} = \exp\Big(-\frac{\beta}{m}\hat{H}_1\Big) \quad (6.81)$$

where, as usual, δ_{ij} denotes the Kronecker delta. The kinetic part, $\hat{K}^{(\tau)}$, is a one-particle operator whereas $\hat{V}^{(\tau)}$ affects two particles if located at the same lattice site. In order to continue the calculation, we want to map the entire many particle problem on a one-particle problem with stochastic fields. This mapping is achieved with the *Discrete Hubbard Stratonovich transformation* presented next.

6.3.1 Discrete Hubbard Stratonovich Transformation

In this section we present a simplified version of the *Siegert transformation* outlined in Sec. 6.3.6. The two-particle term $\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$ in the operator $\hat{H}_1$ is the cause of our troubles. We tackle it with a trick. Consider the square of the operator of the *magnetization* $\hat{m}_i$ at site i

$$\begin{aligned}\hat{m}_i^2 = (\hat{n}_{i\uparrow}-\hat{n}_{i\downarrow})^2 =& \hat{n}_{i\uparrow}^2 + \hat{n}_{i\downarrow}^2 - 2\,\hat{n}_{i\uparrow}\,\hat{n}_{i\downarrow}\\ =& \underbrace{\hat{n}_{i\uparrow}+\hat{n}_{i\downarrow}}_{\hat{n}_i} - 2\,\hat{n}_{i\uparrow}\,\hat{n}_{i\downarrow}\end{aligned} \quad (6.82)$$

In arriving at the last equation, we have exploited the fact that particle number operators commute and are projectors for fermions, i.e. $\hat{n}_{i\sigma}^2 = \hat{n}_{i\sigma}$. The operator $\hat{n}_i$ measures the number of electrons at site i independent of their spin. Inserting the above information into the interaction part of the Hamiltonian, i.e. $\hat{H}_1$, we obtain

$$\hat{H}_1 = U\sum_i \hat{n}_{i\uparrow}\,\hat{n}_{i\downarrow} = \frac{U}{2}\sum_i\big(\hat{n}_i - \hat{m}_i^2\big)\ . \quad (6.83)$$

The sum over $\hat{n}_i$ measures the total number of electrons and is henceforth abbreviated by $\hat{N}_e$. In what follows, its contribution will be added to $\hat{H}_0$. Thus we decompose the Hamiltonian as

$$\hat{H} = \underbrace{\hat{H}_0 + \frac{U}{2}\hat{N}_e}_{\tilde{H}_0}\underbrace{-\frac{U}{2}\hat{m}_i^2}_{\tilde{H}_1}\ . \quad (6.84)$$

Since all commutators between different $\hat{m}_i$ vanish, the exponential function of the new interaction Hamiltonian, $\tilde{H}_1$, is given by the product

$$\exp\big(-\frac{\beta}{m}\tilde{H}_1\big) = \exp\Big(\frac{\beta U}{2m}\sum_i \hat{m}_i^2\Big) = \prod_i \exp\Big(\frac{\beta U}{2m}\hat{m}_i^2\Big)\,. \tag{6.85}$$

Now comes the crucial step. We apply the *Hubbard Stratonovich transformation* to every factor of the product by making the ansatz

$$\exp\Big(\frac{\beta U}{2m}\hat{m}_i^2\Big) = \frac{1}{2}\sum_{S=\pm 1} \mathrm{e}^{\lambda \hat{m}_i S}\,. \tag{6.86}$$

The new quantities S are called *auxiliary fields* since at each lattice site a separate $S = S_i$ is needed. Since the S_i's can assume the values ± 1, they are Ising spins. The parameter λ can be inferred from the matrix elements summarized in Table 6.2. For positive U the equation

$n_{i\uparrow}$	$n_{i\downarrow}$	m_i	$\exp\big(\frac{\beta}{2m}Um_i^2\big)$	$\frac{1}{2}\sum_{S=\pm1}\mathrm{e}^{\lambda m_i S}$
0	0	0	1	1
1	1	0	1	1
1	0	1	$\exp\big(\frac{\beta}{2m}U\big)$	$\cosh(\lambda)$
0	1	-1	$\exp\big(\frac{\beta}{2m}U\big)$	$\cosh(\lambda)$

Table 6.2. Matrix elements for the evaluation of the parameter λ in the Hubbard Stratonovich transformation

$$\cosh(\lambda) = \exp\big(\frac{\beta U}{2m}\big) \tag{6.87}$$

determines $\cosh(\lambda)$ uniquely. We insert the information of (6.2) into the expression of the exponential function of the interaction Hamiltonian. This yields a sum over all *Ising spin* configurations forming the auxiliary fields:

$$\exp\Big(-\frac{\beta}{m}\tilde{H}_1\Big) = 2^{-N}\sum_{S_1\ldots S_N=\pm 1}\exp\Big(\lambda\sum_{i=1}^{N}\hat{m}_i S_i\Big) \tag{6.88}$$

Now the term *stochastic field* displays its justification: These fields S couple to the magnetization similar to a magnetic field. Moreover, they are generated by the random *Ising Spin* configurations $\{S_1 \ldots S_N\}$. Equation (6.88) has an intuitive interpretation: The field $\{S_1 \ldots S_N\}$ generates a static spin-dependent potential for the particles. This can be seen by splitting the operator $\hat{m}_i$ into its components. Then (6.88) reads

$$\exp\Big(-\frac{\beta}{m}\tilde{H}_1\Big) = 2^{-N}\sum_{S_1\ldots S_N=\pm 1}\exp\Big(\lambda\sum_{i=1}^{N}\hat{n}_{i\uparrow}S_i - \lambda\sum_{i=1}^{N}\hat{n}_{i\downarrow}S_i\Big) \tag{6.89}$$

Suppose $S_i = +1$ for a given i. Then the energy λ has to be paid if only one electron of spin $\uparrow$ occupies the site i. Conversely, if only a spin $\downarrow$ electron sits on site i the system gains the energy λ because of the minus sign in front of the last sum. If site i is filled with two electrons, their energy contributions cancel. For $S_i = -1$ the same considerations apply, only the role of the $\uparrow$ and $\downarrow$ electrons are exchanged.

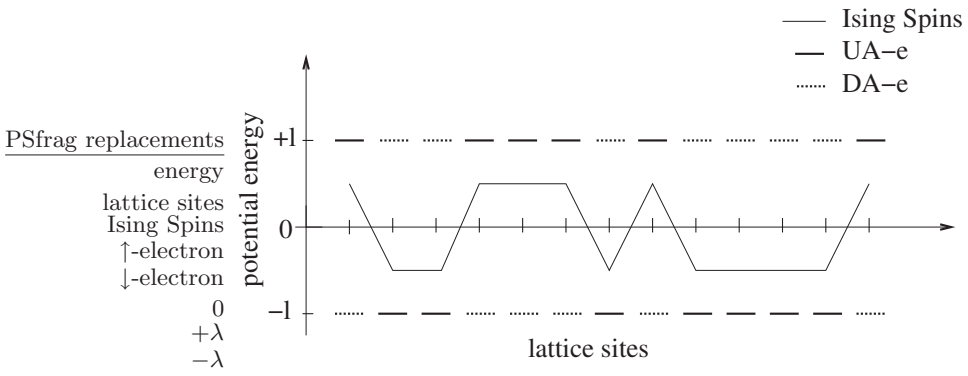

Fig. 6.6. Stochastic potential introduced by the Ising spins acting on $\uparrow$-electrons (full lines) and $\downarrow$-electrons (dashed lines)

We observe a remarkable feature of (6.88). Within one Trotter slice the interaction Hamiltonian $\tilde{H}_1$ has been replaced by a sum of non-interacting one-particle operators

$$\tilde{H}_1^{HS} = \sum_i \hat{m}_i \, S_i \; .$$

This, however, has to be paid with additional degrees of freedom which have to be summed over, namely the stochastic field.
We separate the two different spin orientations $\sigma = \uparrow\downarrow \equiv \pm 1$ and decompose the one-particle Hamiltonians as

$$\tilde{H}_0 = \sum_{\sigma=\uparrow\downarrow} \sum_{i,j} \big(-t_{ij\sigma} + \frac{U}{2}\delta_{ij} \big) \, \hat{a}^\dagger_{i\sigma} \hat{a}_{j\sigma} \stackrel{\text{def}}{=} \sum_{\sigma=\uparrow\downarrow} \tilde{H}_{0\sigma} \tag{6.90}$$

$$\tilde{H}_1^{HS} = \sum_{\sigma=\uparrow\downarrow} \sigma \sum_i \underbrace{\hat{a}^\dagger_{i\sigma} \hat{a}_{i\sigma}}_{\hat{n}_{i\sigma}} S_i \stackrel{\text{def}}{=} \sum_{\sigma=\uparrow\downarrow} \tilde{H}'_\sigma(\underline{S}) \; . \tag{6.91}$$

This has the consequence that the following commutators vanish

$$[\tilde{H}_{0\sigma}, \tilde{H}_{0\bar{\sigma}}] = 0 \; , \quad [\tilde{H}_{0\sigma}, \tilde{H}'_{\bar{\sigma}}] = 0 \; , \quad [\tilde{H}'_\sigma, \tilde{H}'_{\bar{\sigma}}] = 0 \; . \tag{6.92}$$

We decompose the operators $\hat{K}$ and $\hat{V}$ in a similar manner and define in analogy to (6.81) the kinetic and potential part of each spin orientation

$$\tilde{K}_\sigma^{(\tau)} = \exp\Big(- \frac{\beta}{m(1+\delta_{\tau,1})} \tilde{H}_{0\sigma} \Big) \,, \quad \tilde{V}_\sigma(\underline{S}^{(\tau)}) = \exp\Big(\lambda\sigma \sum_{i=1}^{N} \hat{n}_{i\sigma} S_i^{(\tau)} \Big) \,. \tag{6.93}$$

The operator $\mathrm{e}^{-\beta H}$ can now be written as a sum over all possible Ising–Spin configurations of the auxiliary field, $\underline{S}^{(\tau)} = \{S_1^{(\tau)} \dots S_N^{(\tau)}\}$ at every Trotter–Time τ.

$$\mathrm{e}^{-\beta\hat{H}} = \sum_{\{S_i^{(\tau)}\}=\pm 1} \prod_{\tau=1}^{m} \tilde{K}_\uparrow^{(\tau)} \tilde{V}_\uparrow\big(\underline{S}^{(\tau)}\big) \prod_{\tau=1}^{m} \tilde{K}_\downarrow^{(\tau)} \tilde{V}_\downarrow\big(\underline{S}^{(\tau)}\big) \,. \tag{6.94}$$

This is the desired result. We have expressed the exponential of the Hamiltonian of the Hubbard model as a sum over products of one-particle operators.

6.3.2 Choice of the Trial Function $|\psi_T\rangle$ and Time–Evolution

Since we have separated the spin orientations in the operators $\tilde{V}$ and $\tilde{K}$, it is logical to do the same in the trial function. Thus we choose the trial function as a Tensor–product of a pure spin $\uparrow$ state with a pure spin $\downarrow$ state writing

$$|\psi_T\rangle = |\psi_{T\uparrow}\rangle \otimes |\psi_{T\downarrow}\rangle \,. \tag{6.95}$$

The spin $\uparrow$ part of $\mathrm{e}^{-\beta\hat{H}}$ acts only on the spin $\uparrow$ factor of $|\psi_T\rangle$ whereas its spin $\downarrow$ part affects only on the spin $\downarrow$ factor. Therefore, the frozen state $|\psi_\beta\rangle$ reads

$$\begin{aligned} |\psi_\beta\rangle &= \mathrm{e}^{-\beta\hat{H}} |\psi_T\rangle \\ &= \sum_{\{S_i^{(\tau)}\}=\pm 1} \prod_{\tau=1}^{m} \tilde{K}_\uparrow^{(\tau)} \tilde{V}_\uparrow\big(\underline{S}^{(\tau)}\big) |\psi_{T\uparrow}\rangle \otimes \prod_{\tau=1}^{m} \tilde{K}_\downarrow^{(\tau)} \tilde{V}_\downarrow\big(\underline{S}^{(\tau)}\big) |\psi_{T\downarrow}\rangle \,. \end{aligned} \tag{6.96}$$

The simplest choice for the trial functions $|\psi_{T\sigma}\rangle$ are *Slater determinants* representing independent particles. Since only one-particle operators are involved in (6.96), for each auxiliary-field configuration, independent particles stay independent particles by application of the product of K's and V's. Correlations come into play only through the sum over all auxiliary-field configurations. We generate the trial state $|\psi_{T\sigma}\rangle$ by application of ladder operators $\hat{b}_{\alpha,\sigma}^\dagger$ on the vacuum state $|0\rangle$ writing

$$|\psi_{T\sigma}\rangle = \big|\det\big(\varphi_\sigma^\alpha\big)\big\rangle = \prod_{\alpha=1}^{N_\sigma} \hat{b}_{\alpha,\sigma}^\dagger |0\rangle \,. \tag{6.97}$$

The symbol N_σ denotes the number of electrons of spin σ. The operator $\hat{b}^\dagger_{\alpha,\sigma}$ generates an electron in the state $|\varphi^\alpha_\sigma\rangle$. It is possible to express $\hat{b}^\dagger_{\alpha,\sigma}$ in terms of the operators $\hat{a}^\dagger_{i,\sigma}$ appearing in the Hamiltonian: The former is a linear combination of the latter,

$$\hat{b}^\dagger_{\alpha\sigma} = \sum_{i=1}^{N} \varphi^\alpha_{i\sigma} \hat{a}^\dagger_{i\sigma} \; . \tag{6.98}$$

The quantities $\varphi^\alpha_{i\sigma}$ have a direct physical interpretation: They denote the amplitude of probability of finding the generated electron at lattice site i.
Having found an appropriate trial function, in the in the next step we concentrate on its evolution towards $|\psi_\beta\rangle$. We confine the following considerations to one spin orientation and thus drop the subscript σ. In a first step, according to (6.94) we consider the application of the operators $\tilde{K}^{(\tau)}$ and $\tilde{V}\big(S^{(\tau)}\big)$ on the trial state. To this end, we notice that both operators are of the form

$$\tilde{U}^{K/V}_\tau \stackrel{\text{def}}{=} \mathrm{e}^{-\Delta\tau\tilde{H}} \qquad \text{with} \qquad \tilde{H} = \sum_{ij} h_{ij} \hat{a}^\dagger_i \hat{a}_j \; , \tag{6.99}$$

and $\Delta\tau = \beta/m$. The relevant matrix elements h_{ij} are inferred from (6.90) and (6.91). They are given by

$$\tilde{K}^{(\tau)} : \tilde{U}^K_\tau \qquad h_{ij} \to k^{(\tau)}_{ij} = \frac{1}{1+\delta_{\tau,1}} \big(- t_{ij\sigma} + \frac{U}{2}\, \delta_{ij} \big) \tag{6.100a}$$

$$\tilde{V}\big(\underline{S}^{(\tau)}\big) : \tilde{U}^V_\tau \qquad h_{ij} \to v^{(\tau)}_{ij} = \lambda\, \sigma\, \delta_{ij}\, S^{(\tau)}_i / \Delta\tau \tag{6.100b}$$

The operators $\tilde{U}^{K/V}_\tau$, albeit not unitary, display formal analogies to time evolution operators. Therefore, τ is called an *imaginary time* and the composition

$$\tilde{U}_\tau \stackrel{\text{def}}{=} \tilde{U}^K_\tau\, \tilde{U}^V_\tau = \tilde{K}^{(\tau)} \tilde{V}\big(\underline{S}^{(\tau)}\big) \tag{6.101}$$

propagates $\hat{b}^\dagger_i$ from time τ to $\tau - \Delta\tau$ according to

$$\hat{b}^\dagger_i(\Delta\tau) = \tilde{U}_\tau\, \hat{b}^\dagger_i\, \tilde{U}^{-1}_\tau \; .$$

The last factor ($\tau = m$) of the Hubbard Stratonovich decomposition, (6.96), can thus be cast in the form

$$\begin{aligned} &\tilde{K}^{(m)} \tilde{V}\big(\underline{S}^{(m)}\big) \hat{b}^\dagger_1\, \hat{b}^\dagger_2 \ldots \hat{b}^\dagger_{N_\sigma} |0\rangle \\ &\qquad = \tilde{U}_\tau\, \hat{b}^\dagger_1 \tilde{U}^{-1}_\tau \tilde{U}_\tau \hat{b}^\dagger_2 \tilde{U}^{-1}_\tau \ldots \hat{b}^\dagger_N \tilde{U}^{-1}_\tau \tilde{U}_\tau\, |0\rangle \\ &\qquad = \hat{b}^\dagger_1(\Delta\tau)\, \hat{b}^\dagger_2(\Delta\tau) \ldots \hat{b}^\dagger_N(\Delta\tau)\, |0\rangle \; . \end{aligned} \tag{6.102}$$

To arrive at this expression, we have inserted unit operators of the form $\mathbb{I} = \tilde{U}^{-1}_\tau \tilde{U}_\tau$. Moreover, we made use of the identity $\tilde{U}_\tau |0\rangle = |0\rangle$. The operators $\hat{b}^\dagger_\alpha(\Delta\tau)$ can be expressed in terms of the operators $\hat{a}^\dagger_i$ constituting the Hamiltonian,

$$\hat{b}^\dagger_\alpha(\Delta\tau) = \sum_i \varphi_i^{(\alpha)}\, \hat{a}^\dagger_i(\Delta\tau)\ . \tag{6.103}$$

This is called the *Wannier representation*. We can infer an ODE for the time evolution of the ladder operators $\hat{a}^\dagger_l(\Delta\tau)$ by differentiation with respect to time

$$\frac{\partial}{\partial\Delta\tau}\hat{a}^\dagger_l(\Delta\tau) = \frac{\partial}{\partial\Delta\tau}\Big(\mathrm{e}^{-\Delta\tau\tilde{H}}\hat{a}^\dagger_l\,\mathrm{e}^{\Delta\tau\tilde{H}}\Big) = -\mathrm{e}^{-\Delta\tau\tilde{H}}[\tilde{H},\hat{a}^\dagger_l]\mathrm{e}^{\Delta\tau\tilde{H}}\ . \tag{6.104}$$

Since the exponential of the Hamiltonian commutes with the Hamiltonian, this can be cast as

$$\frac{\partial}{\partial\Delta\tau}\hat{a}^\dagger_l(\Delta\tau) = -\big[\tilde{H},\hat{a}^\dagger_l(\Delta\tau)\big]\ . \tag{6.105}$$

We are thus led to calculate the commutators $[\tilde{H},\hat{a}^\dagger_l]$. This can be done remembering the representation of $\tilde{H}$ in terms of the operators $\hat{a}^\dagger_i$ and $\hat{a}_j$.

$$\begin{aligned}
\Big[\tilde{H},\hat{a}^\dagger_l\Big] &= \Big[\sum_{ij} h_{ij}\hat{a}^\dagger_i\hat{a}_j,\hat{a}^\dagger_l\Big] \\
&= \sum_{ij} h_{ij}\hat{a}^\dagger_i\hat{a}_j\hat{a}^\dagger_l - \sum_{ij} h_{ij}\hat{a}^\dagger_l\hat{a}^\dagger_i\hat{a}_j \\
&= \sum_{ij} h_{ij}\hat{a}^\dagger_i\hat{a}_j\hat{a}^\dagger_l - \sum_{ij} h_{ij}\big(-\hat{a}^\dagger_i\hat{a}^\dagger_l + \overbrace{\{\hat{a}^\dagger_i,\hat{a}^\dagger_l\}}^{=0}\big)\,\hat{a}_j \\
&= \sum_{ij} h_{ij}\hat{a}^\dagger_i\hat{a}_j\hat{a}^\dagger_l - \sum_{ij} h_{ij}\hat{a}^\dagger_i\big(\hat{a}_j\hat{a}^\dagger_l - \underbrace{\{\hat{a}_j,\hat{a}^\dagger_l\}}_{=\delta_{j,l}}\big) \\
&= \sum_i h_{il}\hat{a}^\dagger_i
\end{aligned} \tag{6.106}$$

The fermionic anti-commutator relations were applied two times. The linear ODE for the evolution of $\hat{a}^\dagger_i(\Delta\tau)$ is thus given by

$$\frac{\partial}{\partial\Delta\tau}\hat{a}^\dagger_l(\Delta\tau) = -\sum_i h_{il}\hat{a}^\dagger_i(\Delta\tau)\ . \tag{6.107}$$

In a quite analogous manner the evolution of the operator $\hat{a}_i(\Delta\tau)$ can be derived. Carrying through the anti-commutator relations, it turns out that the RHS of the evolution equation has opposite sign. Thus the ODE reads

$$\frac{\partial}{\partial\Delta\tau}\hat{a}_l(\Delta\tau) = +\sum_i h_{il}\hat{a}_i(\Delta\tau)\ . \tag{6.108}$$

Summarizing $\hat{a}^\dagger_l(\Delta\tau)$ to the vector $\mathbf{a}^\dagger(\Delta\tau) = \{\hat{a}^\dagger_1(\Delta\tau),\ldots,\hat{a}^\dagger_N(\Delta\tau)\}$, we obtain the ODE (6.107) in vector form

$$\frac{\partial}{\partial \Delta\tau}\,\mathbf{a}^\dagger(\Delta\tau) = -H\,\mathbf{a}^\dagger(\Delta\tau)\,, \qquad \text{with the matrix} \quad H = \{h_{ij}\}\,. \tag{6.109}$$

Its solution for the initial condition $\mathbf{a}^\dagger(\Delta\tau = 0) = \mathbf{a}^\dagger$ is given by

$$\mathbf{a}^\dagger(\Delta\tau) = \mathrm{e}^{-\Delta\tau H}\mathbf{a}^\dagger\,. \tag{6.110}$$

Inserting this information into (6.103), we obtain the *time evolution* of the operators $\hat{b}^\dagger_\alpha$ as

$$\begin{aligned}\hat{b}^\dagger_\alpha(\Delta\tau) &= \sum_i \varphi_i^{(\alpha)}\hat{a}_i^\dagger(\Delta\tau) = \sum_{ij}\varphi_i^{(\alpha)}\left(\mathrm{e}^{-\Delta\tau H^{(m)}}\right)_{ij}\hat{a}_j^\dagger \\ &= \sum_j\Big(\sum_i\left(\mathrm{e}^{-\Delta\tau H^{(m)}}\right)_{ji}\varphi_i^{(\alpha)}\Big)\,\hat{a}_j^\dagger \overset{\text{def}}{=} \sum_j \tilde{\varphi}_j^{(\alpha)}\hat{a}_j^\dagger \overset{\text{def}}{=} \tilde{b}^\dagger_\alpha\,.\end{aligned} \tag{6.111}$$

We observe the important feature of the algorithm: Due to the bilinear form of the decoupled Hamiltonian, the one-particle operator $\hat{b}^\dagger_\alpha$ at a later time $\Delta\tau$ can be expressed in terms of the one-particle operator $\tilde{b}^\dagger_\alpha$. The decoupling of the interaction term was achieved by application of the Hubbard Stratonovich transformation.
The quantities $\tilde{\varphi}_j^{(\alpha)}$ are called *modified one–particle orbitals*. Using the definition (6.101), they can also be summarized in the vector

$$\tilde{\boldsymbol{\varphi}}^{\,(\alpha)} = U_m\,\boldsymbol{\varphi}^{(\alpha)} = K^{(m)}V^{(m)}\boldsymbol{\varphi}^{(\alpha)}\,. \tag{6.112}$$

Here, $U_m, K^{(m)}$ and $V^{(m)}$ denote the matrices of the matrix elements of the respective operators in the basis $\{\hat{a}_i^\dagger|0\rangle\}$. The term (6.102) finally reads

$$\tilde{K}^{(m)}\tilde{V}\big(\underline{S}^{(m)}\big)|\psi_T\rangle = \tilde{b}_1^\dagger\,\tilde{b}_2^\dagger\ldots\tilde{b}_{N_\sigma}^\dagger\,|0\rangle\,. \tag{6.113}$$

Having treated the last factor of the Trotter decomposition, we now consider the last two factors. They can be written as

$$\begin{aligned}&\tilde{K}^{(m-1)}\tilde{V}\big(\underline{S}^{(m-1)}\big)\tilde{K}^{(m)}\tilde{V}\big(\underline{S}^{(m)}\big)\hat{b}_1^\dagger\,\hat{b}_2^\dagger\ldots\hat{b}_{N_\sigma}^\dagger\,|0\rangle \\ &\quad= \tilde{K}^{(m-1)}\tilde{V}\big(\underline{S}^{(m-1)}\big)\tilde{b}_1^\dagger\,\tilde{b}_2^\dagger\ldots\tilde{b}_{N_\sigma}^\dagger\,|0\rangle \\ &\quad= U(\Delta\tau)\,\tilde{b}_1^\dagger U^{-1}(\Delta\tau)U(\Delta\tau)\tilde{b}_2^\dagger U^{-1}(\Delta\tau)\ldots\tilde{b}_N^\dagger U^{-1}(\Delta\tau)U(\Delta\tau)|0\rangle \\ &\quad= \tilde{b}_1^\dagger(\Delta\tau)\,\tilde{b}_2^\dagger(\Delta\tau)\ldots\tilde{b}_N^\dagger(\Delta\tau)\,|0\rangle\,.\end{aligned} \tag{6.114}$$

Of course, the arguments developed for the evolution of $\hat{b}^\dagger$ apply also for the evolution of $\tilde{b}^\dagger$. Thus we obtain

$$\tilde{b}^\dagger_\alpha(\Delta\tau) = \sum_i \tilde{\varphi}_i^{(\alpha)}\hat{a}_i^\dagger(\Delta\tau) \overset{\text{def}}{=} \sum_j \tilde{\tilde{\varphi}}_j^{(\alpha)}\hat{a}_j^\dagger \overset{\text{def}}{=} \tilde{\tilde{b}}^\dagger_\alpha\,, \tag{6.115}$$

with the vector

$$\begin{aligned}\tilde{\tilde{\boldsymbol{\varphi}}}^{(\alpha)} &= \mathrm{e}^{-\Delta\tau H^{(m-1)}}\tilde{\boldsymbol{\varphi}}^{(\alpha)} \\ &= \mathrm{e}^{-\Delta\tau H^{(m-1)}}\mathrm{e}^{-\Delta\tau H^{(m)}}\boldsymbol{\varphi}^{(\alpha)} \\ &= K^{(m-1)}V^{(m-1)}K^{(m)}V^{(m)}\boldsymbol{\varphi}^{(\alpha)}\ .\end{aligned} \tag{6.116}$$

Consequently, the last two factors can be written as

$$\tilde{K}^{(m-1)}\tilde{V}\big(\underline{S}^{(m-1)}\big)\tilde{K}^{(m)}\tilde{V}\big(\underline{S}^{(m)}\big)|\psi_T\rangle = \tilde{\tilde{b}}_1^\dagger\,\tilde{\tilde{b}}_2^\dagger\ldots\tilde{\tilde{b}}_{N_\sigma}^\dagger\,|0\rangle\ . \tag{6.117}$$

6.3.3 General Formulae for Observables

By continuing the applied strategy through times τ, we are able to evaluate all factors in the Trotter–decomposition of (6.96). For a given Ising-spin field $\{S_i^{(\tau)}\}$, the result is

$$\begin{aligned}\big|\psi_\sigma(S_i^{(\tau)})\big\rangle &\stackrel{\mathrm{def}}{=} \prod_{\tau=1}^{m}\tilde{K}_\sigma^{(\tau)}\tilde{V}\big(\underline{S}_\sigma^{(\tau)}\big)|\psi_{T\sigma}\rangle \\ &= \prod_{\tau=1}^{m}\tilde{K}_\sigma^{(\tau)}\tilde{V}\big(\underline{S}_\sigma^{(\tau)}\big)\big(\hat{b}_{1,\sigma}^\dagger\,\hat{b}_{2,\sigma}^\dagger\ldots\hat{b}_{N_\sigma,\sigma}^\dagger\big)|0\rangle = \bar{b}_{1,\sigma}^\dagger\ \ldots\ \bar{b}_{N_\sigma,\sigma}^\dagger|0\rangle\end{aligned} \tag{6.118}$$

where we have re-introduced the spins σ of the fermions. For both spin orientation the combined ket reads

$$\big|\psi(S_i^{(\tau)})\big\rangle = \big|\psi_\uparrow(S_i^{(\tau)})\big\rangle \otimes \big|\psi_\downarrow(S_i^{(\tau)})\big\rangle\ . \tag{6.119}$$

The operators $\bar{b}$ are the result of the evolution of the original $\hat{b}$'s constituting the trial function. Again, they can be written as a linear combination of the $\hat{a}$'s,

$$\bar{b}_{\alpha,\sigma}^\dagger = \sum_i \bar{\varphi}_{i,\sigma}^{(\alpha)}\hat{a}_{i,\sigma}^\dagger\ . \tag{6.120}$$

The vectors $\bar{\boldsymbol{\varphi}}^{(\alpha)}$ are generated by consecutive application of the evolution operators

$$\bar{\boldsymbol{\varphi}}^{(\alpha)} = U_1\cdot U_2\cdot\cdots U_m\boldsymbol{\varphi}^{(\alpha)} = \underbrace{K^{(1)}\cdot V^{(1)}\cdots K^{(m)}\cdot V^{(m)}}_{\text{matrices}}\boldsymbol{\varphi}^{(\alpha)}\ . \tag{6.121}$$

The $N\times N$ matrices K and V are of the form of (6.99), where K is independent of the spin–field $\underline{S}^{(\tau)}$. The matrix V is diagonal but depends on $\underline{S}^{(\tau)}$. These matrices are inferred from (6.100a) and (6.100b) and read

$$K_{ij} = \left\{\mathrm{e}^{\frac{\Delta\tau}{1+\delta_{\tau,1}}(-t_{hk\sigma}+\frac{U}{2}\delta_{h,k})}\right\}_{ij}\ ,\quad V_{ij} = \mathrm{e}^{\lambda\sigma S_i^{(\tau)}}\,\delta_{i,j}\ . \tag{6.122}$$

They can be calculated before the actual run of the simulation. The dimension of K and V equals the number of lattice sites of the problem.

Thus, we have achieved a mapping of the Quantum–Mechanical problem on a classical Ising Spin problem. The expectation value of the operator $\hat{O}$, which we started to calculate at the beginning of this section, has thus the form

$$< \hat{O} >= \frac{\langle \psi_\beta | \hat{O} | \psi_\beta \rangle}{\langle \psi_\beta \, | \psi_\beta \, \rangle} = \frac{\sum_{\{S_i^\tau\},\{S_i'^\tau\}} \langle \psi(\underline{S}') | \hat{O} | \psi(\underline{S}) \rangle}{\sum_{\{S_i^\tau\},\{S_i'^\tau\}} \langle \psi(\underline{S}') \, | \psi(\underline{S}) \, \rangle} \; . \tag{6.123}$$

By multiplying numerator and denominator with $\langle \psi(\underline{S}') \, | \psi(\underline{S}) \, \rangle$, we obtain

$$\begin{aligned} < \hat{O} > &= \sum_{\{S_i^\tau\}} \sum_{\{S_i'^\tau\}} \frac{\langle \psi(\underline{S}') | \hat{O} | \psi(\underline{S}) \rangle}{\langle \psi(\underline{S}') \, | \psi(\underline{S}) \, \rangle} \frac{\langle \psi(\underline{S}') \, | \psi(\underline{S}) \, \rangle}{\sum_{\{S_i^\tau\},\{S_i'^\tau\}} \langle \psi(\underline{S}') \, | \psi(\underline{S}) \, \rangle} \\ &= \sum_{\{S_i^\tau\}} \sum_{\{S_i'^\tau\}} O(\underline{S}', \underline{S}) \cdot \rho(\underline{S}', \underline{S}) \end{aligned} \tag{6.124}$$

where we have introduced the abbreviations $O(\underline{S}', \underline{S})$ for the first factor and $\rho(\underline{S}', \underline{S})$ for the last. Cast in this form, ρ can be interpreted as the statistical weight of the spin fields $\underline{S}$ and $\underline{S}'$. Notice, however, that ρ is a matrix element and can thus be a *complex* number. This is called the *sign–problem* of the QMC–simulation. It is the cause of severe troubles that are not yet overcome. Usually, this sign is absorbed in the first factor $O(\underline{S}', \underline{S})$ so that ρ becomes a positive density.

$$O(\underline{S}', \underline{S}) \cdot \rho(\underline{S}', \underline{S}) \Longrightarrow O(\underline{S}', \underline{S}) \, \mathrm{e}^{i \arg(\rho(\underline{S}', \underline{S}))} \cdot |\rho(\underline{S}', \underline{S})|$$

6.3.4 Explicit Expressions for Matrix Elements

In this subsection we provide explicit expressions needed to evaluate (6.124).

The matrix elements $\langle \psi(\underline{S}') \, | \psi(\underline{S}) \, \rangle$. Let us first consider the matrix element needed for the weight $\rho(\underline{S}', \underline{S})$. We will again suppress the spin index and treat the expression

$$\langle \psi(\underline{S}') \, | \psi(\underline{S}) \, \rangle = \langle 0 | \prod_{\nu=N_e}^{1} \bar{b}'_\nu \prod_{\nu=1}^{N_e} \bar{b}^\dagger_\nu | 0 \rangle \; , \tag{6.125}$$

where $\bar{b}'_\nu$ and $\bar{b}^\dagger_\nu$ denotes the propagated $\hat{b}$'s with the Ising fields $\underline{S}'$ and $\underline{S}$, respectively.
Let's, for simplicity, consider the case of only two particles ($N_e = 2$). Then we find

$$\langle \psi(\underline{S}') \, | \psi(\underline{S}) \, \rangle = \langle 0 | \bar{b}'_2 \bar{b}'_1 \bar{b}^\dagger_1 \bar{b}^\dagger_2 | 0 \rangle \; . \tag{6.126}$$

In order to simplify this expression, we pull $\bar{b}'_1$ to the right-most position. Then its application to $|0\rangle$ yields zero. We had to interchange $\bar{b}'_1$ twice with creation operators. This can be done by using anti-commutators which yields

$$\langle 0|\bar{b}'_2\bar{b}'_1\bar{b}^\dagger_1\bar{b}^\dagger_2|0\rangle = \langle 0|\bar{b}'_2\{\bar{b}'_1,\bar{b}^\dagger_1\}\bar{b}^\dagger_2|0\rangle - \langle 0|\bar{b}'_2\bar{b}^\dagger_1\{\bar{b}'_1,\bar{b}^\dagger_2\}|0\rangle \tag{6.127}$$

Now the anti-commutator relations for fermions imply that the apperaring anti-commuators are proportional to the unit operator. This can be seen by expanding $\bar{b}^\dagger_\alpha$ and $\bar{b}'_\beta$ as a linear combination of the $\hat{a}_h$'s. Consequently, the anti-commutators can be treated as numbers. These numbers can be evaluated as expectation values of the anti-commutator in any normalized state, thus also in the vacuum state:

$$\langle 0|\{\bar{b}'_\alpha,\bar{b}^\dagger_\beta\}|0\rangle = \langle 0|\bar{b}'_\alpha\bar{b}^\dagger_\beta|0\rangle \; .$$

By substituting this into (6.126), we obtain a special form of Wick's theorem

$$\begin{aligned}\langle \psi(\underline{S}')\,|\psi(\underline{S})\,\rangle &= \langle 0|\bar{b}'_2\bar{b}'_1\bar{b}^\dagger_1\bar{b}^\dagger_2|0\rangle \\ &= \langle 0|\bar{b}'_1\bar{b}^\dagger_1|0\rangle\langle 0|\bar{b}'_2\bar{b}^\dagger_2|0\rangle - \langle 0|\bar{b}'_1\bar{b}^\dagger_2|0\rangle\langle 0|\bar{b}'_2\bar{b}^\dagger_1|0\rangle \; .\end{aligned} \tag{6.128}$$

Upon introducing the overlap matrix $G_{\alpha\beta}(\underline{S}',\underline{S}) = \langle 0|\bar{b}'_\alpha\bar{b}^\dagger_\beta|0\rangle$ this can also be cast in the form

$$\langle \psi(\underline{S}')\,|\psi(\underline{S})\,\rangle = G_{11}\,G_{22} - G_{12}\,G_{21} = \begin{vmatrix} G_{11} & G_{12} \\ G_{21} & G_{22}\end{vmatrix} \; . \tag{6.129}$$

In a straight forward way, the above procedure can be generalized for higher particles numbers N_e. Wick's theorem splits the product of N_e annihilition operators and N_e creation operators in sums over N_e pairs of one annihilition operator and one creation operator. We obtain

$$\langle \psi(\underline{S}')\,|\psi(\underline{S})\,\rangle = \det(G(\underline{S}',\underline{S})) \; . \tag{6.130}$$

The overlap matrix G can be obtained from the modified one-particle orbitals. By using (6.120), we get

$$G_{\alpha\beta} = \langle 0|\bar{b}'_\alpha\bar{b}^\dagger_\beta|0\rangle = \sum_{i,j}\left(\bar{\varphi}'^{(\alpha)}_i\right)^\star\bar{\varphi}^{(\beta)}_j\underbrace{\langle 0|\hat{a}_i\hat{a}^\dagger_j|0\rangle}_{=\delta_{ij}} = \sum_i\left(\bar{\varphi}'^{(\alpha)}_i\right)^\star\bar{\varphi}^{(\beta)}_i \; . \tag{6.131}$$

Of course, $\bar{\boldsymbol{\varphi}}'^{(\alpha)}$ means the orbital α propagated with the Ising spin field $\underline{S}'$ and $\bar{\boldsymbol{\varphi}}^{(\beta)}$ is the result of the propagation of the orbital β determined by the field $\underline{S}$.

The matrix elements $\langle\boldsymbol{\psi(\underline{S}')}|\hat{\boldsymbol{a}}_{\boldsymbol{\nu}}\hat{\boldsymbol{a}}^\dagger_{\boldsymbol{\mu}}|\boldsymbol{\psi(\underline{S})}\rangle$. In what follows we consider the expectation values of one-particle operators of the form $\hat{O} = \hat{a}_\nu\hat{a}^\dagger_\mu$ in the propagated states, i.e.

$$O(\underline{S}',\underline{S}) = g_{\nu\mu}(\underline{S}',\underline{S}) = \frac{\langle\psi(\underline{S}')|\hat{a}_\nu\hat{a}^\dagger_\mu|\psi(\underline{S})\rangle}{\langle\psi(\underline{S}')\,|\psi(\underline{S})\,\rangle} \; . \tag{6.132}$$

Combinations of these operators constitute e.g. the one-particle Greens function, thus the notation $g_{\nu\mu}$. The denominator of $g_{\nu\mu}$ has already been evaluated above. The numerator can be written in the form

$$\begin{aligned}\big\langle\psi(\underline{S}')\big|\hat{a}_\nu\hat{a}_\mu^\dagger\big|\psi(\underline{S})\big\rangle =& \big\langle 0\big|\prod_{\alpha=N_e}^{1}\bar{b}'_\alpha\hat{a}_\nu\hat{a}_\mu^\dagger\prod_{\beta=1}^{N_e}\bar{b}_\beta^\dagger\big|0\big\rangle \\ =& \big\langle 0\big|\bar{b}'_{N_e}\cdots\bar{b}'_2\,\bar{b}'_1\,\bar{b}'_0\,\bar{b}_0^\dagger\,\bar{b}_1^\dagger\,\bar{b}_2^\dagger\cdots\bar{b}_{N_e}^\dagger\big|0\big\rangle\end{aligned} \tag{6.133}$$

where we have substituted

$$\begin{aligned}\bar{b}_0^\dagger &= \sum_{i=1}^{N_e}\bar{\varphi}_i^{(0)}\hat{a}_i^\dagger \qquad \text{with } \bar{\varphi}_i^{(0)} = \delta_{i,\mu} \\ \bar{b}'_0 &= \sum_{i=1}^{N_e}\bar{\varphi}_i'^{(0)\star}\hat{a}_i \quad \text{with } \bar{\varphi}_i'^{(0)\star} = \delta_{i,\nu}\end{aligned} \tag{6.134}$$

for the operators $\hat{a}$. In doing so, we have formally arrived at the same expression as in (6.125). The only difference is that now the product runs from 0 to N_e. Therefore the same arguments apply and Wick's theorem entails that the numerator can be written as a determinant,

$$\big\langle 0\big|\prod_{\alpha=N_e}^{0}\bar{b}'_\alpha\prod_{\beta=0}^{N_e}\bar{b}_\beta^\dagger\big|0\big\rangle = \det G^O\ . \tag{6.135}$$

The overlap matrix G^O is evaluated by using (6.131) along with (6.134) for the zero components. It depends on the auxiliary-field configuration, i.e. $G^O = G^O(\underline{S},\underline{S}')$, and is given by

$$G^O_{l,l'} = \left(\begin{array}{c|ccc} \delta_{\nu,\mu} & \bar{\varphi}_\mu^{(1)} & \cdots & \bar{\varphi}_\mu^{(N_e)} \\ \hline \bar{\varphi}_\nu'^{(1)\star} & & & \\ \vdots & & G_{l,l'} & \\ \bar{\varphi}_\nu'^{(N_e)\star} & & & \end{array}\right)\ . \tag{6.136}$$

Therefore, $g_{\nu\mu}$ can be written as the ratio of the two determinants

$$g_{\nu\mu}(\underline{S}',\underline{S}) = \frac{\big\langle\psi(\underline{S}')\big|\hat{a}_\nu\hat{a}_\mu^\dagger|\psi(\underline{S})\big\rangle}{\big\langle\psi(\underline{S}')\,|\psi(\underline{S})\,\big\rangle} = \frac{\det G^O(\underline{S}',\underline{S})}{\det G(\underline{S}',\underline{S})}\ . \tag{6.137}$$

In order to evaluate this formula efficiently, it is expedient to perform linear manipulations on the matrix G^O that leave the determinant invariant and reduce the zeroth column to zero except for the element $(0,0)$. After adding a suitable linear combination of the last N_e columns to the zeroth column, G^O takes the form

$$G^{O\prime}_{l,l'} = \left(\begin{array}{c|ccc} g^O & \bar{\varphi}^{(1)}_\mu & \cdots & \bar{\varphi}^{(N_e)}_\mu \\ \hline 0 & & & \\ \vdots & & G_{l,l'} & \\ 0 & & & \end{array}\right) \tag{6.138}$$

with g^O given by

$$g^O = \delta_{\nu,\mu} - \sum_{i,j=1}^{N_e} \bar{\varphi}^{(i)}_\mu \big(G^{-1}\big)_{ij} \bar{\varphi}'^{(j)}_\nu = \delta_{\nu,\mu} - \bar{\boldsymbol{\varphi}}^T_\mu \cdot G^{-1} \bar{\boldsymbol{\varphi}'}_\nu \, . \tag{6.139}$$

The determinat can now be expanded along the first column and is given by $\det G^{O\prime} = \det G^O = g^O \, \det G$. Then $g_{\nu\mu}$ simplifies to

$$g_{\nu\mu}(\underline{S}', \underline{S}) = \frac{g^O \, \det G}{\det G} = g^O = \delta_{\nu,\mu} - \bar{\boldsymbol{\varphi}}^T_\mu \cdot G^{-1} \bar{\boldsymbol{\varphi}'}_\nu \, . \tag{6.140}$$

Matrix elements of higher order operators. In order to calculate matrix elements $O(\underline{S}, \underline{S}')$ of higher order operators, we follow the same lines as for matrix elements of one-particle operators. Here, we will demonstrate this procedure only for two-particle operators. A generalization is straight forward.
A matrix element of a general two-particle operator can be cast in the form

$$O(\underline{S}', \underline{S}) = g_{\nu\mu\eta\xi}(\underline{S}', \underline{S}) = \frac{\big\langle \psi(\underline{S}') \big| \hat{a}_\nu \hat{a}_\mu \hat{a}^\dagger_\eta \hat{a}^\dagger_\xi \big| \psi(\underline{S}) \big\rangle}{\big\langle \psi(\underline{S}') \, \big| \psi(\underline{S}) \, \big\rangle} \, . \tag{6.141}$$

The numerator can be written as

$$g_{\nu\mu\eta\xi} = \big\langle 0 \big| \prod_{\alpha=N_e}^{-1} \bar{b}'_\alpha \prod_{\beta=-1}^{N_e} \bar{b}^\dagger_\beta \big| 0 \big\rangle \tag{6.142}$$

with $\bar{b}_0$'s and $\bar{b}_{-1}$'s given by expressions analogous to (6.134). Now we apply Wick's theorem reducing the last equation to the determinant $g_{\nu\mu\eta\xi} = \det G^O / \det G$ of a matrix

$$G^O_{l,l'} = \left(\begin{array}{cc|ccc} \delta_{\eta,\mu} & \delta_{\eta,\nu} & \bar{\varphi}^{(1)}_\eta & \cdots & \bar{\varphi}^{(N_e)}_\eta \\ \hline \delta_{\xi,\mu} & \delta_{\xi,\nu} & \bar{\varphi}^{(1)}_\xi & \cdots & \bar{\varphi}^{(N_e)}_\xi \\ \hline \bar{\varphi}'^{(1)\star}_\mu & \bar{\varphi}'^{(1)\star}_\nu & & & \\ \vdots & \vdots & & G_{l,l'} & \\ \bar{\varphi}'^{(N_e)\star}_\mu & \bar{\varphi}'^{(N_e)\star}_\mu & & & \end{array}\right) \, . \tag{6.143}$$

We can now eliminate the elements $G^O_{0,-1}$ to $G^O_{N_e,-1}$ and $G^O_{1,0}$ to $G^O_{N_e,0}$ by adding linear combinations of the last N_e columns to the first two columns. This leaves the determinant of the matrix invariant and yields

$$G^O_{l,l'} = \left(\begin{array}{c|c|ccc} g^O_{-1} & r^O & \bar\varphi^{(1)}_\eta & \cdots & \bar\varphi^{(N_e)}_\eta \\ \hline 0 & g^O_0 & \bar\varphi^{(1)}_\xi & \cdots & \bar\varphi^{(N_e)}_\xi \\ \hline 0 & 0 & & & \\ \vdots & \vdots & & G_{l,l'} & \\ 0 & 0 & & & \end{array}\right) . \tag{6.144}$$

The new symbols are given by

$$g^O_0 = \delta_{\xi,\nu} - \bar{\boldsymbol{\varphi}}^T_\xi G^{-1} \bar{\boldsymbol{\varphi}}'_\nu \tag{6.145}$$

$$r^O = \delta_{\eta,\nu} - \bar{\boldsymbol{\varphi}}^T_\eta G^{-1} \bar{\boldsymbol{\varphi}}'_\nu \tag{6.146}$$

and

$$g^O_{-1} = \delta_{\eta,\mu} - \frac{r^O}{g^O_0} \left(\delta_{\xi,\mu} - \bar{\boldsymbol{\varphi}}^T_\eta G^{-1} \bar{\boldsymbol{\varphi}}'_\mu\right) - \bar{\boldsymbol{\varphi}}^T_\eta G^{-1} \bar{\boldsymbol{\varphi}}'_\mu \tag{6.147}$$

Now the expectation value of the two-particle operator is easily calculated. By expanding the determinant of G^O along the first two columns we obtain

$$g_{\nu\mu\eta\xi}(\underline{S}', \underline{S}) = \frac{\det G^O}{\det G} = \frac{g^O_{-1} g^O_0 \det G}{\det G} = g^O_{-1} g^O_0 \ . \tag{6.148}$$

6.3.5 Example: Simulation of the Hubbard Model

6.3.6 Siegert Transformation

As mentioned at the discussion of the Hubbard Stratonovich transformation, there exists a general method of decomposing the exponential of the square of an operator. This map is called the *Siegert transformation* and is outlined in this subsection.
We consider a self–adjoint bounded operator $\hat{O}$ with discrete spectrum. The eigenvectors $\{|n\rangle\}_{n\geq 0}$ span a complete basis. Invoking the spectral theorem, we can calculate the integral

$$\begin{aligned} \int_{-\infty}^{\infty} \mathrm{e}^{-(\hat{O}+x\mathbb{I})^2}\, dx &= \int_{-\infty}^{\infty} \sum_{n\geq 0} |n\rangle\, \mathrm{e}^{-(O_n+x)^2}\, \langle n|\, dx \\ &= \sum_{n\geq 0} |n\rangle\langle n| \int_{-\infty}^{\infty} \mathrm{e}^{-(O_n+x)^2}\, dx \ . \end{aligned} \tag{6.149}$$

We have inserted a complete set of eigenstates of the observable $\hat{O}$ and in the second step exchanged integration with summation. In each integral we substitute $t = O_n + x$. The bounds of integration remain the unchanged. Thus we obtain the standard integral

$$\int_{-\infty}^{\infty} \mathrm{e}^{-(O_n+x)^2}\, dx = \int_{-\infty}^{\infty} \mathrm{e}^{-t^2}\, dt = \sqrt{\pi} \tag{6.150}$$

and consequently

$$\int_{-\infty}^{\infty} \mathrm{e}^{-(\hat{O}+x\mathbb{I})^2}\, dx = \sqrt{\pi} \sum_{n\geq 0} |n\rangle\langle n| = \sqrt{\pi}\, \mathbb{I}\,. \tag{6.151}$$

On the other hand we can as well expand the exponent and write

$$\int_{-\infty}^{\infty} \mathrm{e}^{-(\hat{O}+x\mathbb{I})^2}\, dx = \int_{-\infty}^{\infty} \mathrm{e}^{-(\hat{O}^2+2x\hat{O}+x^2)}\, dx = \mathrm{e}^{-\hat{O}^2} \int_{-\infty}^{\infty} \mathrm{e}^{-2x\hat{O}} \mathrm{e}^{-x^2}\, dx\,. \tag{6.152}$$

Substituting $y = 2x$ and inserting the result of (6.151), we obtain the *Siegert transformation*

$$\mathrm{e}^{\hat{O}^2} = \frac{1}{2\sqrt{\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-y\hat{O}} \mathrm{e}^{-\frac{y^2}{4}}\, dy\,. \tag{6.153}$$

To illustrate this map, we reconsider the magnetization formerly treated with the Hubbard Stratonovich transformation. In this case, the Siegert transformation yields

$$\mathrm{e}^{\frac{\beta U}{2m}\hat{m}_i^2} = \mathrm{e}^{(\sqrt{\frac{\beta U}{2m}}\hat{m}_i)^2} = \mathrm{e}^{\hat{O}^2} = \frac{1}{2\sqrt{\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-\sqrt{\frac{\beta U}{2m}}\hat{m}_i\, x} \mathrm{e}^{-\frac{x^2}{4}}\, dx\,. \tag{6.154}$$

Instead of the sum over two discrete values we now have an integral over infinitely many points. The quantity x corresponds to the auxiliary fields S of the Hubbard Stratonovich transformation. This looks more complicated but has, nevertheless, sometimes its advantages.

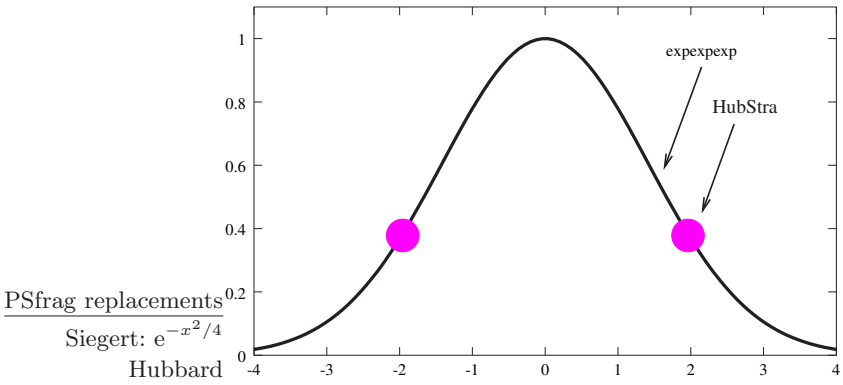

Fig. 6.7. Comparison between the Siegert– and the Hubbard Stratonovich transformation. Filled circles indicate the points at which the exponent is evaluated in the case of the Hubbard Stratonovich transformation.

6.4 Grand Canonical QMC Method

Historical remarks ... up to $\beta = 1$ which corresponds to a temperature of 10.000 Kelvin ...
We want to calculate the expectation value of an observable $\hat{O}$. In the grand canonical ensemble it is given by the trace

$$< \hat{O} >_T = \frac{1}{\mathrm{tr}(\exp(-\beta\hat{H}))} \ \mathrm{tr}\left(\hat{O}\mathrm{e}^{-\beta\hat{H}}\right) . \tag{6.155}$$

First we turn to investigate the grand canonical partition function Z appearing in the denominator of (6.155).

$$Z = \ \mathrm{tr}(\exp(-\beta\hat{H})) = \sum_{|\psi\rangle} \langle\psi| \exp(-\beta\hat{H})|\psi\rangle . \tag{6.156}$$

The sum has to be extended over a whole basis $|\psi\rangle$ of the Hilbert space (i.e. Fock space) of the system. We will demonstrate the application of the Grand Canonical QMC on the Hubbard model. The grand canonical Hamiltonian of the Hubbard model is a sum of the kinetic (or hopping) part $\hat{K}$, the on site interaction part $\hat{V}$ representing the short range part of the Coulomb repulsion and a part proportional to the particle number $\hat{N}_e$. Thus, the Hamiltonian reads

$$\hat{H} = \underbrace{-t \sum_{<i,j>,\sigma} \hat{c}^\dagger_{i,\sigma}\hat{c}_{j,\sigma}}_{\hat{K}} + \underbrace{U \sum_{i=1}^{N} \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}}_{\hat{V}} \underbrace{-\mu \sum_{i,\sigma} \hat{n}_{i\sigma}}_{\hat{N}_e} \tag{6.157}$$

where μ is the chemical potential of the system. Hopping is only possible between nearest neighbours, as usually indicated by the symbol $< i, j >$ in the sum of the kinetic part. Since the components $\hat{K}$ and $\hat{V}$ of the Hamiltonian do *not* commute, we perform a Suzuki Trotter decomposition of the exponential function $\exp(-\beta\hat{H})$) with m Trotter slices,

$$\mathrm{e}^{-\beta\hat{H}} = \left(\mathrm{e}^{-\Delta\tau\hat{H}}\right)^m \approx \prod_{\tau=1}^{m} \mathrm{e}^{-\Delta\tau\hat{K}}\, \mathrm{e}^{\Delta\tau\mu\hat{N}_e}\, \mathrm{e}^{\Delta\tau\hat{V}} + O(\Delta\tau^2) \tag{6.158}$$

with $\Delta\tau = \beta/m$. Inserting this approximation into the expression for the partition function, (6.156) yields a trace of m products of Trotter slices,

$$Z = \mathrm{tr} \prod_{\tau=1}^{m} \mathrm{e}^{-\Delta\tau\hat{K}}\, \mathrm{e}^{\Delta\tau\mu\hat{N}_e}\, \mathrm{e}^{\Delta\tau\hat{V}} + O(\Delta\tau^2)\ . \tag{6.159}$$

In what follows, we want to deal with one particle operators. Thus the next step is to carry out a discrete Hubbard Stratonovich transformation in the potential part of the Hamiltonian. To this end, we introduce the auxiliary spins S and write

$$\mathrm{e}^{\Delta\tau U\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}} = \frac{1}{2}\sum_{S=-1}^{+1} \mathrm{e}^{\lambda S(\hat{n}_{i\uparrow}-\hat{n}_{i\downarrow})}\, \mathrm{e}^{\frac{\Delta\tau U}{2}(\hat{n}_{i\uparrow}+\hat{n}_{i\downarrow})} \tag{6.160}$$

with the parameter λ given by

$$\lambda = 2\,\mathrm{atanh}\sqrt{\tanh\left(\frac{\Delta\tau U}{2}\right)}\ . \tag{6.161}$$

The many particle operator is transformed in a sum over one particle operators with an auxiliary field consisting of N Ising spins S_i. This is possible, because different $\hat{n}_i$ operators commute.

$$\mathrm{e}^{-\Delta\tau\hat{V}} = \prod_{i=1}^{N} \mathrm{e}^{-\Delta\tau U\,\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}} = \prod_{i=1}^{N}\Big(\frac{1}{2}\sum_{S_i=\pm1} \mathrm{e}^{\lambda S_i(\hat{n}_{i\uparrow}-\hat{n}_{i\downarrow})}\Big)\, \mathrm{e}^{\frac{\Delta\tau U}{2}\sum_{i=1}^{N}(\hat{n}_{i\uparrow}+\hat{n}_{i\downarrow})} \tag{6.162}$$

Exchanging sum and product and identifying the last sum as the operator of the electron number, $\hat{N}_e$, yields

$$\mathrm{e}^{-\Delta\tau\hat{V}} = 2^{-N}\sum_{S_1,\ldots S_N=\pm1} \mathrm{e}^{\lambda\sum_{i=1}^{N} S_i(\hat{n}_{i\uparrow}-n_{i\downarrow})}\, \mathrm{e}^{-\frac{\Delta\tau U}{2}\hat{N}_e}\ . \tag{6.163}$$

Since the operators of different spin orientation commute, we separate them and split

$$\hat{K} = \hat{K}_\uparrow + \hat{K}_\downarrow \,, \quad \hat{V} = \hat{V}_\uparrow + \hat{V}_\downarrow \,, \quad \hat{N}_e = \hat{N}_{e\uparrow} + \hat{N}_{e\downarrow} \,. \tag{6.164}$$

Now we can write the exponential functions as products of exponentials of each spin orientation. Furthermore, we insert the Hubbard Stratonovich transformation in each Trotter slice X of (6.170),

$$\begin{aligned} X &\stackrel{\text{def}}{=} \mathrm{e}^{-\Delta\tau\hat{K}}\,\mathrm{e}^{\Delta\tau\hat{V}}\,\mathrm{e}^{\Delta\tau\mu\hat{N}_e} \\ &= \mathrm{e}^{-\Delta\tau\hat{K}_\uparrow}\,\mathrm{e}^{-\Delta\tau\hat{K}_\downarrow} 2^{-N} \sum_{\underline{S}} \mathrm{e}^{\lambda\sum_{i=1}^{N} S_i\hat{n}_{i\uparrow}}\,\mathrm{e}^{-\lambda\sum_{i=1}^{N} S_i\hat{n}_{i\downarrow}}\,\mathrm{e}^{\Delta\tau(\mu-\frac{U}{2}\hat{N}_e)} \,. \end{aligned} \tag{6.165}$$

We observe that the chemical potential μ is altered by the interaction. Separating the two spin orientations entirely, we obtain

$$\begin{aligned} X = 2^{-N} \sum_{\underline{S}} &\mathrm{e}^{-\Delta\tau\hat{K}_\uparrow}\,\mathrm{e}^{\lambda\sum_{i=1}^{N} S_i\hat{n}_{i\uparrow}+\Delta\tau(\mu-\frac{U}{2}\hat{N}_{e\uparrow})} \\ &\mathrm{e}^{-\Delta\tau\hat{K}_\downarrow}\,\mathrm{e}^{-\lambda\sum_{i=1}^{N} S_i\hat{n}_{i\downarrow}+\Delta\tau(\mu-\frac{U}{2}\hat{N}_{e\downarrow})} \,. \end{aligned} \tag{6.166}$$

We introduce two matrices K_{ij} and V_{ij} for the kinetic and potential part, respectively. They are of the form

$$\begin{aligned} K_{ij} &= -t\delta_{<i,j>} = -t \begin{cases} 1 \ldots x_i, x_j \text{ n. n.} \\ 0 \ldots \text{ otherwise} \end{cases} \\ V_{ij}^{\sigma}(\underline{S}) &= \delta_{ij}\Big(\lambda\sigma S_i + \Delta\tau\Big(\mu - \frac{U}{2}\Big)\Big) \end{aligned} \tag{6.167}$$

For each spin orientation $\sigma = \pm 1$ we define the operator

$$\hat{D}^{\sigma}(\underline{S}) = \mathrm{e}^{\Delta\tau\sum_{ij} K_{ij}\hat{c}_{i\sigma}^{\dagger}\hat{c}_{j\sigma}}\mathrm{e}^{\sum_{ij} V_{ij}\hat{c}_{i\sigma}^{\dagger}\hat{c}_{j\sigma}} \tag{6.168}$$

with the help of which we can express the Trotter slice X as

$$X = 2^{-N} \sum_{\underline{S}} \hat{D}^{\uparrow}(\underline{S})\,\hat{D}^{\downarrow}(\underline{S}) \,. \tag{6.169}$$

Since the auxiliary fields S are different for each Trotter time τ, we have to distinguish them. Thus we introduce the superscript (τ). Inserting (6.169) into the partition function Z (6.156) we obtain

$$Z = 2^{-mN}\,\mathrm{tr}\prod_{\tau=1}^{m}\Big(\sum_{\underline{S}^{(\tau)}} \hat{D}^{\uparrow}(\underline{S}^{(\tau)})\,\hat{D}^{\downarrow}(\underline{S}^{(\tau)})\Big) \,. \tag{6.170}$$

Exchanging the order of the sum and the product and exploiting the fact that the operators $\hat{D}$ commute for different spin orientations, we obtain

$$Z = 2^{-mN}\,\mathrm{tr}\sum_{\underline{S}^{(1)}\ldots\underline{S}^{(m)}} \underbrace{\Big(\prod_{\tau=1}^{m}\hat{D}^{\uparrow}(\underline{S}^{(\tau)})\Big)}_{(\Uparrow)} \underbrace{\Big(\prod_{\tau=1}^{m}\hat{D}^{\downarrow}(\underline{S}^{(\tau)})\Big)}_{(\Downarrow)} \,. \tag{6.171}$$

Upon introducing a basis of elementary tensors

$$|\psi_{lk}\rangle = |\psi_{l\uparrow}\rangle \otimes |\psi_{k\downarrow}\rangle \tag{6.172}$$

the trace decomposes in the product of two sums, one for each spin orientation:

$$\begin{aligned}
\mathrm{tr}\Big((\Uparrow)(\Downarrow)\Big) &= \sum_{lk} \Big(\langle\psi_{l\uparrow}| \otimes \langle\psi_{k\downarrow}|\Big)\Big((\Uparrow) \otimes (\Downarrow)\Big)\Big(|\psi_{l\uparrow}\rangle \otimes |\psi_{k\downarrow}\rangle\Big) \\
&= \sum_{lk} \langle\psi_{l\uparrow}|(\Uparrow)|\psi_{l\uparrow}\rangle \, \langle\psi_{k\downarrow}|(\Downarrow)|\psi_{k\downarrow}\rangle \\
&= \Big(\sum_{l} \langle\psi_{l\uparrow}|(\Uparrow)|\psi_{l\uparrow}\rangle\Big)\Big(\sum_{k} \langle\psi_{k\downarrow}|(\Downarrow)|\psi_{k\downarrow}\rangle\Big) \\
&= \mathrm{tr}(\Uparrow)\ \mathrm{tr}(\Downarrow)
\end{aligned} \tag{6.173}$$

Therefore, the whole partition function Z can be written as

$$Z = 2^{-mN} \sum_{\underline{S}^{(1)} \ldots \underline{S}^{(m)}} \Big[\ \mathrm{tr} \prod_{\tau=1}^{m} \hat{D}^{\uparrow}(\underline{S}^{(\tau)})\Big]\Big[\ \mathrm{tr} \prod_{\tau=1}^{m} \hat{D}^{\downarrow}(\underline{S}^{(\tau)})\Big] \tag{6.174}$$

Since the above expression is symmetric in the spin index, we will investigate only one spin orientation and drop its index. Thus we have to deal with

$$\mathrm{tr} \prod_{\tau=1}^{m} \hat{D}(\underline{S}^{(\tau)}) \ , \ \text{ with } \ D(\underline{S}) = \mathrm{e}^{\Delta\tau \sum_{ij} K_{ij} \hat{c}_i^{\dagger} \hat{c}_j} \mathrm{e}^{\sum_{ij} V_{ij} \hat{c}_i^{\dagger} \hat{c}_j} \ . \tag{6.175}$$

This has the form of an exponential function of a combination of one particle operators. We will look at the general structure of its application to wave functions in n particle subspaces of the Fock space.

Only one electron:. If only one electron is present, its wave function can be spanned up as a sum over one particle wave functions located at the lattice sites i. Thus it is given by

$$|\psi\rangle = \sum_{i=1}^{N} d_i \, c_i^{\dagger}|0\rangle \ , \ \text{ with the vector } \ \underline{d} = \{d_1, \ldots d_N\} \ . \tag{6.176}$$

An exponential function of creation and annihilation operators acts on such a wave function $|\psi\rangle$ as

$$\begin{aligned}
\mathrm{e}^{\sum_{ij} A_{ij} \hat{c}_i^{\dagger} c_j}|\psi\rangle &= \sum_{k=1}^{N} d_k \mathrm{e}^{\sum_{ij} A_{ij} \hat{c}_i^{\dagger} c_j} c_k^{\dagger}|0\rangle \\
&= \sum_{k=1}^{N} \sum_{l=1}^{N} d_k \hat{c}_l^{\dagger}|0\rangle \underbrace{\langle 0|\hat{c}_l \mathrm{e}^{\sum_{ij} A_{ij} \hat{c}_i^{\dagger} c_j} c_k^{\dagger}|0\rangle}_{\stackrel{\mathrm{def}}{=} \{\mathrm{e}^A\}_{lk}} \\
&= \sum_{l=1}^{N} \sum_{k=1}^{N} \{\mathrm{e}^A\}_{lk} \, d_k \, c_l^{\dagger}|0\rangle \ .
\end{aligned} \tag{6.177}$$

We have inserted a complete set of one particle states and defined the matrix e^{A}. Therefore we conclude that by application of e^{A}, the vector $\underline{d}$ is transformed in

$$\underline{\tilde{d}} = \mathrm{e}^{A}\,\underline{d} \tag{6.178}$$

and describes the new one particle state. The new state is subjected to a new application of $\mathrm{e}^{A'}$ in the same way. Thus, in the one particle subspace we are able to evaluate

$$\prod_{\tau=1}^{m} \hat{D}(\underline{S}^{(\tau)})|\psi\rangle = \sum_{i=1}^{N} \tilde{d}_i \hat{c}_i^{\dagger}|0\rangle\ , \quad \text{with the vector } \underline{\tilde{d}} = \Big(\prod_{\tau=1}^{m} \mathrm{e}^{-\Delta\tau K}\mathrm{e}^{V}\Big)\,\underline{d}\,. \tag{6.179}$$

Two electrons:. In the two electron subspace, a complete basis is given by the elementary tensors $\left|\psi^{(1)}\right\rangle \otimes \left|\psi^{(2)}\right\rangle$ and each state can be spanned up as a linear combination of these basis states.

$$|\psi\rangle = \left|\psi^{(1)}\right\rangle \otimes \left|\psi^{(2)}\right\rangle = \Big(\sum_{i=1}^{N} d_i^{(1)}\hat{c}_i^{\dagger})\Big)\Big(\sum_{i=1}^{N} d_i^{(2)}\hat{c}_i^{\dagger})\Big)\,|0\rangle \tag{6.180}$$

Since the operator $\exp\{\sum_{ij} A_{ij}\hat{c}_i^{\dagger}\,\hat{c}_j\}$ contains no interaction, its application to $\left|\psi^{(1)}\right\rangle \otimes \left|\psi^{(2)}\right\rangle$ is given by the product

$$\begin{aligned}\mathrm{e}^{\sum_{ij} A_{ij}\hat{c}_i^{\dagger}\hat{c}_j}\left|\psi^{(1)}\right\rangle \otimes \left|\psi^{(2)}\right\rangle &= \Big(\mathrm{e}^{\sum_{ij} A_{ij}\hat{c}_i^{\dagger}\hat{c}_j}\left|\psi^{(1)}\right\rangle\Big) \otimes \Big(\mathrm{e}^{\sum_{ij} A_{ij}\hat{c}_i^{\dagger}\hat{c}_j}\left|\psi^{(2)}\right\rangle\Big) \\ &= \Big(\sum_{i=1}^{N} \tilde{d}_i^{(1)}\,\hat{c}_i^{\dagger}\Big)\Big(\sum_{i=1}^{N} \tilde{d}_i^{(2)}\,\hat{c}_i^{\dagger}\Big)\,|0\rangle\ .\end{aligned} \tag{6.181}$$

Thus we can use the same formula as in the one particle case.

$$\underline{\tilde{d}}^{(\alpha)} = \mathrm{e}^{A}\underline{d}^{(\alpha)} = \prod_{\tau=1}^{m} \mathrm{e}^{\Delta\tau K}\,\mathrm{e}^{V(\underline{S}^{(\tau)}}\,d^{(\alpha)}\ , \qquad \alpha = 1, 2\ . \tag{6.182}$$

More particles:. The above considerations can easily be extended to any arbitrary number of particle. Thus we obtain the operator identity in the whole Fock space

$$\mathrm{tr}\prod_{\tau=1}^{m} \hat{D}(\underline{S}^{(\tau)}) = \ \mathrm{tr}\,\mathrm{e}^{\sum_{ij}\tilde{A}_{ij}\hat{c}_i^{\dagger}\hat{c}_j} \ = \ \mathrm{tr}\,\mathrm{e}^{\underline{\hat{c}}^{\dagger}\tilde{A}\underline{\hat{c}}}\ , \tag{6.183}$$

with the vectors of operators $\underline{\hat{c}}^{\dagger} = \{\hat{c}_1^{\dagger}\ldots\hat{c}_N^{\dagger}\}$ and $\underline{\hat{c}} = \{\hat{c}_1\ldots\hat{c}_N\}$. Since the matrix $\tilde{A}$ is a Hermitian matrix, we can decompose it into a product of a diagonal matrix Δ containing its eigenvalues ε_i and a unitary matrix U containing the eigenvectors $\underline{U}_j$.

$$\tilde{A} = U\,\Delta\,U^\dagger\ , \quad \Delta_{ij} = \delta_{ij}\,\varepsilon_i\ ,\ U = \{\underline{U}_1, \ldots, \underline{U}_N\}\ . \tag{6.184}$$

Upon defining the vector of annihilation operators $\underline{\hat{f}} = U^\dagger \underline{\hat{c}}$ and its adjoint $\underline{\hat{f}}^\dagger = \underline{\hat{c}}^\dagger\, U$, the trace of the exponential function can be expressed as

$$\mathrm{tr}\,\mathrm{e}^{\underline{\hat{c}}^\dagger \tilde{A} \underline{\hat{c}}} = \mathrm{tr}\,\mathrm{e}^{\underline{\hat{c}}^\dagger U\,\Delta\,U^\dagger\,\underline{\hat{c}}} \tag{6.185}$$

$$= \mathrm{tr}\,\mathrm{e}^{\underline{\hat{f}}^\dagger \Delta \underline{\hat{f}}} = \mathrm{tr}\,\mathrm{e}^{\sum_{i=1}^N \varepsilon_i\,\hat{f}_i^\dagger \hat{f}_i} = \mathrm{tr}\,\mathrm{e}^{\sum_{i=1}^N \varepsilon_i\,\hat{n}_i^f} \tag{6.186}$$

It is not difficult to show that the operators $\hat{f}$ and $\hat{f}^\dagger$ fulfill the fermionic anti–commutator relations and are thus annihilation and creation operators of fermions:

$$\{\hat{f}_i, \hat{f}_j^\dagger\} = \sum_{l,k} U_{li}^\dagger\, U_{jk} \underbrace{\{\hat{c}_i, \hat{c}_j^\dagger\}}_{=\delta_{ij}} = \sum_l U_{li}^\dagger\, U_{jl} = \delta_{ij}\ , \tag{6.187}$$

$$\{\hat{f}_i, \hat{f}_j\} = \sum_{l,k} U_{il}^\dagger\, U_{jk}^\dagger \underbrace{\{\hat{c}_i, \hat{c}_j\}}_{=0} = 0\ , \tag{6.188}$$

$$\{\hat{f}_i^\dagger, \hat{f}_j^\dagger\} = \sum_{l,k} U_{li}\, U_{kj} \underbrace{\{\hat{c}_i^\dagger, \hat{c}_j^\dagger\}}_{=0} = 0\ . \tag{6.189}$$

The operator $\hat{n}_i^f$ measures the occupation number of the state f. It has thus the eigenvalues 0 and 1. It is convenient to choose the basis of the occupation numbers of states f for the evaluation of the trace

$$\mathrm{tr}\,\mathrm{e}^{\sum_i \varepsilon_i\,\hat{n}_i^f} = \prod_{i=1}^N \mathrm{tr}\,\mathrm{e}^{\varepsilon_i\,\hat{n}_i^f} = \prod_{i=1}^N \sum_{|n\rangle} \langle n|\mathrm{e}^{\varepsilon_i\,\hat{n}_i^f}|n\rangle \tag{6.190}$$

$$= \prod_{i=1}^N \left(1 + \mathrm{e}^{\varepsilon_i}\right) = \det\left(1 + \mathrm{e}^{\tilde{A}}\right)\ . \tag{6.191}$$

Therefore, the partition function Z reads

$$Z = \mathrm{e}^{-mN} \sum_{\underline{S}^{(1)} \ldots \underline{S}^{(m)}} \prod_{\sigma=\pm 1} \det\left(\mathbb{I} + \prod_{\tau=1}^m \mathrm{e}^{-\Delta\tau K}\,\mathrm{e}^{V(\underline{S}^{(\tau)})}\right)\ . \tag{6.192}$$

Thus we have to evaluate determinants of products of matrix exponential functions. The occurring matrices are of the dimension $N \times N$. The whole product of determinants will be the weight in the Monte Carlo simulation.
In analogy to (6.170) we can formulate the expectation value of an operator $\hat{O}$ with the Hubbard Stratonovich fields $\underline{S}$ and the decomposition of the exponential functions in m Trotter slices. This yields

$$< \hat{O} >_T = \frac{1}{Z} \sum_{\underline{S}^{(1)} \ldots \underline{S}^{(m)}} \mathrm{tr}\left\{\hat{O} \prod_{\tau=1}^m \left(\hat{D}^\uparrow(\underline{S}^{(\tau)})\,\hat{D}^\downarrow(\underline{S}^{(\tau)})\right)\right\} \tag{6.193}$$

$$= \sum_{\underline{S}^{(1)} \ldots \underline{S}^{(m)}} O(\underline{S}^{(1)} \ldots \underline{S}^{(m)})\ . \tag{6.194}$$

The quantities $O(\underline{S}^{(1)} \dots \underline{S}^{(m)})$ represent expectation values of $\hat{O}$ for a given Hubbard Stratonovich field distribution. They are obviously defined as

$$O(\underline{S}^{(1)} \dots \underline{S}^{(m)}) = \frac{1}{Z} \ \mathrm{tr}\left\{\hat{O} \prod_{\tau=1}^{m} \left(\hat{D}^{\uparrow}(\underline{S}^{(\tau)})\, \hat{D}^{\downarrow}(\underline{S}^{(\tau)})\right)\right\} . \tag{6.195}$$

In order to apply a Monte Carlo algorithm, this expression has to be decomposed in a sum over a density function $\rho(\underline{S}^{(1)} \dots \underline{S}^{(m)})$ (to be sampled) times a factor $g^{O}(\underline{S}^{(1)} \dots \underline{S}^{(m)})$ involving the operator $\hat{O}$. The major part of the variation should be within the density ρ. The density $\rho(\underline{S}^{(1)} \dots \underline{S}^{(m)})$ can be decomposed in a product of the contributions of either spin orientation $\rho_{\uparrow}$ and $\rho_{\downarrow}$. It is chosen to be equal to

$$\begin{aligned} \rho(\underline{S}^{(1)} \dots \underline{S}^{(m)}) &= \rho_{\uparrow}(\underline{S}^{(1)} \dots \underline{S}^{(m)})\, \rho_{\downarrow}(\underline{S}^{(1)} \dots \underline{S}^{(m)}) \\ &= \frac{1}{Z^{\uparrow}} \ \mathrm{tr} \prod_{\tau=1}^{m} \hat{D}^{\uparrow}(\underline{S}^{(\tau)})\, \frac{1}{Z^{\downarrow}} \ \mathrm{tr} \prod_{\tau=1}^{m} \hat{D}^{\downarrow}(\underline{S}^{(\tau)}) . \end{aligned} \tag{6.196}$$

Upon defining the function

$$\begin{aligned} g^{O}(\underline{S}^{(1)} \dots \underline{S}^{(m)}) &= \frac{1}{\rho(\underline{S}^{(1)} \dots \underline{S}^{(m)})} \ \mathrm{tr}\Big\{\hat{O} \prod_{\tau=1}^{m} \left(\hat{D}^{\uparrow}(\underline{S}^{(\tau)})\, \hat{D}^{\downarrow}(\underline{S}^{(\tau)})\right)\Big\} \\ &= \frac{1}{\rho(\underline{S}^{(1)} \dots \underline{S}^{(m)})} \ \mathrm{tr}\Big\{\hat{O} \underbrace{\mathrm{e}^{\sum_{ij} A^{\uparrow}_{ij} \hat{c}^{\dagger}_{i\uparrow} \hat{c}_{j\uparrow}} \mathrm{e}^{\sum_{ij} A^{\downarrow}_{ij} \hat{c}^{\dagger}_{i\downarrow} \hat{c}_{j\downarrow}}}_{\stackrel{\mathrm{def}}{=} \hat{X}}\Big\} . \end{aligned} \tag{6.197}$$

we can write the expectation value of $\hat{O}$ in the presence of the Hubbard Stratonovich fields $\underline{S}^{(1)} \dots \underline{S}^{(m)}$ as

$$O(\underline{S}^{(1)} \dots \underline{S}^{(m)}) = g^{O}(\underline{S}^{(1)} \dots \underline{S}^{(m)})\, \rho(\underline{S}^{(1)} \dots \underline{S}^{(m)}) . \tag{6.198}$$

The exponential functions in $\hat{X}$ contain only one particle operators and preserve the particle number of each spin orientation $N_{\uparrow}, N_{\downarrow}$ separatly. Evaluating the trace of $\hat{X}$ in the basis of the occupation number yields

$$\mathrm{tr}\,\{\hat{O}\hat{X}\} = \sum_{n=0}^{N} \sum_{|\psi\rangle^{(n)}} \left\langle \psi_m^{(n)} \middle| \hat{O}\hat{X} \middle| \psi_m^{(n)} \right\rangle \tag{6.199}$$

where the kets $\left\{\left|\psi_m^{(n)}\right\rangle\right\}$ denote a complete basis in the subspace of n particles. If the operator $\hat{O}$ does not preserve the particle numbers $N_{\uparrow}, N_{\downarrow}$ individually, the above trace will be zero. This implies that Green's functions such as $<< c_i^{\dagger} c_j^{\dagger} >>$ vanish. Thus we only look at one and two particle Green's functions.

6.4.1 Evaluation of One particle Green's Functions

In real space the one particle Green's functions have the general structure

$$g^{ji} =<< \hat{c}_{j\sigma}\hat{c}^{\dagger}_{i\sigma} >>= \frac{1}{Z}\ \mathrm{tr}\left\{\hat{c}_{i\sigma}\hat{c}^{\dagger}_{j\sigma}\,\mathrm{e}^{-\beta\hat{H}}\right\}. \tag{6.200}$$

In our notation this corresponds to the expectation value of the operator

$$\hat{O} = \hat{c}_{j\sigma}\hat{c}^{\dagger}_{i\sigma}\ . \tag{6.201}$$

With the auxiliary fields $\underline{S}^{(1)}\ldots\underline{S}^{(m)}$ this can be written as

$$g^{ji} = \sum_{\underline{S}^{(1)}\ldots\underline{S}^{(m)}} g^{ji}(\underline{S}^{(1)}\ldots\underline{S}^{(m)})\rho^{\uparrow}(\underline{S}^{(1)}\ldots\underline{S}^{(m)})\,\rho^{\downarrow}(\underline{S}^{(1)}\ldots\underline{S}^{(m)})\ , \tag{6.202}$$

with the symbols

$$g^{ji}(\underline{S}^{(1)}\ldots\underline{S}^{(m)}) = \frac{\mathrm{tr}\left\{\hat{c}_{j\sigma}\hat{c}^{\dagger}_{i\sigma}\prod_{\tau=1}^{m}\hat{D}^{\sigma}(\underline{S}^{(\tau)})\prod_{\tau=1}^{m}\hat{D}^{\overline{\sigma}}(\underline{S}^{(\tau)})\right\}}{\rho^{\sigma}(\underline{S}^{(1)}\ldots\underline{S}^{(m)})\rho^{\overline{\sigma}}(\underline{S}^{(1)}\ldots\underline{S}^{(m)})}\ . \tag{6.203}$$

As usually, we separate the trace of the product in a product of traces and observe that the trace over $\overline{\sigma}$ is just equal to $\rho^{\overline{\sigma}}(\underline{S}^{(1)}\ldots\underline{S}^{(m)})$. Thus it cancels out with $\rho^{\overline{\sigma}}(\underline{S}^{(1)}\ldots\underline{S}^{(m)})$ in the denominator. This yields the expression

$$g^{ji}(\underline{S}^{(1)}\ldots\underline{S}^{(m)}) = \frac{\mathrm{tr}\left\{\hat{c}_{j\sigma}\hat{c}^{\dagger}_{i\sigma}\prod_{\tau=1}^{m}\hat{D}^{\sigma}(\underline{S}^{(\tau)})\right\}}{\rho^{\sigma}(\underline{S}^{(1)}\ldots\underline{S}^{(m)})} \tag{6.204}$$

From now on we drop the spin index σ. As in (6.184), we diagonalize the matrix $\mathbb{A}$ and expand the operators $\hat{c}_j$ and $\hat{c}^{\dagger}_i$ in a sum over $\hat{f}_\nu$ and $\hat{f}^{\dagger}_\mu$, respectively.

$$\hat{c}_j = \sum_{\nu}\underbrace{\langle j\,|\nu\rangle}_{\stackrel{\mathrm{def}}{=} d_{j\nu}}\hat{f}_\nu\ , \quad \text{and} \quad \hat{c}^{\dagger}_i = \sum_{\mu}\underbrace{\langle\mu\,|j\rangle}_{\stackrel{\mathrm{def}}{=} d^{*}_{\mu i}}\hat{f}^{\dagger}_\mu\ . \tag{6.205}$$

This transformation simplifies the expression for the Green's function to

$$g^{ij} = \frac{1}{\sum_\nu(1+\mathrm{e}^{\varepsilon_i})}\sum_{\mu,\nu} d^{*}_{i\mu}d_{i\nu}\ \mathrm{tr}\left\{f_\mu f^{\dagger}_\nu \mathrm{e}^{\sum_\alpha \varepsilon_\alpha \hat{n}^{f}_{\alpha}}\right\}. \tag{6.206}$$

The evaluation of the trace is easiest in the basis of the occupation numbers of the states $|n_1\ldots n_N\rangle$ generated by $\hat{f}^{\dagger}$. The exponential function can be directly applied to such a state yielding the exponential function of the weighted sum of eigenvalues n_α.

$$\begin{aligned}\mathrm{tr}\left\{\hat{f}_\mu \hat{f}_\nu^\dagger \mathrm{e}^{\sum_\alpha \varepsilon_\alpha \hat{n}_\alpha^f}\right\} &= \sum_{n_1,\ldots n_N=0}^{1} \langle n_1 \ldots n_N| \hat{f}_\mu \hat{f}_\nu^\dagger \mathrm{e}^{\sum_\alpha \varepsilon_\alpha \hat{n}_\alpha^f} |n_1 \ldots n_N\rangle \\ &= \sum_{n_1,\ldots n_N=0}^{1} \langle n_1 \ldots n_N| \hat{f}_\mu \hat{f}_\nu^\dagger |n_1 \ldots n_N\rangle \, \mathrm{e}^{\sum_\alpha \varepsilon_\alpha n_\alpha} \; .\end{aligned} \tag{6.207}$$

The matrix element of the operator $\hat{f}_\mu \hat{f}_\nu^\dagger$ is only unequal to zero if there is no electron in the state ν, $n_\nu = 0$. Furthermore, the orthogonality of the basis states $|n_1 \ldots n_N\rangle$ implies that the created electron must be annihilated to yield a non vanishing matrix element. Thus we conclude that

$$\langle n_1 \ldots n_N| \hat{f}_\mu \hat{f}_\nu^\dagger |n_1 \ldots n_N\rangle = \delta_{\mu,\nu} \, \delta_{n_\nu,0} \tag{6.208}$$

must be fulfilled which implies for the trace

$$\begin{aligned}\mathrm{tr}\left\{\hat{f}_\mu \hat{f}_\nu^\dagger \mathrm{e}^{\sum_\alpha \varepsilon_\alpha \hat{n}_\alpha^f}\right\} =& \delta_{\mu,\nu} \prod_{\substack{\mu=1 \\ \mu\neq\nu}}^{N} \sum_{\nu=0}^{1} \mathrm{e}^{\varepsilon_\mu n_\mu} \sum_{\nu=0}^{1} \delta_{n_\nu,0} \, \mathrm{e}^{\varepsilon_\nu n_\nu} \\ =& \delta_{\mu,\nu} \prod_{\substack{\mu=1 \\ \mu\neq\nu}}^{N} (1 + \mathrm{e}^{\varepsilon_\mu}) \; .\end{aligned} \tag{6.209}$$

Therefore, the whole Green's function reads

$$g^{ji} = \sum_{\mu,\nu} d_{j\mu}^* d_{i\nu} \, \delta_{\nu,\mu} \, \frac{1}{1 + \mathrm{e}^{\varepsilon_\nu}} = \sum_\nu d_{j\mu}^* \frac{1}{1 + \mathrm{e}^{\varepsilon_\nu}} d_{i\nu} \; . \tag{6.210}$$

Inserting the expansion of $\hat{f}$, (6.205) and applying the spectral theorem, we obtain

$$g^{ji} = \langle j| \Big(\sum_\nu |\nu\rangle \frac{1}{1 + \mathrm{e}^{\varepsilon_\nu}} \langle\nu| \Big) |i\rangle = \left\{ \left(\mathbb{I} + \mathrm{e}^{\mathbb{A}} \right)^{-1} \right\}_{ji} \; . \tag{6.211}$$

This result shows us that the Green's function g^{ji} is just the matrix element of the operator $\left(\mathbb{I} + \mathrm{e}^{\mathbb{A}} \right)^{-1}$.

6.4.2 Evaluation of Two particle Green's Functions

6.4.3 Numerics

In this subsection we will consider some numerical problems we are confronted with in the grand canonical monte Carlo. We will treat only single spin flip algorithms, where one Markov step consists in proposing (and accepting or

rejecting) to alter one Hubbard Stratonovich Spin with index I at Trotter time T. Applying the Metropolis Hastings method, we have to deal with the ratio q given by

$$q = \frac{\rho(S')}{\rho(S)} = \frac{\rho^{\uparrow}(S')\rho^{\downarrow}(S')}{\rho^{\uparrow}(S)\rho^{\downarrow}(S)} = q^{\uparrow}\, q^{\downarrow} \; . \tag{6.212}$$

Since the densities ρ factorize in the components of either spin orientation, q also has this property. Now the classical Metropolis algorithm accepts a trial with the probability

$$\alpha = \min\{1, q\} \tag{6.213}$$

whereas a heat bath approach accepts with

$$\alpha = \frac{q}{1+q} \; . \tag{6.214}$$

If only one single spin flip is proposed, the new spin configuration $\underline{S}'$ equals the old one $\underline{S}$ with the exception of one mere spin S at time T and site I. This means that we propose

$$S'_I\prime(T) = -S_I^{(T)} \; . \tag{6.215}$$

The impact of this small change on $\hat{D}^{\sigma}(\underline{S}^{(\tau)})$ has to be evaluated. Since in this quantity

$$\hat{D}^{\sigma}(\underline{S}^{(\tau)}) = \mathrm{e}^{-Delta\tau K^{\sigma}}\, \mathrm{e}^{V(\underline{S}^{(\tau)})} \tag{6.216}$$

only the potential part V^{σ} (which is diagonal in addition!!) actually depends on the Hubbard Stratonovich field, the investigations simplify a lot. The element ij of the matrix V^{σ} is given by

$$V^{\sigma}(\underline{S}^{(\tau)})_{ij} = \sigma\, \lambda\, S_i^{(\tau)}\, \delta_{i,j} \; . \tag{6.217}$$

Thus the exponential function of V is also diagonal. Evaluated with the spin field $\underline{S}'^{(T)}$ it reads

$$
\mathrm{e}_{ij}^{V(\underline{S}'^{(T)})} = \begin{pmatrix}
\mathrm{e}^{\sigma\lambda S_1^{(T)}} & . & . & \ddots & \ddots & \vdots \\
. & \mathrm{e}^{\sigma\lambda S_2^{(T)}} & . & \ddots & \ddots & \vdots \\
. & . & \ddots & . & \ddots & \vdots \\
. & . & \dots & \mathrm{e}^{-\sigma\lambda S_I^{(T)}} & \ddots & \vdots \\
. & . & \dots & \ddots & \ddots & \vdots \\
. & . & \dots & \dots & \dots & \mathrm{e}^{\sigma\lambda S_N^{(T)}}
\end{pmatrix}
$$

$$
= \mathrm{e}^{V(S^{(T)})} \cdot \begin{pmatrix}
1 & . & . & \ddots & \ddots & \vdots \\
. & 1 & . & \ddots & \ddots & \vdots \\
. & . & \ddots & . & \ddots & \vdots \\
. & . & \dots & \mathrm{e}^{-2\sigma\lambda S_I^{(T)}} & \ddots & \vdots \\
. & . & \dots & \ddots & \ddots & \vdots \\
. & . & . & \dots & \dots & 1
\end{pmatrix} \tag{6.218}
$$

The last diagonal matrix expressing effect of the difference of the spin fields will be denoted by Δ. Therefore we can write

$$
\mathrm{e}^{V(\underline{S}'^{(T)})} = \mathrm{e}^{V(\underline{S}^{(T)})}\, \Delta\,, \quad \text{with } \Delta_{ij} = \delta_{ij} \begin{cases} 1 & \dots i \neq I \\ \mathrm{e}^{-2\sigma\lambda S_I^{(T)}} & \dots i = I \end{cases} \tag{6.219}
$$

Including the kinetic (hopping) term K for $\tau = T$ we can write

$$
D(\underline{S}'^{(T)}) = D(\underline{S}^{(T)})\, \Delta\,. \tag{6.220}
$$

These terms appear in the expression of the determinant forming the density ρ. Since the trace is invariant under cyclic permutations, we have the equality for all $L \in \mathbb{N}$

$$
\mathrm{tr} \prod_{\tau=1}^{m} D(\underline{S}^{(\tau)}) = \mathrm{tr} \prod_{\tau=1}^{m} D(\underline{S}^{(\tau+L)})\,. \tag{6.221}
$$

For this formula we have to introduce cyclic boundary conditions $\underline{S}^{(\tau+m)} = \underline{S}^{(\tau)}$ for the time dependence of the Hubbard Stratonovich field. With these results, we can rotate the Ds within the product until obtain Δ as the last factor. This corresponds to exactly T rotations. Then the quantity q reads

$$
q = \frac{\det\left(\mathbb{I} + \prod_{\tau=1}^{m} D(\underline{S}'^{(\tau+T)})\right)}{\det\left(\mathbb{I} + \prod_{\tau=1}^{m} D(\underline{S}^{(\tau+T)})\right)} = \frac{\det\left(\mathbb{I} + \prod_{\tau=1}^{m} D(\underline{S}^{(\tau+T)})\, \Delta\right)}{\det\left(\mathbb{I} + \prod_{\tau=1}^{m} D(\underline{S}^{(\tau+T)})\right)} \tag{6.222}
$$

Now we exploit the fact that the determinant of the product of two quadratic matrices $\mathbb{A}$ and $\mathbb{B}^{-1}$ is given by the product of the individual determinants.

Furthermore, the determinant of the inverse of a matrix is one over the determinant of the matrix. This means

$$\det \mathbb{A}\, \mathbb{B}^{-1} = \det \mathbb{A}\, \det \mathbb{B}^{-1} = \frac{\det \mathbb{A}}{\det \mathbb{B}} \,. \tag{6.223}$$

With this information the quantity q becomes

$$q = \det \Big(\big(\mathbb{I} + \prod_{\tau=1}^{m} D(\underline{S}^{(\tau+T)})\big)^{-1} \, \big(\mathbb{I} + \prod_{\tau=1}^{m} D(\underline{S}^{(\tau+T)}) \Delta\big) \,. \tag{6.224}$$

The first factor corresponds to the Green's function for a given Hubbard Stratonovich field configuration $\underline{S}$ at Trotter time T,

$$g_{ij}^{\underline{S}}(T) =< c_i(T)\, c_j^{\dagger}(T) >_{\underline{S}} = \big(\mathbb{I} + \prod_{\tau=1}^{m} D(\underline{S}^{(\tau+T)})\big)^{-1} \,. \tag{6.225}$$

Furthermore, the second factor is identified with the inverse of a Green's function for the Hubbard Stratonovich field $\underline{S}'$ at Trotter time T. Therefore we obtain the equation

$$q = \det \Big(g^{\underline{S}} \, \big(g^{\underline{S}'}\big)^{-1} \Big) \,. \tag{6.226}$$

Now we turn to investigating the effect of Δ. Physically speaking, Δ corresponds to a defect in the lattice of the Hubbard Stratonovich fields. This effect is described best with the *Dyson equation* which we derive next.

Dyson Equation:. We want to evaluate the effect of one differently oriented spin on the Green's function. To this end we start with the expression for the inverse of the Green's function introducing the abbreviations X,

$$\big(g^{\underline{S}'}\big)^{-1} = \mathbb{I} + \underbrace{\prod_{\tau=1}^{m} D(\underline{S}^{(\tau+T)})}_{\stackrel{\text{def}}{=} X} \, \Delta = \mathbb{I} + X\, \Delta \,. \tag{6.227}$$

The newly introduced quantity X is a part of the non–perturbed Green's function $g^{\underline{S}}$. Actually, its inverse is given by

$$\big(g^{\underline{S}}\big)^{-1} = \mathbb{I} + X \implies X = \big(g^{\underline{S}}\big)^{-1} - \mathbb{I} \,. \tag{6.228}$$

Inserting the last identity in (6.227) yields

$$\begin{aligned} \big(g^{\underline{S}'}\big)^{-1} &= \mathbb{I} \qquad\quad + \Big(\big(g^{\underline{S}}\big)^{-1} - \mathbb{I} \Big) \, \Delta \\ &= \big(g^{\underline{S}}\big)^{-1} g^{\underline{S}} + \big(g^{\underline{S}}\big)^{-1} \big(\mathbb{I} - g^{\underline{S}}\big) \, \Delta \\ &= \big(g^{\underline{S}}\big)^{-1} \Big(g^{\underline{S}} + \big(\mathbb{I} - g^{\underline{S}}\big) \, \Delta \Big) \,. \end{aligned} \tag{6.229}$$

In the first step we have expressed the identity operator as the product of the Green's function with its inverse. Adding and subtracting $\mathbb{I}$ in the second factor yields after factorization

$$\left(g^{\underline{S}'}\right)^{-1} = \left(g^{\underline{S}}\right)^{-1}\Big(\mathbb{I} + (\mathbb{I} - g^{\underline{S}})(\Delta - \mathbb{I})\Big) \,. \tag{6.230}$$

This is the Dyson equation stated in the form we need it to calculate q.

Calculation of q:. Inserting this equation in the expression of q, (6.226), we observe that the leading two factors $g^{\underline{S}}$ and $\left(g^{\underline{S}}\right)^{-1}$ of the determinant cancel. Therefore we obtain

$$q = \det\Big(\mathbb{I} + \underbrace{(\mathbb{I} - g^{\underline{S}})\,(\Delta - \mathbb{I})}_{\stackrel{\text{def}}{=} Y}\Big) \,. \tag{6.231}$$

Now we turn to the evaluation of the above determinant. In the following we will only be concerned with the Green's function evaluated with the original Hubbard Stratonovich fields $\underline{S}$. Thus we will drop the index $\underline{S}$ of the Green's function and simply write

$$g \stackrel{\text{def}}{=} g^{\underline{S}} \,. \tag{6.232}$$

In order to evaluate the determinant it is useful to exploit the identity

$$\log\big(\det(\mathbb{I} + Y)\big) = \ \mathrm{tr}\,\big(\log(\mathbb{I} + Y)\big)$$

and consequently

$$\det(\mathbb{I} + Y) = \exp\big(\ \mathrm{tr}\,\big(\log(\mathbb{I} + Y)\big)\big) \,. \tag{6.233}$$

The logarithm of the matrix $\mathbb{I}+Y$ can be evaluated with the Taylor expansion. This involves the powers of the matrix Y multiplied by some real constants c_n. Exchanging trace and sum yields

$$\det(\mathbb{I} + Y) = \exp\Big(\mathrm{tr}\,\big(\sum_{n=1}^{\infty} c_n\, Y^n\big)\Big) = \exp\Big(\sum_{n=1}^{\infty} c_n\, \mathrm{tr}\,(Y^n)\Big) \,. \tag{6.234}$$

Now we derive an expression for $\mathrm{tr}(Y^n)$. Naturally, we start with $n = 1$

$$\mathrm{tr}X = \sum_i X_{ii} = \sum_{l,i} (\mathbb{I} - g^{\underline{S}})_{il} \underbrace{(\Delta_{li} - \delta_{li})}_{=\alpha\,\delta_{li}\delta_{iI}} = \alpha\,(\mathbb{I} - g^{\underline{S}})_{II} \,. \tag{6.235}$$

where α stands for the difference between Δ and δ in the component I and T, namely

$$\alpha = \mathrm{e}^{-2\sigma\lambda S_I^{(T)}} - 1 \,. \tag{6.236}$$

Evaluating the indices II, the trace of Y turns out to be essentially given by one diagonal element of the Green's function g,

$$\mathrm{tr}Y = \alpha\,(1 - g^{\underline{S}}_{II})\;. \tag{6.237}$$

A diagonal element of the n–th power of Y has the structure

$$(Y^n)_{ii} = Y_{il_1}\,Y_{l_1l_2}\,Y_{l_2l_3}\,\ldots\,Y_{l_{n-1}i}\;. \tag{6.238}$$

Let's examine the product of the first two matrices corresponding to the element il_2 of the square of Y. Inserting the explicit form of Y we obtain

$$\begin{aligned}(YY)_{il_2} = Y_{il_1}\,Y_{l_1l_2} &= (\mathbb{I} - g^{\underline{S}})_{iI}\alpha\,\delta_{l_1I}\,Y_{l_1l_2} = (\mathbb{I} - g^{\underline{S}})_{iI}\alpha\,Y_{Il_2} \\ &= (\mathbb{I} - g^{\underline{S}})_{iI}\alpha\,\Big[(\mathbb{I} - g)_{II}\alpha\Big]\,\delta_{l_2I}\end{aligned} \tag{6.239}$$

Performing completely analog steps, we derive the third power of Y. It is given by

$$(YYY)_{il_3} = (\mathbb{I} - g^{\underline{S}})_{iI}\alpha\,\Big[(\mathbb{I} - g)_{II}\alpha\Big]^2\,\delta_{l_2I}\;. \tag{6.240}$$

Now it is easy to guess what the n–th power of Y might be. Complete induction proves the identity

$$(Y^n)_{ij} = (\mathbb{I} - g^{\underline{S}})_{iI}\alpha\,\Big[(\mathbb{I} - g)_{II}\alpha\Big]^{n-1}\,\delta_{jI} = \Big[(\mathbb{I} - g)_{II}\alpha\Big]^{n-1}\,Y_{ij}\;. \tag{6.241}$$

The last identity stems from the definition of the matrix Y. A diagonal element of Y^n has an even simpler form because the Kronecker–delta then acts on the index i in the first factor. Therefore the sum in the trace of Y^n is easily evaluated and the trace is given by

$$\mathrm{tr}\,Y^n = \sum_i (Y^n)_{ii} = \sum_i \Big[(\mathbb{I} - g)_{II}\alpha\Big]^n\,\delta_{iI} = \Big[(\mathbb{I} - g)_{II}\alpha\Big]^n \tag{6.242}$$

for all $n \in \mathbb{N}$. Inserting the above identity into (6.234) and observing that the sum represents the Taylor expansion of the logarithm, the determinant of $\mathbb{I} + Y$ is given by

$$\begin{aligned}\det(\mathbb{I} + Y) &= \exp\Big(\sum_{n=1}^{\infty} c_n\big[(\mathbb{I} - g)_{II}\alpha\big]^n\Big) \\ &= \exp\Big(\log\big(1 + \big[(\mathbb{I} - g)_{II}\alpha\big]\big)\Big) \\ &= 1 - (1 - g_{II})\,\alpha\;,\end{aligned} \tag{6.243}$$

where the exponential function cancelled the logarithm. Inserting the definition of α, q^σ eventually turns out to be equal to

$$q^\sigma = 2 + \big(1 - g^{\underline{S}}_{II\sigma}(T)\big)\,\big(\mathrm{e}^{-2\sigma\lambda S^{(T)}_{II}} - 1\big)\;. \tag{6.244}$$

These considerations reduce the computational cost of the algorithm from originally $o(mN^3)$ to merely $o(1)$!!

Updating of the Green's functions:. If the new configuration of the Hubbard Stratonovich spins $\underline{S}'$ is accepted in the Markov chain, the Green's functions $g^{\underline{S}}(T)$ has to be updated. To this end we can also use the Dyson Equation (6.230), although now not for the inverse but for the actual Green's function.

$$\begin{aligned} g^{\underline{S}'}(T) &= \left((\mathbb{I} + (\mathbb{I} - g^{\underline{S}}(T))\,(\Delta - \mathbb{I}) \right)^{-1} g^{\underline{S}}(T) \\ &= \left(\mathbb{I} + Y \right)^{-1} g^{\underline{S}}(T) \end{aligned} \tag{6.245}$$

We expand the inverse of $\mathbb{I} + Y$ in a geometric series. This yields

$$\left(\mathbb{I} + Y \right)^{-1} = \sum_{\nu=0}^{\infty} (-1)^{\nu} Y^{\nu} = \mathbb{I} - \sum_{\nu=1}^{\infty} (-1)^{\nu-1} Y^{\nu} \; . \tag{6.246}$$

Inserting the derived formula for the ν–th power of Y, (6.241), we find

$$\left(\left(\mathbb{I} + Y \right)^{-1} \right)_{ij} = \mathbb{I} - \sum_{\nu=1}^{\infty} (-1)^{\nu-1} \left[\alpha\,(1 - g_{II}) \right]^{\nu-1} Y_{ij} \tag{6.247}$$

Substituting the index ν by $\mu = \nu - 1$, we remark that the complete geometric series is reproduced, now for the numbers $-\alpha\,(1 - g_{II})$. Inserting its sum we find

$$\left(\left(\mathbb{I} + Y \right)^{-1} \right)_{ij} = \mathbb{I} - \left[1 + \alpha\,(1 - g_{II}) \right]^{-1} Y_{ij} \; . \tag{6.248}$$

Finally we obtain the the correct expression for the altered Green's function. Inserting the last equation in (6.245) we find

$$g^{\underline{S}'}(T) = \mathbb{I} - \left[1 + \alpha\,(1 - g_{II}) \right]^{-1} Y g^{\underline{S}}(T) \; . \tag{6.249}$$

This formula involves only one matrix multiplication, namely $Y\, g^{\underline{S}}(T)$. The original computational cost of $O(m\,N^3)$ is thus reduced to $O(N^2)$.
But not only the Green's function at time $\tau = T$ has to be updated. All the Green's function have to be calculated. This is most efficiently done by a procedure called *wrapping*. This is presented next.
Remember that the one particle Green's function at time $\tau_{L'} = L'\,\Delta\tau$ for spin–orientation σ is given by (6.225). We abbreviate the product over m Trotter slices by X writing

$$g^{\underline{S}}_{ij}(L'\,\Delta\tau) = \Big[\mathbb{I} + \underbrace{\prod_{\tau=1}^{m} D(\underline{S}^{(\tau+L')})}_{X_{L'}} \Big]^{-1} = \left[\mathbb{I} + X_{L'} \right]^{-1} \; . \tag{6.250}$$

Again, this expression can be viewed as the sum of the geometric series. We obtain

$$g_{ij}^{\underline{S}}(L'\,\Delta\tau) = \mathbb{I} + \sum_{\nu=1}^{\infty}(-1)^{\nu} X_{L'}^{\nu} \tag{6.251}$$

In order to simplify the above equation, we have to examine the powers of $X_{L'}$. Writing these powers as products and inserting the definition of $X_{L'}$ we find the relation

$$X_{L'}^{\nu} = D_{L'+1}\, D_{L'+2} \cdots X_0^{\nu-1}\, D_1 \cdots D_{L'} \; . \tag{6.252}$$

Inserting (6.252) into the product of (6.251) we obtain for the Green's function at time $L'\,\Delta\tau$

$$g_{ij}^{\underline{S}}(L'\,\Delta\tau) = \mathbb{I} + D_{L'+1} \cdots D_m \Big(\sum_{\nu=1}^{\infty}(-1)^{\nu} X_0^{\nu-1} \Big)\, D_1 \cdots D_{L'} \; . \tag{6.253}$$

Applying the same strategy for $g_{ij}^{\underline{S}}((L'+1)\,\Delta\tau)$, we derive

$$X_{L'}^{\nu} = D_{L'+2}\, D_{L'+3} \cdots X_0^{\nu-1}\, D_1 \cdots D_{L'+1} \; . \tag{6.254}$$

Therefore, the Green's function at time $(L'+1)\,\Delta\tau$ is given by

$$\begin{aligned} g_{ij}^{\underline{S}}((L'+1)\,\Delta\tau) &= \mathbb{I} + D_{L'+2} \cdots D_m \Big(\sum_{\nu=1}^{\infty}(-1)^{\nu} X_0^{\nu-1} \Big)\, D_1 \cdots D_{L'+1} \; . \\ &= \mathbb{I} + D_{L'+1}^{-1} \Big(D_{L'+1} \cdots D_m \Big(\sum_{\nu=1}^{\infty}(-1)^{\nu} X_0^{\nu-1} \Big)\, D_1 \cdots D_{L'} \Big) D_{L'+1} \\ &= \mathbb{I} + D_{L'+1}^{-1} \Big(g_{ij}^{\underline{S}}(L'\,\Delta\tau) - \mathbb{I} \Big)\, D_{L'+1} \end{aligned} \tag{6.255}$$

Simplifying the content of the above parenthesis, we finally obtain a recursion expression for the updating. It reads

$$g^{\underline{S}'}(\tau+1) = D^{-1}(S^{(\tau+1)})\, g^{\underline{S}}(\tau)\, D(S^{(\tau+1)}) \; . \tag{6.256}$$

Thus, beginning with $\tau = T$, all Green's functions can be updated with the above simple formula. From time to time the Green's function has to be evaluated ab initio due to accumulation of numerical round off errors.

Time dependent Green's functions:. Now we consider an operator $\hat{O}$ depending on the Trotter time τ. This is for instance the case of the time dependent one particle Green's function

$$\hat{O}(\tau) = \hat{c}_i(\tau)\, \hat{c}_j^{\dagger} \tag{6.257}$$

The formalism generalizes best for Trotter times τ that are a multiple of $\Delta\tau$. Therefore we tackle the trace

$$< \hat{c}_i(\tau)\, \hat{c}_j^{\dagger} >= \; \mathrm{tr} \left(\hat{c}_i(\tau)\, \hat{c}_j^{\dagger} \prod_{\tau=1}^{m} D(\underline{S}^{(\tau)}) \right) , \qquad \text{for } \; \tau = n\,\Delta\tau \; , \tag{6.258}$$

where is a natural number $n \in \mathbb{N}$ much smaller than m Using the Heisenberg time evolution for the operators $\hat{c}_i(\tau)$, we obtain the equation

$$\hat{c}_i(\tau) = \mathrm{e}^{\tau\,\hat{H}}\,\hat{c}_i\,\mathrm{e}^{-\tau\,\hat{H}}\ . \tag{6.259}$$

For the expectation value in the canonical ensembles this yields

$$< \hat{c}_i(\tau)\,\hat{c}_j^\dagger >= \frac{1}{Z}\ \mathrm{tr}\left(\mathrm{e}^{\tau\hat{H}}\mathrm{e}^{-\beta\hat{H}}\hat{c}_i\mathrm{e}^{-\tau\hat{H}}\hat{c}_j^\dagger\right) = \frac{1}{Z}\ \mathrm{tr}\left(\mathrm{e}^{-(\beta-\tau)\hat{H}}\,\hat{c}_i\mathrm{e}^{-\tau\hat{H}}\hat{c}_j^\dagger\right). \tag{6.260}$$

Introducing the discretization of the Trotter time $\Delta\tau$, we can write the Green's function as a product

$$< \hat{c}_i(\tau)\,\hat{c}_j^\dagger >= \frac{1}{Z}\ \mathrm{tr}\Big(\prod_{l=1}^{(m-n)}\ \mathrm{e}^{-\Delta\tau\hat{H}}\,\hat{c}_i\,\mathrm{e}^{-\Delta\tau\hat{H}}\Big)\,. \tag{6.261}$$

We introduce a sequence of propagators $\hat{U}(\Delta\tau) = \mathrm{e}^{\Delta\tau\hat{H}}$ to obtain

$$\hat{c}_i(\tau) = U(\Delta\tau)^n\,\hat{c}_i\,U(\Delta\tau)^{-n} \tag{6.262}$$

and

$$\begin{aligned} < \hat{c}_i(\tau)\,\hat{c}_j^\dagger > \Big|_{\tau=n\,\Delta\tau} &= < \left(\hat{U}(\Delta\tau)\right)^n\,\hat{c}_i\ \hat{c}_j^\dagger > \\ &= \sum_{\underline{S}} \rho(\underline{S})\,\Big(\prod_{l=m-n+1}^{m} D(\underline{S}^{(l)})\,g\Big)_{ij} \end{aligned} \tag{6.263}$$

Numerical Stability of Matrix Products:. In early years the Grand Canonical Quantum Monte Carlo was only of academic usefulness because numerical instability spoilt its application at lower (below 10.000 K) temperatures. The crucial point in the algorithm is the evaluation of the matrix product

$$\prod_{l=1}^{m} D(\underline{S}^{(l)}) \tag{6.264}$$

because this has to be done for an as big number of Trotter slices as $m \approx 1000$. In real applications the eigenvalue of the matrices $D(\underline{S}^{(l)})$ range within the interval $(10^{-100}, 10^{100})$. This means that the condition number of $D(\underline{S}^{(l)})$ (given by the ratio of the largest and the smallest eigenvalue) is up to 10^{200}. Therefore, successive matrix multiplication as in (6.264) is an extremely ill posed process. This is the case, because a matrix multiplication mixes all magnitudes of the entries of the involved matrices.
There is a way of stabilizing matrix multiplications by separating different magnitudes of eigenvalues. This approach lifts many of the restrictions of the Grand Canonical QMC. It consists of successive application of the *singular value decomposition* (SVD) outlined in the following.

In a first step we directly carry out as many matrix multiplications (say n) of (6.264) as reasonably possible. The products are referred to as matrices $A^{(k)}$, $k = 1 \dots m/n$. In the worst case no multiplication is possible and $A^{(k)}$ corresponds to $D(\underline{S}^{(l)})$.

$$\underbrace{D(\underline{S}^{(1)}) \cdots D(\underline{S}^{(n)})}_{A^{(m/n)}} \cdot \underbrace{D(\underline{S}^{(n+1)}) \cdots D(\underline{S}^{(2n)})}_{A^{(m/n-1)}} \cdots \underbrace{D(\underline{S}^{(m-n)}) \cdots D(\underline{S}^{(m)})}_{A^{(1)}} . \tag{6.265}$$

Thus the product of (6.264) is partially carried out. It simplifies to a product of m/n factors counted from $k = m/n$ down to $k = 1$,

$$\prod_{l=1}^{m} D(\underline{S}^{(l)}) = \prod_{k=m/n}^{1} A^{(k)} = A^{(m/n)} \cdots A^{(2)} \cdot A^{(1)} . \tag{6.266}$$

The product of the matrices $A^{(k)}$ is now stabilized by the following scheme: Matrix $A^{(1)}$ is subjected to a SVD. This yields a decomposition of $A^{(1)}$ in a product of three matrices $U^{(1)}$, $\Delta^{(1)}$ and $V^{(1)}$,

$$A^{(1)} = U^{(1)} \, \Delta^{(1)} \, V^{(1)\dagger} \tag{6.267}$$

with the unitary matrices $U^{(1)}$ and $V^{(1)}$ and the diagonal matrix $\Delta^{(1)}$. Now all eigenvalues of a unitary matrix are situated on the unit circle. Thus its condition number is 1 and a product of any matrix A with a unitary matrix doesn't worsen the condition number of A. Therefore, we can safely multiply $A^{(2)}$ with $U^{(1)}$. Furthermore, $\Delta^{(1)}$ is a diagonal matrix and its multiplication to $A^{(2)} \, U^{(1)}$ is trivial. The product of these three matrices is subjected to a SVD decomposition. This yields

$$A^{(2)} \cdot A^{(1)} = \underbrace{A^{(2)} \, U^{(1)} \, \Delta^{(1)}}_{U^{(2)} \, \Delta^{(2)} \, V^{(2)\dagger}} V^{(1)\dagger} = U^{(2)} \, \Delta^{(2)} \, V^{(2)\dagger} \, V^{(1)\dagger} \tag{6.268}$$

The same procedure is applies for the product of the matrix $A^{(3)}$ with (6.268). A SVD of the matrix $A^{(3)} \, U^{(2)} \, \Delta^{(2)}$ yields

$$A^{(3)} \cdot A^{(2)} \cdot A^{(1)} = U^{(3)} \, \Delta^{(3)} \, V^{(3)\dagger} \, V^{(2)\dagger} \, V^{(1)\dagger} . \tag{6.269}$$

Successive application of this strategy finally yields the stable formula for the product

$$\prod_{l=1}^{m} D(\underline{S}^{(l)}) = U^{(m/n)} \, \Delta^{(m/n)} \prod_{l=m/n}^{1} V^{(l)\dagger} . \tag{6.270}$$

This evaluation involves m/n singular value decompositions. The computational cost of one such operation is ???

7. Maximum Entropy

7.1 Ill–Posed Inversion Problems

In this section we will show a way to the famous *maximum entropy* principle. To motivate this principle, we consider a set of linear equations with the vector of unknowns $\mathbf{x}$, matrix M and the vector of known data $\mathbf{d}$:

$$M \cdot \mathbf{x} = \mathbf{d} \; . \tag{7.1}$$

It often occurs that the data $\mathbf{d}$ derived from an experiment or a computer simulation suffer from noise which will be denoted by $\boldsymbol{\eta}$. Furthermore, the condition of the matrix M given by the ratio of biggest to smallest eigenvalue can be rather high. That means that the problem

$$M \cdot \mathbf{x} = \mathbf{d} + \boldsymbol{\eta} \tag{7.2}$$

is ill posed and cannot be solved by direct inversion of M. Small eigenvalues of M amplify the noise significantly. This is best seen when considering a quadratic matrix M that can be cast in the form

$$M = \sum_i a_i \mathbf{u}_i \, \mathbf{u}_i^\dagger \tag{7.3}$$

with eigenvalues a_i and eigenvectors $\mathbf{u}_i$. Application of the inverse of M to $\mathbf{d} + \boldsymbol{\eta}$ yields

$$M^{-1}(\mathbf{d} + \boldsymbol{\eta}) = \sum_i \frac{1}{a_i} \mathbf{u}_i \, \mathbf{u}_i^\dagger (\mathbf{d} + \boldsymbol{\eta}) = \mathbf{x} + \sum_i \mathbf{u}_i \, \frac{\mathbf{u}_i^\dagger \boldsymbol{\eta}}{a_i} \, , \tag{7.4}$$

with $\mathbf{x}$ being the underlying exact solution. In case of a large overlap $\mathbf{u}_i^\dagger \boldsymbol{\eta}$, between the eigenvectors $\mathbf{u}_i^\dagger$ and the noise vector $\boldsymbol{\eta}$ the error is drastically amplified. If M originates from an experimental apparatus–function of a general point spread function, small eigenvalues correspond to rapidly oscillating eigenfunctions which couple stronger to noise contributions $\boldsymbol{\eta}$ than to the exact data $\mathbf{d}$.
To illustrate this point consider some measurements of the Greens function along the imaginary axes of which we want to infer the spectral function $A(\omega)$. The relation between the two functions is given by

$$g(\tau_i) = \int_0^\infty A(\omega)\, e^{-\omega\tau_i}\, d\omega \; . \tag{7.5}$$

The exponential part of the integrand decreases rapidly as ω becomes large. This means that the shape of $A(\omega)$ for $\omega > 1$ influences only very weakly the integral $g(\tau_i)$. Reversely, since we are given the data $g(\tau_i)$, we can say little about this part of $A(\omega)$. Worse, direct inversion of Eq. (7.5) amplifies the noise of $g(\tau_i)$ giving rise to huge oscillations of the spectral function (cf. Figure 7.1). In the example illustrated in Fig. 7.1, the largest eigenvalue is approximately 74 and the smallest 3×10^{-19}.

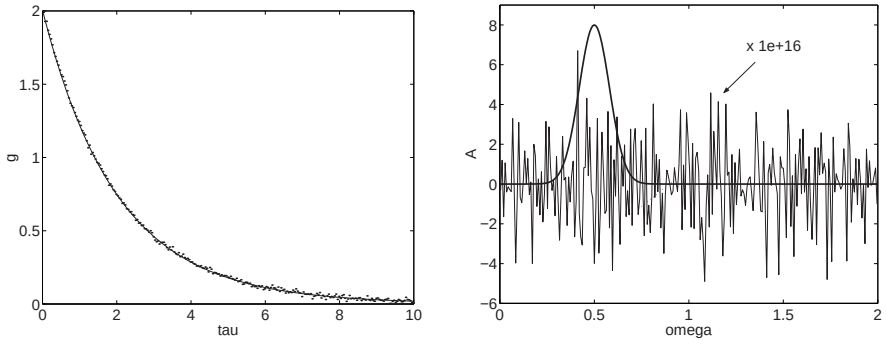

Fig. 7.1. The smooth line in the left–hand plot corresponds to the image of the smooth peak in the right–hand plot. After adding a small noise to $g(\tau)$, the inversion $A(\omega)$ has lost all resemblence to the actual peak.

Since this direct approach is not feasible, we will raise a different question: Given the data $g(\tau_i)$ and some prior knowledge I what is the *most likely* spectral function $A(\omega)$?? The Bayes' Theorem yields

$$p(A(\omega) \,|\, g(\tau_i)\, I) = \frac{1}{Z}\, p(g(\tau_i) \,|\, A(\omega)\, I)\, p(A(\omega) \,|\, I)$$

with the normalization Z. In order to apply this formula, we have to determine the prior probability $p(A(\omega) \,|\, I)$. In this case it will be an entropic prior. The general problem of the correct assignment of priors is the contents of the subsequent section.

7.2 Quantified Maximum Entropy

We next assign the probabilities in the case of noisy testable infromation. Either data are obtained from a computer experiment or from a real physical experiment. In both cases the data suffer from random noise. In what follows

we want to derive a formfree reconstruction of the distribution function $\rho(x)$. This procedure is called *quantified maximum entropy*.
We will derive the probability $p(\rho(x) \,|\, \mathbf{d}, I)$ that a distribution $\rho(x)$ is the real one in the light of noisy data $\mathbf{d}$. A number of N_d data points d_ν will be taken into account. The result is derived in four steps.

7.2.1 Step One

We discretize the possible values of x leading to

$$\rho(x) \to \rho_i = \rho(x_i)\, \Delta V_i \,. \tag{7.6}$$

This discrete set is called the *set of pixels*.

7.2.2 Step Two

We introduce a small unit of ρ_i denoted by $\Delta\rho$. This *quantization* maps the probability density onto integers n_i

$$\rho_i \to n_i \qquad \text{with} \quad \rho_i \approx n_i\, \Delta\rho \,. \tag{7.7}$$

I.e., instead of $p(\rho|\ldots)$ we are dealing with $p(\{n_i\}|\ldots)$, which simplifies the argumentation considerably.

7.2.3 Step Three

We derive the *prior probability* $P(\mathbf{n} \,|\, I)$. To this end we introduce the *default model* by assuming that that the mean number of points in every pixel i is given by μ_i. More precisely, we assume that every $\Delta\rho$ we add has the probability $\mu_i / \sum \mu_i$ to fall into pixel i. This gives rise to a *Poisson process* whose distribution reads

$$P(n_i \,|\, \mu_i\, I) = \frac{\mu_i^{n_i}}{n_i!}\, e^{-\mu_i} \,, \qquad n_i = 0, 1, 2, \ldots \,. \tag{7.8}$$

The combined probability $P(\mathbf{n} \,|\, \boldsymbol{\mu}, I)$ for all N pixels is given by the product

$$P(\mathbf{n} \,|\, \boldsymbol{\mu}, I) = \prod_{i=1}^{N} P(n_i \,|\, \mu_i, I) = e^{-\sum_i \mu_i} \prod_{i=1}^{N} \frac{\mu_i^{n_i}}{n_i!} \,. \tag{7.9}$$

Assuming large numbers $n_i \gg 1$ we employ Stirling's formula and obtain

$$P(\mathbf{n} \,|\, I) = \frac{1}{Z}\, \frac{1}{\prod_i \sqrt{n_i}}\, e^{S} \,, \tag{7.10}$$

where Z is the normalization factor and S stands for the *entropy*.

$$S = \sum_{i=1}^{N} S_i = \sum_{i=1}^{N} n_i - \mu_i - n_i \log(n_i/\mu_i) \tag{7.11}$$

7.2.4 Step Four

We undo the quantization

$$n_i = \frac{\rho_i}{\Delta\rho} \quad \Rightarrow \quad \mu_i = \frac{m_i}{\Delta\rho} \tag{7.12}$$

The prior probability for n_i, i.e. Eq. (7.10), and thus the prior for ρ_i can be expressed in terms of ρ_i and m_i. In fact, by inserting Eq. (7.12) into Eq. (7.10) we obtain

$$p(\boldsymbol{\rho}\,|\alpha,\, I) = \frac{1}{Z(\alpha)}\,\frac{1}{\prod_i \sqrt{\rho_i}}\, e^{\alpha S}\ . \tag{7.13}$$

We have introduced the regularization parameter $\alpha = \frac{1}{\Delta\rho}$ that is also called *nuisance parameter* or *hyper-parameter*. It has to be fixed later on, and meanwhile we add it to the set of conditions.

7.2.5 The Steepest Descent Approximation

The normalization of $p(\boldsymbol{\rho}\,|\,\alpha, I)$ can actually be computed numerically. For the posterior means we encounter, however, more complex integrals which can no longer be evaluate analytically and one either resorts to the MCMC approach or to the *steepest descent approximation*, which we will discuss now. The general idea behind this method is to approximate integrals whose integrand is a product of a weakly varying function $f(\boldsymbol{\rho})$ and a sharply peaked factor $\exp(\Phi(\boldsymbol{\rho}))$ (as illustrated in Fig. 7.2) by making a Taylor expansion of the exponent $\Phi(\boldsymbol{\rho})$ around its global maximum $\boldsymbol{\rho}^*$

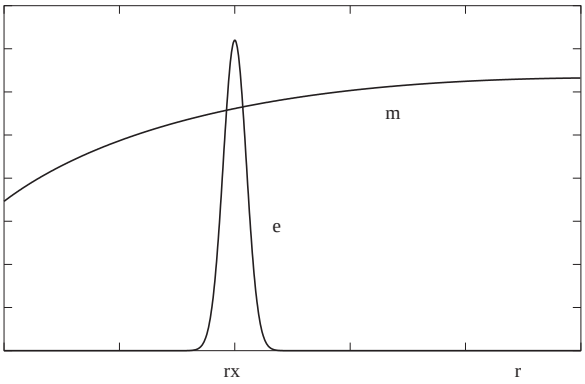

Fig. 7.2. Illustration of the steepest descent method: The flat measure $\mu(\rho)$ compared with the strongly peaked exponential function

$$\int_{\mathbb{R}_+^N} e^{\Phi(\boldsymbol{\rho})}\, f(\boldsymbol{\rho})\, d\boldsymbol{\rho} \approx f(\boldsymbol{\rho}^*) \int_{\mathbb{R}^N} e^{\Phi(\boldsymbol{\rho}^*)+\frac{1}{2}\sum_{i,j}\Delta\rho_i \frac{\partial^2}{\partial\rho_i\partial\rho_j}\Phi\Big|_{\boldsymbol{\rho}^*}\Delta\rho_j}\, d\boldsymbol{\rho}\,. \quad (7.14)$$

This approximation is possible whenever the maximum is sharply peaked and far enough away from the origin to allow the extension of the volume of integration to the entire $\mathbb{R}^N$. All the eigenvalues of the Hessian H_{ij}

$$H_{ij} = -\frac{\partial^2}{\partial\rho_i\partial\rho_j}\Phi\Big|_{\boldsymbol{\rho}^*} \quad (7.15)$$

have to be positive. Otherwise the integral does not converge. Due to the convexity of the function $\Phi(\boldsymbol{\rho})$, this condition is fulfilled in the present case. The steepest descent approximation yields a gaussian integral which is readily evaluated

$$\int_0^\infty e^{\Phi(\boldsymbol{\rho})}\, f(\boldsymbol{\rho})\, d\boldsymbol{\rho} \approx f(\boldsymbol{\rho}^*)\, e^{\Phi(\boldsymbol{\rho}^*)}\, (2\pi)^{N/2}\, |H|^{-1/2}\,. \quad (7.16)$$

7.2.6 Normalization of $p(\boldsymbol{\rho}\,|\,\alpha\, I)$

The application of the steepest descent approximation to the normalization of the entropic prior yields

$$Z(\alpha) = \prod_{i=1}^{N} \frac{1}{\sqrt{m_i}} \sqrt{2\pi\, m_i/\alpha} = (2\pi)^{N/2}\, \alpha^{-N/2}\,, \quad (7.17)$$

and the normalized entropic prior reads

$$p(\boldsymbol{\rho}\,|\,\alpha\, I) = \left(\frac{\alpha}{2\pi}\right)^{N/2} \Big(\prod_i \rho_i^{-\frac{1}{2}}\Big)\, e^{\alpha S}\,. \quad (7.18)$$

If we increase the regularization parameter α, the entropic prior becomes an increasingly narrow peak at $\rho = \mu$. Since the norm is fixed to 1, we eventually have

$$\lim_{\alpha\to\infty} p(\boldsymbol{\rho}\,|\,\alpha\, I) = \delta(\rho - \mu) \quad (7.19)$$

7.2.7 Posterior probability density

Next we discuss the posterior pdf $p(\boldsymbol{\rho}\,|\,\mathbf{d}\, I)$ for $\boldsymbol{\rho}$ in the light of the data $\mathbf{d}$ and prior information I. The marginalization rule yields

$$p(\boldsymbol{\rho}\,|\,\mathbf{d}\, I) = \int p(\boldsymbol{\rho}\,|\,\alpha\,\mathbf{d}\, I)\; p(\alpha\,|\,\mathbf{d}\, I)\, d\alpha\,. \quad (7.20)$$

As a function of α, the first factor $p(\boldsymbol{\rho} \,|\, \alpha\, \mathbf{d}\, I)$ is rather flat whereas $p(\alpha \,|\, \mathbf{d}\, I)$ is strongly peaked even for a fairly small number of five data points. Therefore, we approximate the integral as

$$p(\boldsymbol{\rho} \,|\, \mathbf{d}\, I) \approx p(\boldsymbol{\rho} \,|\, \alpha^* \mathbf{d}\, I) \underbrace{\int p(\alpha \,|\, \mathbf{d}\, I)\, d\alpha}_{=1} = p(\boldsymbol{\rho} \,|\, \alpha^*\, \mathbf{d}\, I)\ . \tag{7.21}$$

As usual, the symbol α^* denotes the peak of $p(\alpha \,|\, \mathbf{d}\, I)$. The approximation used in Eq. (7.21) is called the *evidence approximation*. In order to find the maximum α^*, we have to know the distribution $p(\alpha \,|\, \mathbf{d}\, I)$, that we get as follows

$$\begin{aligned} p(\alpha \,|\, \mathbf{d}\, I) &= \int p(\alpha\, \boldsymbol{\rho} \,|\, \mathbf{d}\, I)\, d\boldsymbol{\rho} = \frac{1}{p(\mathbf{d} \,|\, I)} \int p(\alpha\, \boldsymbol{\rho}\, \mathbf{d} \,|\, I)\, d\boldsymbol{\rho} \\ &= \frac{1}{p(\mathbf{d} \,|\, I)} \int p(\mathbf{d} \,|\, \boldsymbol{\rho}\, \alpha\, I)\, p(\boldsymbol{\rho} \,|\, \alpha\, I)\, p(\alpha \,|\, I)\, d\boldsymbol{\rho} \\ &\propto\ p(\alpha \,|\, I) \int p(\boldsymbol{\rho} | \mathbf{d}\, \alpha\, I)\, d\boldsymbol{\rho} \end{aligned} \tag{7.22}$$

We have used that the probability density $p(\mathbf{d} \,|\, \boldsymbol{\rho}\, \alpha\, I)$ (likelihood) does not depend on α. Since α is scale-parameter $p(\alpha \,|\, I)$ is given by Jeffreys' prior $p(\alpha \,|\, I) \propto 1/\alpha$. The density $p(\boldsymbol{\rho} \,|\, \alpha\, I)$ is given by the entropic prior, as derived above.

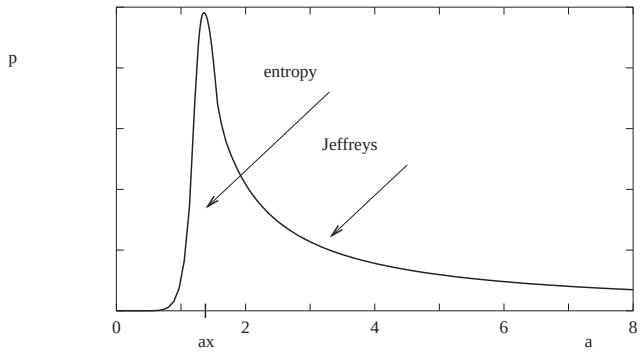

Fig. 7.3. Qualitative behaviour of the function $p(\alpha \,|\, \mathbf{d}\, I)$

In QMC simulations, the model is linear. Then the vector of theoretical data $\mathbf{d}^{\mathrm{th}}$ is obtained by application of a matrix M to the densities $\boldsymbol{\rho}$. Thus, the general form of a QMC model reads

$$\mathbf{d}^{\mathrm{th}}(\boldsymbol{\rho}) \ =\ M \cdot \boldsymbol{\rho}\ . \tag{7.23}$$

A typical example is the above quoted relation between the Greens function and the spectral function, Eq. (7.5).
The deviation of the QMC data from the theoretical prediction is denoted by $\Delta\mathbf{d}$

$$\Delta\mathbf{d} = \mathbf{d} - \mathbf{d}^{\mathrm{th}}(\boldsymbol{\rho}) = \mathbf{d} - M \cdot \boldsymbol{\rho} \,. \tag{7.24}$$

For the QMC data, the likelihood function is the N_d–dimensional multivariate normal distribution

$$p(\mathbf{d} \,|\, \boldsymbol{\rho}\, I) = (2\pi)^{-N_d/2}\, |C|^{1/2}\, e^{-\frac{1}{2}\Delta\mathbf{d}^\dagger C^{-1}\Delta\mathbf{d}} \,. \tag{7.25}$$

The covariance matrix C originates from the errors of the experiment. By substituting this ansatz into Eq. (7.22), we obtain in steepest descent approximation

$$\begin{aligned} p(\alpha \,|\, \mathbf{d}\, I) &= (2\pi)^{-(N_d+N)/2}\, |C|^{1/2}\, \alpha^{N/2-1} \int_0^\infty e^{\overbrace{-\frac{1}{2}\Delta\mathbf{d}^\dagger C^{-1}\Delta\mathbf{d} \,+\, \alpha\, S}^{=:\Phi}} \prod_i \frac{d\rho_i}{\sqrt{\rho_i}} \\ &= (2\pi)^{-N_d/2}\, |C|^{1/2}\, \alpha^{N/2-1}\, |H|^{-1/2}\, \frac{e^{-\Phi^*}}{\prod_i \sqrt{\rho_i^*}} \,. \end{aligned} \tag{7.26}$$

In order to carry out this approximation we have to find the maximum $\boldsymbol{\rho}_i^*$ of the exponent

$$\Phi = -\frac{1}{2} \underbrace{\Delta\mathbf{d}^\dagger C^{-1} \Delta\mathbf{d}}_{\chi^2} + \alpha\, S \tag{7.27}$$

under the positivity constraint. There are a couple of tricks to find the maximum efficiently, but basically it is a modified version of Newton-Raphson.
The quantity χ^2 is called the *misfit* of the data because it is a measure for the deviation of the experimental data from the theoretically predicted data.
At the maximum $\boldsymbol{\rho}_i^*$ the Hessian

$$H_{ij} = -\frac{\partial^2 \Phi}{\partial\rho_i \partial\rho_j} = (M^\dagger C^{-1} M)_{ij} + \frac{\alpha}{\rho_i^*}\, \delta_{ij} \tag{7.28}$$

has to be evaluated. The *posterior* pdf in the evidence approximation is eventually

$$p(\boldsymbol{\rho} \,|\, \mathbf{d}\, I) = p(\boldsymbol{\rho} \,|\, \mathbf{d}\, I\, \alpha^*) = \frac{1}{Z}\, e^{-\frac{1}{2}\chi^2 + \alpha^* S} \,, \tag{7.29}$$

7.3 Examples

In this Section we will illustrate the Maximum Entropy based reconstruction for two different examples. The first example is the inversion of the integral

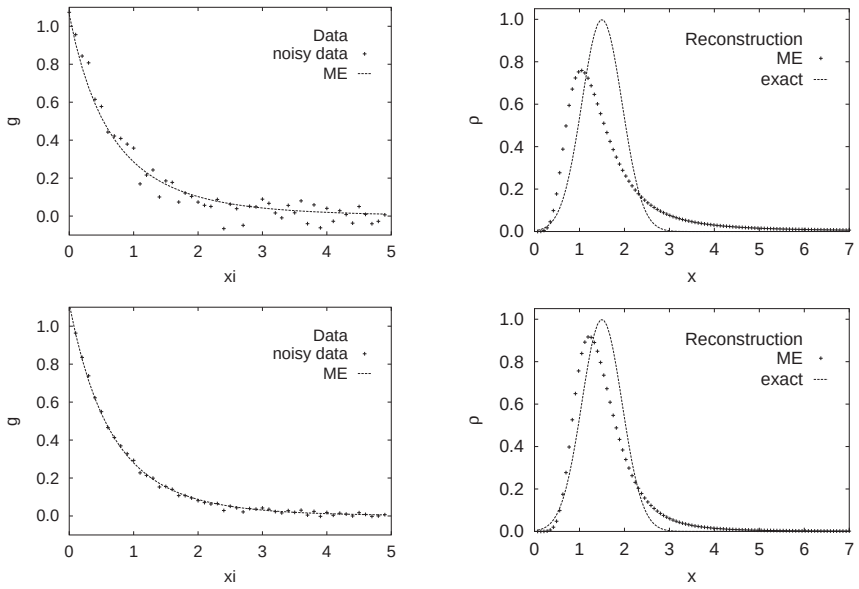

Fig. 7.4. Dependence of the quality of the reconstruction on the noise. The plots at the left–hand side show the data g whose Maximum–Entropy (ME) reconstruction is depicted at the right–hand side. The dashed line at the left–hand side represents g calculated with ρ from the ME reconstruction.

transformation with an exponential kernel. This is a typical problem arising in Quantum Monte Carlo methods. As a second example we will consider an optical application, namely the Abel inversion.

7.3.1 Laplace Transformation

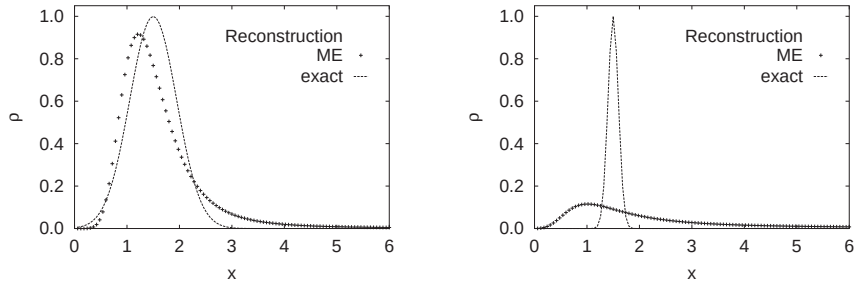

Fig. 7.5. Reconstruction of noisy data. The quality of the reconstruction dependends on the the width of the peak.

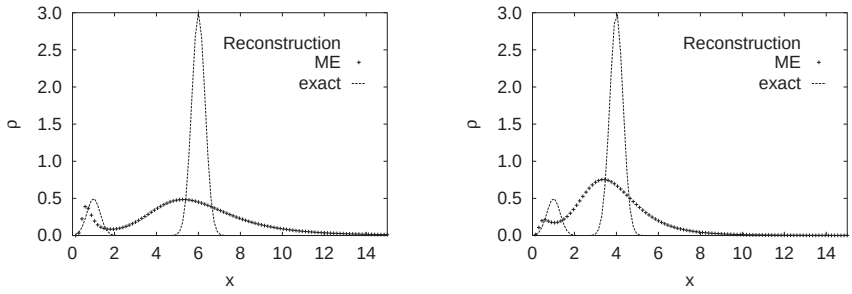

Fig. 7.6. Resolution of two neighbouring peaks. The farther the peaks are separated, the better they are resolved in the reconstruction process.

We assume that the experimental data g are related to the desired physical quantity $\rho(x)$ via the integral

$$g(\xi) = \int_0^\infty e^{-\xi x}\, \rho(x)\, dx\,. \tag{7.30}$$

The data g are given for a set $\xi_1, \ldots, \xi_{N_d}$. The problem is to reconstruct the function $\rho(x)$.
First of all we have to discretize the relation (7.30). The simplest way of doing that is to truncate the integral at $x = x^f$ and then replace it by a finite sum. By introducing a number N of x-knots according to $x_i = (i - 1/2)\, x^f/N$, we obtain

$$\begin{aligned} g_\nu \equiv g(\xi_\nu) &\approx \sum_{i=1}^{N} e^{-\xi_\nu x_i}\, \rho(x_i)\, \Delta x \\ &= \sum_{i=1}^{N} e^{-\xi_\nu x_i}\, \rho_i\, \Delta x\,, \end{aligned} \tag{7.31}$$

with $\rho_i \equiv \rho(x_i)$ and $\Delta x = x^f/N$. Thus the matrix of the model is given by

$$M_{\nu i} = e^{-\xi_\nu x_i}\, \Delta x\,. \tag{7.32}$$

Some results of the Maximum Entropy reconstruction of $\rho(x)$ are shown in Fig. 7.4–7.6. Figure 7.4 illustrates the influence of the noise on the quality of the reconstruction: Due to a higher noise level that can be seen at the left–hand column, the reconstructed peak in the plot in the first row is broarder and smaller than that in the second. Via Eq. (7.31), the reconstruced ρ can be used to obtain a smooth curve approximating the actual data points. This curve is the dashed line in the plots of the left–hand column of Fig. 7.4.
In Fig. 7.5 the influence of the width of a peak on the quality of the reconstruction is depicted. The thinner the peak the poorer the agreement of initial and reconstructed density.

The plots in Fig. 7.6 illustrate the dependence of the resolution of two separated peaks on their separation. Two limiting cases are shown: The reconstructed density of the left–hand plot displays two well separated peaks. In the reconstruction of the right–hand plot, however, the smaller peak is reduced to a shoulder of the bigger one.

7.3.2 Abel Inversion

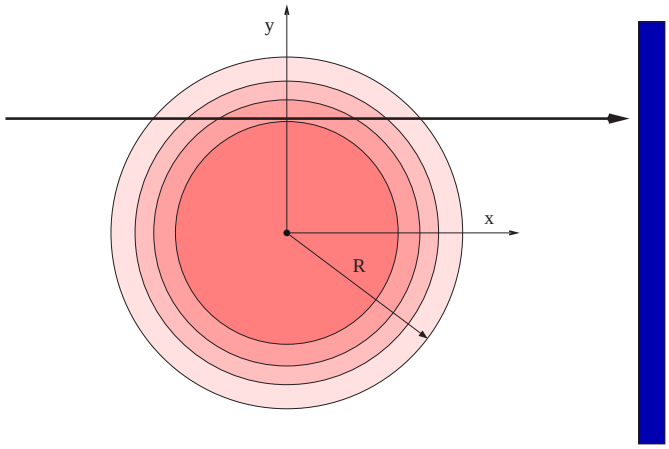

Fig. 7.7. Geometry of the Abel inversion. The density and thus the index of absorption depends only on the radius $r \in [0, R]$.

In this section we illustrate the application of the Maximum Entropy principle to another elementary physical inversion problem, this time in the field of optics. The problem of the Abel inversion presupposes a cylindrically symmetric distribution of an absorbing (or refracting) matter. The data are measured along secants of the absorbant (c.f. Fig. 7.7) where a laser beam penetrates the material.
We assume that the index of absorption is directly proportional to the density denoted by $\rho(r)$, and we suppose that the amount of the absorbed intensity is negligible compared to the laser intensity. Then the problem becomes linear and the absorption is proportional to the integral

$$A(y) = \int_{-\sqrt{R^2-y^2}}^{\sqrt{R^2-y^2}} \rho(\sqrt{x^2+y^2})\, dx\,. \tag{7.33}$$

By performing a simple substitution of variables to rewrite the integral with measure dr, we obtain the expression

$$A(y) = \int_y^R \frac{2r}{\sqrt{r^2 - y^2}}\, \rho(r)\, dr = \int_0^R \Theta(r - y)\, \frac{2r}{\sqrt{r^2 - y^2}}\, \rho(r)\, dr \qquad (7.34)$$

where $\Theta(.)$ denotes the unit step function. Therefore, we have cast our problem in the standard notation for linear models. With the Kernel $K_y(r)$ it reads

$$A(y) = \int_0^R K_y(r)\, \rho(r)\, dr\,, \qquad \text{with} \quad K_y(r) = \Theta(r - y)\, \frac{2r}{\sqrt{r^2 - y^2}}\,. \quad (7.35)$$

The inversion of this integral is very ill posed due to the singularity of the Kernel $K_y(r)$ at the position $r = y$. A sketch of the function $K_y(r)$ for different values of y is given in Fig. 7.8.

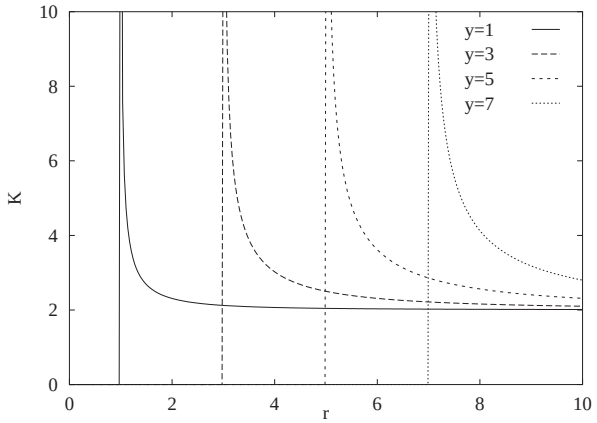

Fig. 7.8. The Kernel $K_y(r)$ of the Abel inversion for different values of y. The points $r = y$ are singularities where the kernel tends towards infinity.

We need a model for the absorbing density. For simplicity we will assume a piecewise constant function of the form

$$\rho(r) = \sum_{j=1}^{N_0} \rho_j\, \chi_j(r)\,. \qquad (7.36)$$

Here χ_j denotes the characteristic function of the interval $[(j–1)R/N_0, jR/N_0)$. The continuity of the density will be accounted for by a spline interpolation. By inserting the model (7.36) into Eq. (7.35), we obtain

$$A(y) = \int_0^R K_y(r)\, \rho(r)\, dr = \int_y^R \frac{2r}{\sqrt{r^2 - y^2}} \sum_{j=1}^{N_0} \rho_j\, \chi_j(r)\,. \qquad (7.37)$$

The integral can be evaluated explicitly, only the bounds of integration deserve a carefull treatment. By exchanging sum and integral, we have

$$A(y) = \sum_{j=1}^{N_0} \rho_j \int_y^R \frac{2r}{\sqrt{r^2 - y^2}} \chi_j(r) = \sum_{j=1}^{N_0} \rho_j \, A_j(y) \tag{7.38}$$

with

$$A_j(y) = \begin{cases} 2\sqrt{r^2 - y^2}\Big|_{r=(j-1)N_0/R}^{jN_0/R} & \dots y \le (j-1)R/N_0 \\ 2\sqrt{(jR/N_0)^2 - y^2} & \dots (j-1)R/N_0 < y \le jR/N_0 \\ 0 & \dots y > jR/N_0 \end{cases} . \tag{7.39}$$

For the discretization of the y variable we choose the simplest possibility and assume an infinitly thin laser beam that yields data at the points

$$y_\nu = \frac{(\nu - 1/2)R}{N_d} , \qquad \nu = 1, \dots, N_d . \tag{7.40}$$

Therefore, the matrix $A_{\nu j} = A_j(y_\nu)$ relating the data with the density reads

$$A_{\nu j} = \begin{cases} 2\sqrt{r^2 - \left(\frac{\nu-1/2}{N_d}\right)^2}\Big|_{r=(j-1)N_0/R}^{jN_0/R} & \dots \frac{\nu-1/2}{N_d} \le \frac{j-1}{N_0} \\ 2\sqrt{\left(\frac{jR}{N_0}\right)^2 - \left(\frac{\nu-1/2}{N_d}\right)^2} & \dots \frac{j-1}{N_0} < \frac{\nu-1/2}{N_d} \le \frac{j}{N_0} \\ 0 & \dots \frac{\nu-1/2}{N_d} > \frac{j}{N_0} \end{cases} . \tag{7.41}$$

In order to obtain the smooth curves for the reconstructed density, an additional spline interpolation of the densities is introduced. The N_0 values of the density are obtained by means of a smooth interpolation from $N < N_0$ density knots.
Since the spline interpolation is linear, it is achieved by means of a matrix $S_{ji}, j = 1, \dots, N_0, \; i = 1, \dots, N$ relating N_0 interpolated density values to N density knots. The actual form of S can be found in [**?**] The matrix M of the model is obtaind by a matrix multiplication and reads

$$M_{\nu i} = \sum_{j=1}^{N_0} A_{\nu j} S_{ji} . \tag{7.42}$$

Some results of the Abel inversion are depicted in Fig. (7.9). The data (left–hand column) have been generated by the direct Abel transformation of the function

$$\rho(r) = r^2 \, (1 - r^2) + \frac{1}{5} \, e^{-250(r-1/4)^2} .$$

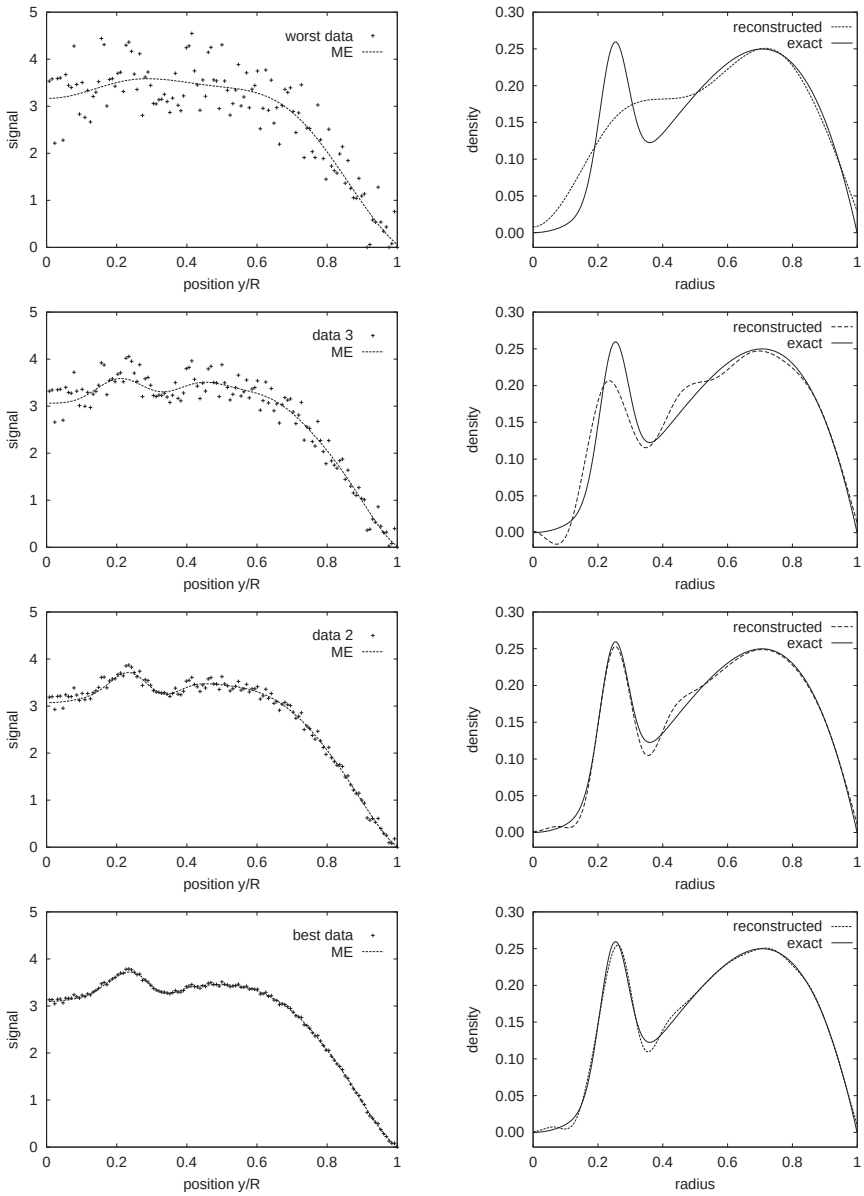

Fig. 7.9. Sampled data and reconstructed densities for four different noise levels.

The noise has been simulated by adding a random error drawn from a normal deviate with zero mean and standard deviation (from top to bottom) of $\sigma = 0.65, 0.46, 0.29, 0.17$, respectively. In all plots the number of data points is $N_d = 128$ and $N_0 = 256$.
For a given number N of density knots, the nuisance parameter α is determined iteratively by resorting to the criterion $\chi^2/N_d \approx 1$. This means that α is adapted in such a way that the mean error of the interpolation approximately equals the standard error of the data points.
The number of intervals N is optimized by maximizing the probability $P(N \,|\, \mathbf{d}, I)$ as explained in the previous Section. This strategy yields $N = 5, 10, 13, 16$, respectively. For N too small, no α can meet the criterion $\chi^2/N_d \approx 1$ because the approximation is too stiff and $\alpha \to 0$. Near the optimal N, the nuisance parameter assumes its maximal value. When increasing N too much, the reconstructed density begins to oscillate as α decreases.