11

Auxiliary Field Quantum Monte Carlo

11.1 Introduction

One of the most important advantages of the Hartree-Fock approach (or more generally any mean-field theory) is that a complete and efficient numerical solution is possible in terms of simple linear algebra operations, possibly including diagonalization of small matrices. However, as discussed in Chapter 1, these techniques, which are based upon independent-electron wave functions, are usually not accurate to describe correlated systems, as for example the Hubbard model. In this respect, projection methods that filter out the ground state by the iterative application of a suitable operator have been introduced; two examples have been discussed in Chapters 8 and 9. Here, we would like to introduce an alternative projection technique, which is particularly suited for the fermionic Hubbard model (Sorella et al., 1989), the so-called auxiliary-field quantum Monte Carlo (AFQMC). The main task of this approach is to reduce the many-body problem to the solution of several mean-field-like calculations, which are affordable by using a stochastic method in the space of Slater determinants. In this way, statistical errors can be controlled, provided the sign problem does not appear during the mentioned transformation; remarkably, this is indeed possible in many interesting cases. Moreover, here, the sign problem is not related to the bosonic-fermionic instability, which has been discussed in section 10.1 since explicitly antisymmetric Slater determinants are sampled within AFQMC) and, therefore, it is often milder than the conventional case, e.g., within the Green's function Monte Carlo, which is defined in configuration space (Fahy and Hamann, 1991).

The general idea is to filter out the ground-state wave function by applying an imaginary-time τ propagation (see section 1.7):

$$\lim_{\tau\to\infty} e^{-\tau\mathcal{H}}|\Psi_0\rangle \propto |\Upsilon_0\rangle, \tag{11.1}$$

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as before, the necessary requirement is to choose an initial state $|\Psi_0\rangle$ such that $\langle\Upsilon_0|\Psi_0\rangle \neq 0$. First of all, as done in section 5.6, we contract the spin index σ and the lattice site i into a single index I running from 1 to $2L$:

$$c_{i,\uparrow} \equiv d_i\,, \tag{11.2}$$

$$c_{i,\downarrow} \equiv d_{i+L}. \tag{11.3}$$

Then, we will specialize to the case in which the Hamiltonian contains kinetic and potential terms:

$$\mathcal{H} = \mathcal{K} + \mathcal{V}, \tag{11.4}$$

where

$$\mathcal{K} = \sum_{I,J} K_{I,J} d_I^\dagger d_J, \tag{11.5}$$

$$\mathcal{V} = U \sum_i n_i n_{i+L}; \tag{11.6}$$

here, we have denoted the densities on site $i = 1, \ldots, L$, for electrons with spin up and down, by:

$$n_i = d_i^\dagger d_i \equiv n_{i,\uparrow} = c_{i,\uparrow}^\dagger c_{i,\uparrow}, \tag{11.7}$$

$$n_{i+L} = d_{i+L}^\dagger d_{i+L} \equiv n_{i,\downarrow} = c_{i,\downarrow}^\dagger c_{i,\downarrow}. \tag{11.8}$$

The kinetic energy is written in terms of a $2L \times 2L$ matrix $\mathbf{K}$; in the simplest case, $K_{i,j} = K_{i+L,j+L} = -t$ if i and j are nearest neighbors and 0 otherwise. In general cases with conserved number of particles, it can be taken as a generic Hermitian matrix. Moreover, extensions to an arbitrary bilinear form in the fermion fields, namely without assuming that the kinetic energy commutes with the number of particles, are also possible within this framework.

In the following, we consider the initial state as a non-interacting wave function with N_e electrons:

$$|\Psi_0\rangle = \prod_{\alpha=1}^{N_e} \left(\sum_I \psi_{I,\alpha} d_I^\dagger \right) |0\rangle, \tag{11.9}$$

which is described by the $2L \times N_e$ matrix $\boldsymbol{\psi}$. This is the general case where the orbitals defined by $\{\psi_{I,\alpha}\}$ do not have a definite spin value (which includes BCS-like states, once a particle-hole transformation has been done on spin-down electrons). By contrast, whenever there is no mixing between spin-up and spin-down components, the matrix $\boldsymbol{\psi}$ can be written in terms of two blocks with dimensions $L \times N_e^\uparrow$ and $L \times N_e^\downarrow$.

In the absence of the interaction term $\mathcal{V}$, the projection technique of Eq. (11.1) can be implemented in a simple and efficient way. Indeed, the one-body propagator

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$\exp(-\tau\mathcal{K})$ transforms an uncorrelated wave function into another state that is still uncorrelated:

$$e^{-\tau\mathcal{K}}|\Psi_0\rangle = \prod_{\alpha=1}^{N_e}\left(\sum_I \psi_{I,\alpha}(\tau)d_I^\dagger\right)|0\rangle, \tag{11.10}$$

where the evolved orbitals are given by:

$$\psi_{I,\alpha}(\tau) = \sum_\beta e^{-\tau\epsilon_\beta}\left(\sum_J \psi_{J,\alpha}U_{J,\beta}^*\right)U_{I,\beta}; \tag{11.11}$$

here $\{\epsilon_\beta\}$ are the eigenvalues of the kinetic term $\mathcal{K}$ and the matrix $\mathbf{U}$ contains its eigenvectors, i.e., $\phi_\beta^\dagger = \sum_I U_{I,\beta}d_I^\dagger$. Therefore, the imaginary-time evolution of a Slater determinant can be conveniently written as a matrix-matrix multiplication of the original $2L \times N_e$ matrix $\boldsymbol{\psi}$ and the $2L \times 2L$ propagation matrix $\mathbf{P}(\tau)$:

$$\boldsymbol{\psi}(\tau) = \mathbf{P}(\tau)\boldsymbol{\psi}, \tag{11.12}$$

where

$$P_{I,J}(\tau) = \sum_\beta e^{-\tau\epsilon_\beta}U_{I,\beta}U_{J,\beta}^*. \tag{11.13}$$

In summary, we have shown that the imaginary-time propagation with only the kinetic operator transforms a Slater determinant into another Slater determinant; in addition, this kind of propagation is achieved by a simple (and efficient) matrix-matrix multiplication. When the interaction term $\mathcal{V}$ is non-zero, the time evolution is no longer so simple, since the application of a many-body propagator $\exp(-\tau\mathcal{H})$ to a Slater determinant does not lead to a single Slater determinant. The AFQMC is based upon the Trotter approximation (Trotter, 1959; Suzuki, 1976a,b), which allows us to express the full evolution $\exp(-\tau\mathcal{H})$ in terms of a sequence of distinct propagations involving either the kinetic or the potential term. Then, the latter one is handled by using the so-called Hubbard-Stratonovich transformation (Hubbard, 1959; Stratonovich, 1957), which replaces a many-body term with a superposition of one-body propagations depending on classical auxiliary variables, which have to be integrated out by means of a stochastic technique.

11.2 Trotter Approximation

Let us consider a small step $\Delta\tau$ in the imaginary-time evolution of Eq. (11.1); then, we can define an effective Hamiltonian $\overline{\mathcal{H}}$ that is close to the original one:

$$\exp\left(-\Delta\tau\overline{\mathcal{H}}\right) = \exp\left(-\frac{\Delta\tau}{2}\mathcal{K}\right)\exp\left(-\Delta\tau\mathcal{V}\right)\exp\left(-\frac{\Delta\tau}{2}\mathcal{K}\right). \tag{11.14}$$

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Indeed, for small values of $\Delta\tau$, a straightforward expansion of both sides of the previous equation allows us to evaluate $\overline{\mathcal{H}}$ as:

$$\overline{\mathcal{H}} = \mathcal{H} + \Delta\tau^2 \mathcal{O}_{\mathrm{Tr}} + \mathcal{O}(\Delta\tau^3), \tag{11.15}$$

where the Hermitian operator $\mathcal{O}_{\mathrm{Tr}}$ is given by:

$$\mathcal{O}_{\mathrm{Tr}} = \frac{1}{12}\left[[\mathcal{K},\mathcal{V}],\mathcal{V}\right] + \frac{1}{24}\left[[\mathcal{K},\mathcal{V}],\mathcal{K}\right]. \tag{11.16}$$

We would like to emphasize that the operator $\mathcal{O}_{\mathrm{Tr}}$ is extensive (i.e., it scales with the number of the sites L). Indeed, given the actual form of the operators $\mathcal{K}$ and $\mathcal{V}$ (which are sums of local operators), the commutator $[\mathcal{K},\mathcal{V}]$ is extensive; more generally, the commutator of two extensive operators is extensive. Therefore, all the properties that we compute with the effective Hamiltonian $\overline{\mathcal{H}}$ at fixed $\Delta\tau$ are related to the ones of the original Hamiltonian $\mathcal{H}$ by a small error in $\Delta\tau^2$. Thus, the error associated to the Trotter decomposition of Eq. (11.14) is perfectly under control, since it can be reduced systematically by decreasing $\Delta\tau$. Moreover, for a given accuracy on thermodynamic quantities (e.g., the energy per site), we do not need to decrease the Trotter time $\Delta\tau$ when increasing the system size, namely, the error associated to the Trotter approximation is size consistent.

11.3 Hubbard-Stratonovich Transformation

The Hubbard-Stratonovich transformation allows us to replace a propagator containing in its exponent two-body interaction terms in the density (or spin), with much simpler one-body propagators. This is obtained at the cost of introducing auxiliary *classical* fields (variables) on each site i, hereafter denoted by $\{\sigma_i\}$. Since $\exp(-\Delta\tau\mathcal{V})$ can be factorized in L terms, each one acting on a single site i, we can focus on every site independently. Let us discuss the decouplings that are usually employed for the repulsive Hubbard model. The simplest example is obtained by using *continuous* auxiliary fields:

$$\exp\left[\frac{g}{2}(n_{i,\uparrow} - n_{i,\downarrow})^2\right] = \int_{-\infty}^{+\infty} \frac{d\sigma_i}{\sqrt{2\pi}} \exp\left[-\frac{1}{2}\sigma_i^2 + \lambda\sigma_i(n_{i,\uparrow} - n_{i,\downarrow})\right], \tag{11.17}$$

with $\lambda^2 = g$. Indeed, in the basis where $(n_{i,\uparrow} - n_{i,\downarrow})$ is diagonal, the r.h.s. of the above equation becomes a standard Gaussian integral, where $(n_{i,\uparrow} - n_{i,\downarrow})$ can be considered just as a number. This transformation can be simplified and extended to *discrete*, i.e., Ising, auxiliary fields $\sigma_i = \pm 1$ by means of the following relation (Hirsch, 1985):

$$\exp\left[\frac{g}{2}(n_{i,\uparrow} - n_{i,\downarrow})^2\right] = \frac{1}{2}\sum_{\sigma_i=\pm 1} \exp\left[\lambda\sigma_i(n_{i,\uparrow} - n_{i,\downarrow})\right], \tag{11.18}$$

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where now $\cosh\lambda = \exp(g/2)$. This expression can be easily proved by expanding $\exp(\lambda n_{i,\sigma})$ and noting that all powers k different from zero contribute with $\lambda^k/k!$ (since $n_{i,\sigma}^k = n_{i,\sigma}$ for $k \geq 1$, as a consequence of the Pauli principle). This fact leads to:

$$\exp(\lambda n_{i,\sigma}) = 1 + \left(e^{\lambda} - 1\right) n_{i,\sigma}. \tag{11.19}$$

Therefore, we have:

$$\exp\left[\frac{g}{2}(n_{i,\uparrow} - n_{i,\downarrow})^2\right] = 1 + \left[\exp\left(\frac{g}{2}\right) - 1\right](n_{i,\uparrow} + n_{i,\downarrow}) + 2\left[1 - \exp\left(\frac{g}{2}\right)\right] n_{i,\uparrow} n_{i,\downarrow}, \tag{11.20}$$

$$\frac{1}{2}\sum_{\sigma_i = \pm 1} \exp\left[\lambda\sigma_i(n_{i,\uparrow} - n_{i,\downarrow})\right] = 1 + (\cosh\lambda - 1)(n_{i,\uparrow} + n_{i,\downarrow}) + 2(1 - \cosh\lambda) n_{i,\uparrow} n_{i,\downarrow}, \tag{11.21}$$

which imply that Eq. (11.18) is indeed verified with $\cosh\lambda = \exp(g/2)$.

The Hubbard-Stratonovich transformation is very useful since it turns a complicated two-body operator, containing in the exponent the square of $(n_{i,\uparrow} - n_{i,\downarrow})$, into a superposition of simple one-body terms, which depend upon an auxiliary field. In particular, by using that $n_{i,\sigma}^2 = n_{i,\sigma}$, the many-body propagator can be recast in a form that is suitable for the Hubbard-Stratonovich transformation:

$$\exp(-\Delta\tau\mathcal{V}) = \exp\left(-\frac{\Delta\tau}{2} U N_e\right) \prod_i \exp\left[\frac{\Delta\tau}{2} U (n_{i,\uparrow} - n_{i,\downarrow})^2\right]. \tag{11.22}$$

In this way, by introducing an independent Ising field $\sigma_i = \pm 1$ for each site, we can write:

$$\exp(-\Delta\tau\mathcal{V}) \propto \sum_{\sigma_i = \pm 1} \exp\left[\lambda \sum_i \sigma_i (n_{i,\uparrow} - n_{i,\downarrow})\right], \tag{11.23}$$

where we have used Eq. (11.18) for $g = U\Delta\tau$, which implies that:

$$\cosh\lambda = \exp\left(\frac{U\Delta\tau}{2}\right). \tag{11.24}$$

In Eq. (11.23), we have omitted an irrelevant constant $\exp(-UN_e\Delta\tau/2)/2^L$, since we assume that the total number of particles N_e is fixed. Therefore, we are now in the position to apply a many-body operator $\exp(-\tau\mathcal{V})$ to the non-interacting state of Eq. (11.9). In fact, by defining:

$$h_\sigma(\lambda) = \lambda \sum_i \sigma_i (n_{i,\uparrow} - n_{i,\downarrow}), \tag{11.25}$$

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such that:

$$\exp(-\Delta\tau\mathcal{V}) \propto \sum_{\sigma_i=\pm 1} \exp\left[h_\sigma(\lambda)\right], \tag{11.26}$$

we obtain:

$$e^{h_\sigma(\lambda)}|\Psi_0\rangle = \prod_{\alpha=1}^{N_e}\left(\sum_I \psi_{I,\alpha}(\lambda)d_I^\dagger\right)|0\rangle, \tag{11.27}$$

where the evolved orbitals are given by:

$$\psi_{I,\alpha}(\lambda) = \begin{cases} \exp(\lambda\sigma_I)\psi_{I,\alpha} & \text{if } I \leq L, \\ \exp(-\lambda\sigma_{I-L})\psi_{I,\alpha} & \text{if } I > L. \end{cases} \tag{11.28}$$

In this way, not only the kinetic term, but also the propagation with the potential energy can be written in terms of a matrix-matrix multiplication, through a diagonal $2L \times 2L$ matrix $\mathbf{V}(\lambda)$:

$$\boldsymbol{\psi}(\lambda) = \mathbf{V}(\lambda)\boldsymbol{\psi}, \tag{11.29}$$

where

$$V_{I,J}(\lambda) = \delta_{I,J}\begin{cases} \exp(\lambda\sigma_I) & \text{if } I \leq L, \\ \exp(-\lambda\sigma_{I-L}) & \text{if } I > L. \end{cases} \tag{11.30}$$

Finally, we would like to remark that there are several other ways for performing the Hubbard-Stratonovich decoupling. For example, the two-body operator can be written as:

$$\mathcal{V} = \frac{U}{2}\sum_i n_i^2 - \frac{UN_e}{2}. \tag{11.31}$$

Then, the propagator $\exp(-\Delta\tau\mathcal{V})$ contains squared one-body operators with a *negative* prefactor; therefore, we can use the transformation of Eq. (11.17) with an *imaginary* constant $\lambda \to i\lambda$. This introduces a *phase problem* in quantum Monte Carlo calculations that can be afforded by using some approximation, e.g., the so-called constrained-path quantum Monte Carlo (Zhang et al., 1995). Remarkably, the phase problem is absent at half filling $N_e = L$. To our knowledge, no systematic studies have been done to identify the most efficient Hubbard-Stratonovich decoupling for a given model, namely the one that minimizes the statistical errors for a given computational time.

11.4 The Path-Integral Representation

Now, we are in the position to compute all the properties of the ground state of the effective Hamiltonian $\overline{\mathcal{H}}$, which can be taken arbitrarily close to the exact

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Hamiltonian, i.e., with an error vanishing as $\Delta\tau^2$. To this purpose we consider the pseudo-partition function:

$$\mathcal{Z} = \langle\Psi_0|e^{-\tau\overline{\mathcal{H}}}|\Psi_0\rangle = \langle\Psi_0|\left[\exp(-\Delta\tau\overline{\mathcal{H}})\right]^{2T}|\Psi_0\rangle, \tag{11.32}$$

where $2T$ is the number of Trotter slices and $\tau = 2T\Delta\tau$. For $T \to \infty$ the many-body state

$$|\Psi_T\rangle = \left[\exp(-\Delta\tau\overline{\mathcal{H}})\right]^{T}|\Psi_0\rangle \tag{11.33}$$

converges to the exact ground state $|\overline{\Upsilon}_0\rangle$ of $\overline{\mathcal{H}}$. Thus, any operator or correlation function $\mathcal{O}$ can be evaluated as:

$$\frac{\langle\overline{\Upsilon}_0|\mathcal{O}|\overline{\Upsilon}_0\rangle}{\langle\overline{\Upsilon}_0|\overline{\Upsilon}_0\rangle} = \lim_{T\to\infty}\frac{\langle\Psi_T|\mathcal{O}|\Psi_T\rangle}{\mathcal{Z}}. \tag{11.34}$$

Then, a path-integral representation can be obtained by replacing in both the numerator and the denominator of Eq. (11.34) the auxiliary-field transformation of Eq. (11.23) for *each* Trotter slice:

$$\mathcal{Z} = \sum_{\sigma_i^q=\pm1}\langle\Psi_0|U_\sigma(2T,0)|\Psi_0\rangle, \tag{11.35}$$

where we have introduced the compact definition of the one-body propagator $U_\sigma(2T,0)$ defined by the auxiliary-field transformation (11.23), which implies a corresponding one-body operator $h_\sigma^q(\lambda) = \lambda\sum_i\sigma_i^q(n_{i,\uparrow} - n_{i,\downarrow})$ for each Trotter slice $1 \le q \le 2T$; here, the field $\sigma_i^q = \pm1$ acquires also a discrete time index q, besides the one associated to the lattice site i. Then, we have that:

$$U_\sigma(2T,0) = \exp\left(-\frac{\Delta\tau}{2}\mathcal{K}\right)\exp\left[h_\sigma^{2T}(\lambda)\right]\exp\left(-\Delta\tau\mathcal{K}\right)\exp\left[h_\sigma^{2T-1}(\lambda)\right]\ldots$$
$$\ldots\exp\left[h_\sigma^{2}(\lambda)\right]\exp\left(-\Delta\tau\mathcal{K}\right)\exp\left[h_\sigma^{1}(\lambda)\right]\left(-\frac{\Delta\tau}{2}\mathcal{K}\right). \tag{11.36}$$

Since $U_\sigma(2T,0)$ is a one-body propagator, when applied to a Slater determinant, it gives back another Slater determinant. Therefore, the quantity $\langle\Psi_0|U_\sigma(2T,0)|\Psi_0\rangle$ can be numerically evaluated for any *fixed* configuration of the Ising fields $\{\sigma_i^q\}$. By using the same fields also in the numerator of Eq. (11.34), we obtain:

$$\frac{\langle\Psi_T|\mathcal{O}|\Psi_T\rangle}{\mathcal{Z}} = \frac{\sum_{\sigma_i^q=\pm1}\langle\Psi_0|U_\sigma(2T,T)\mathcal{O}U_\sigma(T,0)|\Psi_0\rangle}{\sum_{\sigma_i^q=\pm1}\langle\Psi_0|U_\sigma(2T,0)|\Psi_0\rangle}. \tag{11.37}$$

Then, a Monte Carlo scheme can be devised to evaluate the r.h.s. of this equation through the computation of the ratio of the average of two random variables. In particular, we consider the positive weight:

$$\mathcal{W}(\sigma) = |\langle\Psi_0|U_\sigma(2T,0)|\Psi_0\rangle|, \tag{11.38}$$

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such that, the expectation value of any operator or correlation function $\mathcal{O}$ is given by:

$$\frac{\langle \Psi_T|\mathcal{O}|\Psi_T\rangle}{\mathcal{Z}} \approx \frac{\langle\langle \mathcal{O}(\sigma)S(\sigma)\rangle\rangle}{\langle\langle S(\sigma)\rangle\rangle}, \tag{11.39}$$

where $\langle\langle \dots \rangle\rangle$ indicates the statistical average over the distribution defined by the weight (11.38), $S(\sigma)$ is the sign of $\langle \Psi_0|U_\sigma(2T,0)|\Psi_0\rangle$, and

$$\mathcal{O}(\sigma) = \frac{\langle \Psi_0|U_\sigma(2T,T)\mathcal{O}U_\sigma(T,0)|\Psi_0\rangle}{\langle \Psi_0|U_\sigma(2T,T)U_\sigma(T,0)|\Psi_0\rangle}. \tag{11.40}$$

Notice that within the AFQMC technique, the sign (or phase) problem appears whenever $\langle \Psi_0|U_\sigma(2T,0)|\Psi_0\rangle$ has not a definite sign for all the field configurations $\{\sigma_i^q\}$.

All quantities (i.e., random variables and weights) can be computed in polynomial time once the fields σ_i^q are given for each site and time slice q. The forward-propagated state $|\overline{R}_T\rangle = U_\sigma(T,0)|\Psi_0\rangle$ can be written in the same form as in Eq. (11.9) by means of a $2L \times N_e$ matrix:

$$\overline{\mathbf{R}}_T = \mathbf{P}\left(\frac{\Delta\tau}{2}\right)\mathbf{R}_T, \tag{11.41}$$

$$\mathbf{R}_T = \mathbf{V}_T(\lambda)\mathbf{P}(\Delta\tau)\dots\mathbf{P}(\Delta\tau)\mathbf{V}_1(\lambda)\mathbf{P}\left(\frac{\Delta\tau}{2}\right)\boldsymbol{\psi}, \tag{11.42}$$

where $\mathbf{P}(\tau)$ and $\mathbf{V}_q$ are $2L \times 2L$ matrices defined in Eqs. (11.13) and (11.30), for each time slice q, i.e., with fields $\{\sigma_i^q\}$. Notice that, the matrix $\mathbf{R}_T$ can be computed iteratively over the time slices for increasing values of q, by applying matrix-matrix multiplications with $O(8TL^2N_e)$ total operations:

$$\mathbf{R}_{q+1} = \mathbf{V}_{q+1}(\lambda)\mathbf{P}(\Delta\tau)\mathbf{R}_q, \tag{11.43}$$

with the initial condition:

$$\mathbf{R}_1 = \mathbf{V}_1(\lambda)\mathbf{P}\left(\frac{\Delta\tau}{2}\right)\boldsymbol{\psi}. \tag{11.44}$$

The backward-propagated state $\langle \overline{L}_T| = \langle \Psi_0|U_\sigma(2T,T)$ can be computed in an analogous way:

$$\overline{\mathbf{L}}_T = \mathbf{P}\left(-\frac{\Delta\tau}{2}\right)\mathbf{L}_T, \tag{11.45}$$

$$\mathbf{L}_T = \mathbf{P}(\Delta\tau)\mathbf{V}_{T+1}^\dagger(\lambda)\dots\mathbf{P}(\Delta\tau)\mathbf{V}_{2T}^\dagger(\lambda)\mathbf{P}\left(\frac{\Delta\tau}{2}\right)\boldsymbol{\psi}, \tag{11.46}$$

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which can be again computed iteratively:

$$\mathbf{L}_{q-1} = \mathbf{P}(\Delta\tau)\mathbf{V}_q^\dagger \mathbf{L}_q, \tag{11.47}$$

with the initial condition:

$$\mathbf{L}_{2T} = \mathbf{P}\left(\frac{\Delta\tau}{2}\right)\boldsymbol{\psi}. \tag{11.48}$$

Then, the overlap between the two wave functions is just a conventional determinant of an $N_e \times N_e$ matrix:

$$(\overline{\mathbf{L}}_T)^\dagger \overline{\mathbf{R}}_T = (\mathbf{L}_T)^\dagger \mathbf{R}_T = \mathbf{M}, \tag{11.49}$$

which is computable in $O(N_e^3)$ operations by standard numerical libraries. Finally, the quantum expectation value $\mathcal{O}(\sigma)$ of Eq. (11.40) can be also calculated in polynomial time by using the Wick theorem, as shown in section 11.5.

11.4.1 Stable Imaginary-Time Propagation

The imaginary-time evolution of Eqs. (11.42) and (11.46) is defined for an infinite precision arithmetic. Instead, actual computations are affected by truncation errors, which lead to an instability problem when applying the one-body operator to a Slater determinant for large imaginary time τ. Indeed, let us consider the kinetic part of the propagator, for which the evolved orbitals are given by Eq. (11.11). Then, the factor $\exp(-\tau\epsilon_\beta)$ will induce an exponential instability of the algorithm, since all the orbitals will be dominated by the ones corresponding to the lowest eigenvalues; more precisely, in double-precision floating point $1 + 10^{-15} = 1$, and, therefore, whenever $\exp[-\tau(\epsilon_{N_e} - \epsilon_1)] < 10^{-15}$, there will be only $N_e - 1$ linearly independent orbitals within numerical accuracy; this fact leads to a vanishing Slater determinant. In order to overcome this problem, we must take $\Delta\tau$ such that:

$$\Delta\tau(\epsilon_{N_e} - \epsilon_1) \ll \ln 10^{15}. \tag{11.50}$$

Notice that this condition is size consistent, because in a lattice model the single-particle bandwidth is finite in the thermodynamic limit (e.g., it is $4dt$ in the d-dimensional case with nearest-neighbor hopping t). Then, after each short-time evolution, the propagated orbitals can be orthogonalized without loosing information of the Slater determinant. Indeed, by using any linear transformation generated by the matrix $\mathbf{A}$:

$$\psi'_{I,\alpha} = \sum_\beta \psi_{I,\beta} A_{\beta,\alpha}, \tag{11.51}$$

the Slater determinant is not changed, apart from an overall constant $\det \mathbf{A}$, which can be saved and updated during the total propagation. In this context, the

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Gram-Schmidt orthogonalization is the simplest algorithm for this purpose; however, a more efficient one is obtained by applying the Cholesky decomposition. Here, the $N_e \times N_e$ overlap matrix is considered and decomposed:

$$\mathbf{M} = \boldsymbol{\psi}^\dagger \boldsymbol{\psi} = \mathbf{L}^\dagger \mathbf{L}, \tag{11.52}$$

where $\boldsymbol{\psi}$ is now a generic matrix and $\mathbf{L}$ is a lower-triangular matrix. Then, the new orbitals given by:

$$\boldsymbol{\psi}' = \boldsymbol{\psi} \mathbf{L}^{-1} \tag{11.53}$$

will be orthogonal to each other. Indeed, we have that:

$$(\boldsymbol{\psi}')^\dagger \boldsymbol{\psi}' = (\mathbf{L}^\dagger)^{-1} \boldsymbol{\psi}^\dagger \boldsymbol{\psi} \mathbf{L}^{-1} = (\mathbf{L}^\dagger)^{-1} \mathbf{L}^\dagger \mathbf{L} \mathbf{L}^{-1} = \mathbf{1}. \tag{11.54}$$

These orbitals will describe the same determinant apart for an overall constant equal to $\det \mathbf{L}$, which is simple to compute, since it is equal to the product of the diagonal elements of $\mathbf{L}$. In the ground-state technique described here, the normalization of the Slater determinant is an irrelevant constant that does not appear in any physical quantity and, therefore, can be disregarded. After the orthogonalization, another stable propagation can be done without facing any instability problems.

11.5 Sequential Updates

In this section, we describe a simple Markov process that can be used to sample the weight of Eq. (11.38). In particular, for each time slice q, a single Ising variable on the site k is changed. In order to speed up the update, it is important to propose the new values of the auxiliary fields for all sites in a given time slice before moving to the next one. If we flip the field $\sigma_k^q \to -\sigma_k^q$ at the site k (a *sequential* loop over the sites is implied) only the right wave function $|R_q\rangle$ will change in a simple way:

$$|R'_q\rangle = e^{-2\lambda \sigma_k^q (n_{k,\uparrow} - n_{k,\downarrow})} |R_q\rangle = (1 + \lambda_\downarrow n_{k,\downarrow})(1 + \lambda_\uparrow n_{k,\uparrow}) |R_q\rangle, \tag{11.55}$$

where $\lambda_\uparrow = \exp(-2\lambda\sigma_k^q) - 1$ and $\lambda_\downarrow = \exp(2\lambda\sigma_k^q) - 1$. For a proposed flip of the Ising variable, the change of the weight $\mathcal{W}(\sigma) = |\langle L_q | R_q \rangle|$ and the corresponding sign (or phase) $\mathcal{S}(\sigma)$ can be updated by means of the ratio:

$$\mathcal{R}_k^q = \frac{\langle L_q | R'_q \rangle}{\langle L_q | R_q \rangle} = \frac{\langle L_q | (1 + \lambda_\downarrow n_{k,\downarrow})(1 + \lambda_\uparrow n_{k,\uparrow}) | R_q \rangle}{\langle L_q | R_q \rangle}, \tag{11.56}$$

which represents a many-body correlation function computed between two different Slater determinants $\langle L_q|$ and $|R_q\rangle$. Finally, the acceptance probability is obtained by the standard Metropolis algorithm, described in section 3.9; a slightly better scheme, with smaller correlation times and faster equilibration, is given by the

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so-called heat-bath algorithm (Krauth, 2006), where the proposed configuration σ_k' is accepted with probability:

$$A(\sigma_k'|\sigma_k) = \frac{|\mathcal{R}_k^q|}{1+|\mathcal{R}_k^q|}. \tag{11.57}$$

The ratio $\mathcal{R}_k^q$ can be computed in terms of the equal-time Green's function defined by a $2L \times 2L$ matrix:

$$(G_q)_{J,I} = \frac{\langle L_q|d_I^\dagger d_J|R_q\rangle}{\langle L_q|R_q\rangle}. \tag{11.58}$$

In the most general case, $(G_q)_{J,I}$ can be non-zero even for the off-diagonal spin components with $I \leq L$ and $J > L$ or $I > L$ and $J \leq L$, which are present whenever BCS-like wave functions are considered (these elements are related to the anomalous averages, once a particle-hole transformation on the spin-down electrons is performed). Instead, whenever the Slater determinants are factorized into spin-up and spin-down components, $(G_q)_{J,I}$ has a block diagonal form. Having defined the above Green's function, all possible many-body correlation functions between two different determinants can be computed by using the Wick theorem (for the case when *bra* and *ket* states are different).

Let us now compute the Green's function of Eq. (11.58). First of all, the overlap between two Slater determinants is given by the determinant of the corresponding overlap matrix, see Eq. (11.49); for example, the denominator of the r.h.s. of Eq. (11.58) is given by:

$$\langle L_q|R_q\rangle = \det(\mathbf{M}) = \det\left[(\mathbf{L}_q)^\dagger \mathbf{R}_q\right]. \tag{11.59}$$

The numerator can be evaluated in an analogous way, by noticing that it can be written in terms of the overlap between two Slater determinants with $N_e + 1$ electrons:

$$\langle L_q|d_I^\dagger d_J|R_q\rangle = \delta_{I,J}\langle L_q|R_q\rangle - \langle \Psi_J|\Psi_I\rangle, \tag{11.60}$$

with

$$|\Psi_I\rangle = d_I^\dagger|R_q\rangle, \tag{11.61}$$

$$|\Psi_J\rangle = d_J^\dagger|L_q\rangle. \tag{11.62}$$

The new matrix $\mathbf{M}'$ corresponding to the overlap $\langle \Psi_J|\Psi_I\rangle$ can be computed realizing that the extra $N_e + 1$ orbital enter in a particularly simple way:

$$\mathbf{M}' = \begin{pmatrix} \delta_{I,J} & (R_q)_{J,\beta} \\ (L_q)^*_{I,\alpha} & M_{\alpha,\beta} \end{pmatrix} \tag{11.63}$$

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where we have highlighted the contribution of the extra row/column, while all the other matrix elements remain exactly equal to the original $N_e \times N_e$ matrix $\mathbf{M}$. In order to compute the determinant of the above matrix, we use the property that the determinant is unchanged if we add to the left-most column an appropriate linear combination of the other columns. This can be done in a way to cancel all its values but the diagonal one: the coefficients x_β of the linear combination are given by:

$$\sum_\beta M_{\alpha,\beta} x_\beta = -(L_q)^*_{I,\alpha}, \tag{11.64}$$

which leads to:

$$x_\beta = -\sum_\alpha M^{-1}_{\beta,\alpha} (L_q)^*_{I,\alpha}. \tag{11.65}$$

Therefore, we obtain that:

$$\begin{aligned} \det \mathbf{M}' &= \begin{vmatrix} \delta_{I,J} - \sum_{\alpha,\beta} (R_q)_{J,\beta} M^{-1}_{\beta,\alpha} (L_q)^*_{I,\alpha} & (R_q)_{J,\beta} \\ 0 & M_{\alpha,\beta} \end{vmatrix} \\ &= \det \mathbf{M} \times \left[\delta_{I,J} - \sum_{\alpha,\beta} (R_q)_{J,\beta} M^{-1}_{\beta,\alpha} (L_q)^*_{I,\alpha} \right]. \end{aligned} \tag{11.66}$$

By combining this result with Eq. (11.60), we obtain that:

$$(G_q)_{J,I} = \sum_{\alpha,\beta} (R_q)_{J,\beta} M^{-1}_{\beta,\alpha} (L_q)^*_{I,\alpha}, \tag{11.67}$$

which can be cast in a compact form:

$$\mathbf{G}_q = \mathbf{R}_q \mathbf{M}^{-1} \mathbf{L}^\dagger_q. \tag{11.68}$$

This quantity can be evaluated by scratch at the beginning of the calculation by using standard linear algebra operations and then updated whenever a Monte Carlo move is accepted (see below). For stability reasons, it is necessary to perform a re-computation by scratch of the Green's function at selected time slices, e.g., for $q = m \times p$, where m is an integer and p is a fixed small integer.

By performing a similar derivation, we can get the expressions containing four fermion operators:

$$\frac{\langle L_q | d^\dagger_I d_J d^\dagger_K d_N | R_q \rangle}{\langle L_q | R_q \rangle} = (G_q)_{J,I} (G_q)_{N,K} + (G_q)_{N,I} [\delta_{K,J} - (G_q)_{J,K}], \tag{11.69}$$

which allows us to compute the ratio in Eq. (11.56):

$$\mathcal{R}^q_k = [1 + \lambda_\uparrow (G_q)_{k,k}][1 + \lambda_\downarrow (G_q)_{k+L,k+L}] - \lambda_\uparrow \lambda_\downarrow (G_q)_{k+L,k} (G_q)_{k,k+L}; \tag{11.70}$$

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here the last term is only present if the determinants do not factorize into spin-up and spin-down blocks.

Once the trial move $|R_q\rangle \rightarrow |R'_q\rangle$ is accepted, the Green's function must be updated:

$$(G_q)'_{J,I} = \frac{\langle L_q | d_I^\dagger d_J | R'_q \rangle}{\langle L_q | R'_q \rangle}. \tag{11.71}$$

As we will show in the following, this can be done without recomputing it by scratch, but using a simple application of the Wick theorem. Notice that, if the Slater determinants are factorized for spin-up and spin-down electrons, the last term in Eq. (11.70) vanishes and also the updating of the Green's function simplifies. Without assuming a factorized Slater determinant, we obtain the final expression:

$$(G_q)'_{J,I} = (G_q)_{J,I} + a_J^\uparrow (G_q)_{k,I} + a_J^\downarrow (G_q)_{k+L,I}, \tag{11.72}$$

where

$$a_J^\uparrow = \frac{\lambda_\uparrow}{\mathcal{R}_k^q} \left\{ -\overline{(G_q)}_{J,k} + \lambda_\downarrow \left[\overline{(G_q)}_{J,k+L} (G_q)_{k+L,k} - \overline{(G_q)}_{J,k} (G_q)_{k+L,k+L} \right] \right\}, \tag{11.73}$$

$$a_J^\downarrow = \frac{\lambda_\downarrow}{\mathcal{R}_k^q} \left\{ -\overline{(G_q)}_{J,k+L} + \lambda_\uparrow \left[\overline{(G_q)}_{J,k} (G_q)_{k,k+L} - \overline{(G_q)}_{J,k+L} (G_q)_{k,k} \right] \right\}, \tag{11.74}$$

in which $\overline{(G_q)}_{J,I} = (G_q)_{J,I} - \delta_{J,I}$. We would like to mention that whenever the Green's function factorizes into spin up and down components, a much simpler updating, involving each spin part independently, is possible:

$$(G_q)'_{j,i} = (G_q)_{j,i} + a_j^\uparrow (G_q)_{k,i}, \tag{11.75}$$

$$(G_q)'_{j+L,i+L} = (G_q)_{j+L,i+L} + a_{j+L}^\downarrow (G_q)_{k+L,i+L}, \tag{11.76}$$

where now:

$$a_j^\uparrow = -\frac{\lambda_\uparrow}{1 + \lambda_\uparrow (G_q)_{k,k}} \overline{(G_q)}_{j,k}, \tag{11.77}$$

$$a_{j+L}^\downarrow = -\frac{\lambda_\downarrow}{1 + \lambda_\downarrow (G_q)_{k+L,k+L}} \overline{(G_q)}_{j+L,k+L}. \tag{11.78}$$

In summary, the updating scheme for a given time slice q can be done with $O(L^3)$ operations. In order to go from one time slice to the neighboring one, we need to propagate the left Slater determinant $\langle L_q|$ with the matrix-matrix multiplications of Eq. (11.47), which requires again at most $O(L^3)$ operations. Instead, the right Slater determinant $|R_q\rangle$ can be stored at the beginning and saved in memory (otherwise, it can be backward propagated by using Eq. (11.43), i.e., $\mathbf{R}_{q-1} = \mathbf{P}(-\Delta\tau)[\mathbf{V}_q(\lambda)]^{-1}\mathbf{R}_q$). Also the Green's function can be backward propagated from

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time slice q to time slice $q-1$ with analogous matrix-matrix operations. Indeed, from Eq. (11.68) and the propagation of the left and right matrices, we have:

$$\mathbf{G}_{q-1} = \mathbf{P}(-\Delta\tau)[\mathbf{V}_q(\lambda)]^{-1}\mathbf{G}_q\mathbf{V}_q(\lambda)\mathbf{P}(\Delta\tau). \tag{11.79}$$

Thus, a sweep over all the time slices costs at most $O(TL^3)$ operations. Therefore, this algorithm is particularly efficient for ground-state properties since the $T \to \infty$ limit can be reached with a cost that is only linear with the number of time slices.

11.5.1 Delayed Updates

The basic operation in the updating procedure Eq. (11.72) is the rank-1 update of a generic $2L \times 2L$ matrix:

$$(G_q)'_{J,I} = (G_q)_{J,I} + a_J^\sigma b_I^\sigma, \tag{11.80}$$

where a_J^σ is defined in Eqs. (11.73) and (11.74), while $b_I^\uparrow = (G_q)_{k,I}$ and $b_I^\downarrow = (G_q)_{k+L,I}$. As already emphasized in section 5.6, this kind of operation can be computationally inefficient when, for large sizes, the matrix $\mathbf{G}_q$ is not completely contained in the cache of the processor. A way to overcome this drawback is to delay the update of the matrix, without loosing its information. This can be obtained by storing a set of left and right vectors $\mathbf{a}^{(p)}$ and $\mathbf{b}^{(p)}$ with $p = 1, \ldots, 2m$ (including the "spin" index σ), as well as the "initial" matrix, denoted by $\mathbf{G}_q^0$, from which the delayed updates start. Then, the matrix $\mathbf{G}_q$, after m updates is given by:

$$(G_q)_{J,I} = (G_q)^0_{J,I} + \sum_{p=1}^{2m} a_J^{(p)} b_I^{(p)}. \tag{11.81}$$

Every time we accept a new configuration, new vectors $\mathbf{a}^{(m+1)}$, $\mathbf{a}^{(m+2)}$, $\mathbf{b}^{(m+1)}$ $\mathbf{b}^{(m+2)}$ are computed in few operations in term of $\mathbf{G}_q^0$ and the previous vectors with $p = 1, \ldots, 2m$. Notice that, once the matrix $\mathbf{G}_q$ is written in the form of Eq. (11.81), the number of operations required to evaluate the factors in the sum is $O(8mL)$, which is negligible compared to the full update for $m \ll L$.

By performing this kind of delayed update, we can find an optimal $m_{\max}$, for which we can evaluate the full matrix $\mathbf{G}_q$ by a standard matrix multiplication:

$$\mathbf{G}_q = \mathbf{G}_q^0 + \mathbf{A}\mathbf{B}^T, \tag{11.82}$$

where $\mathbf{A}$ and $\mathbf{B}$ are $2L \times 2m_{\max}$ matrices, which are made of the $p = 1, \ldots, 2m_{\max}$ vectors $\mathbf{a}^{(p)}$ and $\mathbf{b}^{(p)}$, respectively. After that, we can continue with a new delayed update with a new $\mathbf{G}_q^0 = \mathbf{G}_q$, by initializing to zero the integer m. The advantage of this updating procedure is that after a cycle of $2m_{\max}$ steps the bulk of the computation is given by the matrix-matrix multiplication in Eq. (11.82), which is

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much more efficient (and is not limited by the dimension of the cache memory) than the $2m_{\max}$ rank-1 updates. For large number of electrons, the delayed update procedure allows us to improve the speed of the Monte Carlo code by about an order of magnitude.

11.6 Ground-State Energy and Correlation Functions

The ground-state energy or any other observable, including correlation functions, can be easily computed by using the Wick theorem that has been discussed in section 11.5. Indeed, let us consider a generic n-body operator:

$$\mathcal{O} = \sum_{I_1,\ldots,I_n} \sum_{J_1,\ldots,J_n} \mathcal{O}_{I_1,\ldots,I_n;J_1,\ldots,J_n} d^\dagger_{I_1} d_{J_1} \ldots d^\dagger_{I_n} d_{J_n}, \tag{11.83}$$

where $d^\dagger_I$ (d_I) creates (destroys) an electron on the site $I = 1,\ldots,2L$. Then, the correlation function of Eq. (11.34) is evaluated by computing $\mathcal{O}(\sigma)$ given by Eq. (11.40), which can be done by using the fact that both $|\overline{R}_T\rangle = U_\sigma(T,0)|\Psi_0\rangle$ and $\langle\overline{L}_T| = \langle\Psi_0|U_\sigma(2T,T)$ are Slater determinants and, therefore, the Wick theorem can be applied.

Finally, it is worth mentioning that the error on the ground-state energy, which is obtained for $T \to \infty$, vanishes as $O(\Delta\tau^4)$. Indeed, given the symmetric Trotter approximation of Eq. (11.14), the effective Hamiltonian $\overline{\mathcal{H}}$ differs from the original one $\mathcal{H}$ by a perturbation that vanishes as $O(\Delta\tau^2)$, see Eq. (11.15). The ground state of $\overline{\mathcal{H}}$, which is obtained by the projection technique of Eq. (11.33), can be related to the exact ground state of $\mathcal{H}$ by using standard perturbation theory, i.e., $|\overline{\Upsilon}_0\rangle = |\Upsilon_0\rangle + \Delta\tau^2|\Upsilon'\rangle + O(\Delta\tau^4)$ (where $|\Upsilon'\rangle$ is orthogonal to $|\Upsilon_0\rangle$). Thus, when computing the expectation value of $\mathcal{H}$ over $|\overline{\Upsilon}_0\rangle$ the leading correction $O(\Delta\tau^2)$ vanishes and we obtain that the leading error is $O(\Delta\tau^4)$.

11.7 Simple Cases without Sign Problem

Let us discuss few examples in which the AFQMC technique does not suffer from the sign problem. First of all, we consider the case of the attractive Hubbard model, i.e., the case with $U < 0$ (and any real kinetic term). In this case, an auxiliary-field transformation is possible with a real field σ_i that is coupled only to the total density $\sigma_i(n_{i,\uparrow}+n_{i,\downarrow}-1)$. Indeed, the discrete transformation of Eq. (11.18) can be modified into:

$$\exp\left[\frac{g}{2}(n_{i,\uparrow}+n_{i,\downarrow}-1)^2\right] = \frac{1}{2}\sum_{\sigma_i=\pm1} \exp\left[\lambda\sigma_i(n_{i,\uparrow}+n_{i,\downarrow}-1)\right], \tag{11.84}$$

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where $\cosh\lambda = \exp(g/2)$ with $g = |U|\Delta\tau$. Then, we take a trial wave function $|\Psi_0\rangle$ with the *same* real orbitals for both spin components, namely $|\Psi_0\rangle = |\Psi_{0,\uparrow}\rangle \bigotimes |\Psi_{0,\downarrow}\rangle$, where:

$$|\Psi_{0,\sigma}\rangle = \prod_{\alpha=1}^{N_e/2} \sum_i \psi_{i,\alpha} c_{i,\sigma}^\dagger |0\rangle. \tag{11.85}$$

In this case, the one-body propagator $U_\sigma(2T,0)$ factorizes into up and down terms, i.e., $U_\sigma(2T,0) = U_\sigma^\uparrow(2T,0) \times U_\sigma^\downarrow(2T,0)$, because the total propagation acts in the same way over the spin-up and the spin-down components of the wave function. The consequence is that the pseudo-partition function $\mathcal{Z}$ of Eq. (11.35) becomes:

$$\mathcal{Z} = \sum_{\sigma_i^q=\pm 1} \left(\langle\Psi_{0,\uparrow}|U_\sigma^\uparrow(2T,0)|\Psi_{0,\uparrow}\rangle\right)^2. \tag{11.86}$$

Therefore, the Monte Carlo weight is strictly positive, being the square of a real number. In summary, the AFQMC has no sign problem for attractive (spin-independent) interactions, for any lattice structure, whenever the number of spin-up particles is exactly equal to the number of spin-down ones.

Another example in which there is no sign problem is the case of the repulsive Hubbard model on bi-partite lattices (e.g., with a kinetic term that only couples opposite sublattices A and B) at half-filling, i.e., when $N_e^\uparrow + N_e^\downarrow = L$. Indeed, we can always map the repulsive model into the attractive one by performing a particle-hole transformation on the spin-down particles:

$$c_{i,\uparrow} \to f_{i,\uparrow}, \tag{11.87}$$

$$c_{i,\downarrow} \to s_i f_{i,\downarrow}^\dagger, \tag{11.88}$$

where $s_i = 1$ ($s_i = -1$) if the site i belongs to the A (B) sublattice; this sign is necessary in order not to change the kinetic term. Then, the number of spin-down electrons is changed by the particle-hole transformation (see section 5.6):

$$u_{i,\uparrow} = f_{i,\uparrow}^\dagger f_{i,\uparrow} = c_{i,\uparrow}^\dagger c_{i,\uparrow} = n_{i,\uparrow}, \tag{11.89}$$

$$u_{i,\downarrow} = f_{i,\downarrow}^\dagger f_{i,\downarrow} = 1 - c_{i,\downarrow}^\dagger c_{i,\downarrow} = 1 - n_{i,\downarrow}, \tag{11.90}$$

which imply that the total number of "new" spin-up electrons is $N_e^\uparrow$, while the total number of "new" spin-down electrons is $L - N_e^\downarrow$. Therefore, based upon the results for the attractive model, we conclude that there is no sign problem when the number of spin-down electrons after the particle-hole transformation is exactly equal to the number of spin-up electrons, namely $N_e^\downarrow + N_e^\uparrow = L$, which is exactly the half-filled condition.

The results for the repulsive Hubbard model with $U/t = 4$ are shown in Fig. 11.1 for $N_e = 42$ on 50 sites. The initial wave function $|\Psi_0\rangle$ is given by the

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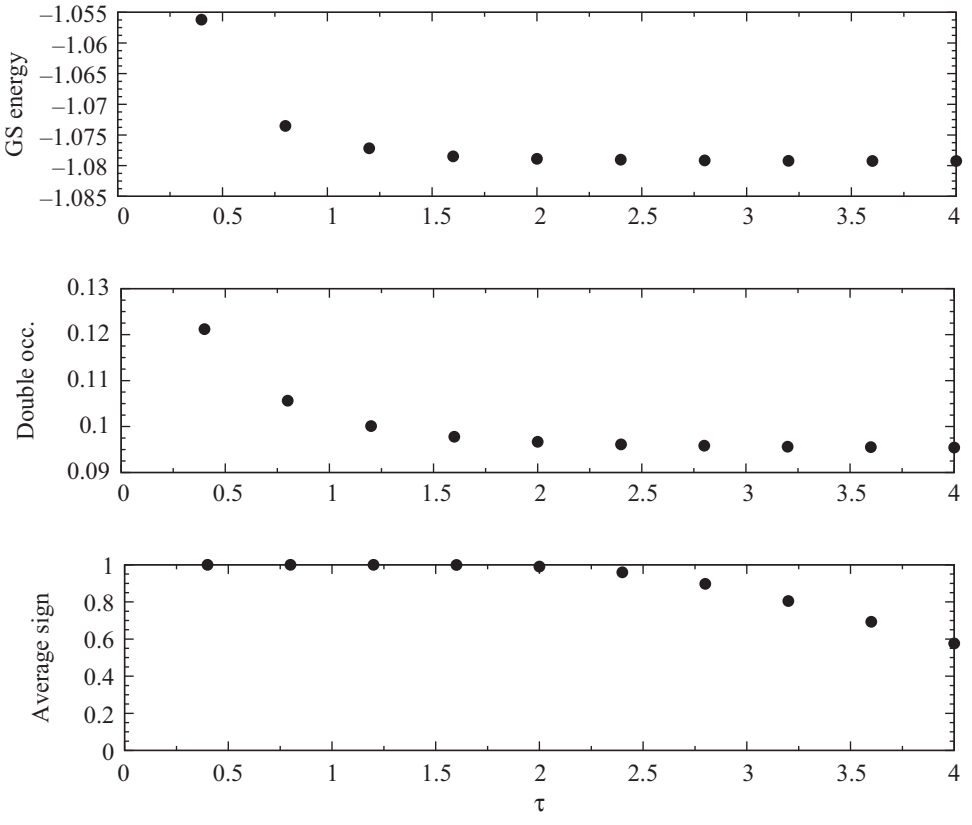

Figure 11.1 Results for the Hubbard model for $N_e = 42$ electrons on 50 sites, with $U/t = 4$; the time discretization in the Trotter approximation is $\Delta\tau = 0.1$ All the quantities are shown as a function of the projection time τ: ground-state energy (upper panel), double occupations $D = 1/L \sum_i n_{i,\uparrow} n_{i,\downarrow}$ (middle panel), and average sign (lower panel).

non-interacting one, which corresponds to a closed-shell configuration (i.e., there is a finite-size gap between the highest occupied and the lowest unoccupied levels). We show the results for the ground-state energy, double occupations $D = 1/L \sum_i n_{i,\uparrow} n_{i,\downarrow}$, and also the average sign $\langle\langle S(\sigma)\rangle\rangle$ along the simulation. We remark that, in this case, a fast convergence to the exact values is obtained as a function of the projection time τ (the discretization time associated to the Trotter decomposition is $\Delta\tau = 0.1$). We would like to emphasize that, given the closed-shell condition, the average sign remains close to 1 up to $\tau \approx 2$ and falls down to 0 very slowly, allowing a precise evaluation of the physical quantities.

Finally, we would like to mention that a sign-free decoupling is possible also when long-range interactions are present (on bi-partite lattices). Indeed, let us take:

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$$\mathcal{V}_{\mathrm{LR}} = \sum_{l,k} U_{l,k}(n_l - 1)(n_k - 1); \tag{11.91}$$

then, we can consider the following Hubbard-Stratonovich transformation for the many-body propagator:

$$\exp\left(-\Delta\tau\,\mathcal{V}_{\mathrm{LR}}\right) = \int \mathbf{d}\boldsymbol{\rho}\,\exp\left[-\frac{1}{2}\sum_{l,k}\rho_l U^{-1}_{l,k}\rho_k + i\sqrt{\Delta\tau}\sum_k \rho_k(n_k - 1)\right], \tag{11.92}$$

where the only constraint is given by the fact that $\mathbf{U}$ must be a positive-definite matrix. Therefore, whenever the kinetic term acts separately on electrons with up and down spin, the propagator is factorized. Moreover, by performing the particle-hole transformation of Eqs. (11.87) and (11.88), we immediately obtain that the spin-up and spin-down propagators are one the complex conjugated of the other, thus leading to a positive weight:

$$\mathcal{Z} = \sum_{\sigma_i^q = \pm 1} \left|\langle \Psi_{0,\uparrow} | U_\sigma^\uparrow(2T, 0) | \Psi_{0,\uparrow}\rangle\right|^2. \tag{11.93}$$

11.8 Practical Implementation

Here, we would like to sketch the important steps in a practical implementation of the auxiliary-field quantum Monte Carlo algorithm.

1. **Initialization** at the beginning of the calculation.
   - Before starting, we have to decide the total number of Trotter slices $2T$ and the number p of time slices between two consecutive orthogonalizations (with the Cholesky algorithm). In particular, p should be chosen small enough to guarantee a sufficient accuracy of the calculation, which can be systematically tested by decreasing p ($p = 1$ being the most accurate case).
   - Start with randomly generated Ising fields for each site and time slice $\sigma_i^q = \pm 1$. The $2L \times 2L$ matrices $\mathbf{P}(\pm\Delta\tau)$ and $\mathbf{P}(\pm\Delta\tau/2)$ must be computed at the beginning and stored in memory by means of Eq. (11.13). Instead, the diagonal matrices $\mathbf{V}_q(\lambda)$ do not need to be stored, since all the calculations can be done efficiently by using the fact that these matrices are diagonal (a diagonal matrix times a full matrix costs only $4L^2$ operations).
2. **Initial propagation**.
   - Propagate forward $\mathbf{R}_q$ for $q = 1, \ldots, 2T$ by using Eq. (11.43) and, for stability reasons, orthogonalize the propagation each p steps; save, in the computer memory, the associated $2L \times N_e$ matrices corresponding to the wave function $|R_q\rangle$ for $q = k \times p$ (where k is an integer). Arrived at the final interval $q = 2T$,

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initialize the back-propagated wave function $\mathbf{L}_{2T}$ of Eq. (11.48) and compute the Green's function $\mathbf{G}_{2T}$ of Eq. (11.68) by scratch.

3. **Markov process** with the Metropolis algorithm.
   - At the time slice q, the sweep on the sites $i = 1, \ldots 2L$ begins. At each step, we can use Eq. (11.70) to compute the ratio between the new and old weights. Then, either the Metropolis algorithm or the heat-bath one can be used to generate a Markov process. Whenever the proposed configuration is accepted, the Green's function is updated according to Eq. (11.72). Delayed updates can be also used for an improved performances with large-size calculations.
   - At the end of the sweep over the lattice sites, we change the backward propagated state from q to $q - 1$, by using Eq. (11.47). Notice that, after p propagations a Cholesky orthogonalization has to be employed for stability reasons. At this stage, it is also necessary to propagate the Green's function according to Eq. (11.79). Only when $\mathbf{L}_q$ is orthogonalized, we compute the Green's function by scratch (by using $\mathbf{R}_q$ that have been saved in the initialization).
   - Go back to the initial propagation and continue the Monte Carlo procedure in order to accumulate statistics. Notice that a minor improvement of the algorithm is to reverse back the direction of the sweep, namely going from $q = 1$ to $q = 2T$, so that the initial propagation can be avoided. This approach typically saves approximately 10% of the total amount of computation.
4. **Computation of observables**.

   Observables (i.e., the total energy) can be computed along the sweeps over the time slices. In particular, for $q \approx T$ (i.e., around the middle interval) we get the expectation value over the state $|\Psi_T\rangle$ of Eq. (11.33). In this case, we should remind that the Green's function $\mathbf{G}_q$ that is used to compute correlation functions has to be propagated by half-time with the kinetic energy:

$$\mathbf{G}_q \to \mathbf{P}\left(\frac{\Delta\tau}{2}\right)\mathbf{G}_q\mathbf{P}\left(-\frac{\Delta\tau}{2}\right), \tag{11.94}$$

   which is particularly important for computing physical quantities with a sufficiently small Trotter error.

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