7

Time-Dependent Variational Monte Carlo

7.1 Introduction

Variational calculations are usually limited to study the ground-state and low-energy states, as discussed in Chapter 1. Here, we present a straightforward generalization of the variational principle to consider non-equilibrium properties of strongly correlated systems. In this regard, the simplest example is given by the time-dependent Hartree-Fock approach, which has been introduced by Dirac (1930) at the dawn of quantum mechanics (Ring and Schuck, 2004). In the following, we present the formalism for a real-time variational approach that is able to incorporate the Jastrow factor (Carleo et al., 2012, 2014); the method has been further generalized to incorporate a time-dependent fermionic part (Ido et al., 2015).

In principle, a time-dependent approach would require solving the full many-body Schrödinger equation:

$$i\frac{d}{dt}|\Phi(t)\rangle = \mathcal{H}|\Phi(t)\rangle, \tag{7.1}$$

where $|\Phi(t)\rangle$ is the wave function at time t. The formal solution (here, we assume that the Hamiltonian does not depend upon time) is given by:

$$|\Phi(t)\rangle = e^{-i\mathcal{H}t}|\Phi(0)\rangle. \tag{7.2}$$

However, an exact treatment of the time evolution is possible only for small systems, since the Hilbert space grows exponentially as the system size increases and, therefore, approximated techniques are needed. In this regard, the time-dependent Hartree-Fock approximation is not accurate for interacting many-body systems because it drastically underestimate correlation effects. In the recent past, few numerical methods have been developed to treat large systems accurately, as time-dependent density matrix renormalization group (White and Feiguin, 2004; Daley et al., 2004) and non-equilibrium dynamical mean-field theory (Aoki et al., 2014). However, both these methods have severe difficulties in treating

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large systems in two or three dimensions. Therefore, alternative techniques are needed and the time-dependent extension of the variational Monte Carlo approach represents a suitable way to follow the exact dynamics of correlated wave functions.

7.2 Real-Time Evolution of the Variational Parameters

The heart of our variational approach is the definition of the time-dependent wave function. Here, we will consider bosonic problems only, where the quantum state has the form of a time-dependent Jastrow factor, but the generalization to fermionic systems is straightforward and can be done by considering a time-dependent Slater determinant (Ido et al., 2015). Therefore, we take:

$$\Psi(x,t) = \langle x|\Psi(t)\rangle = \exp\left[\sum_k \alpha_k(t)\mathcal{O}_k(x)\right]\zeta(x), \tag{7.3}$$

where $\zeta(x)$ is a time-independent bosonic state and $\alpha_k(t) = \alpha_k^R(t) + i\alpha_k^I(t)$ are *complex* variational parameters coupled to the real local excitation operators $\mathcal{O}_k$, which are taken to be diagonal in the chosen basis, i.e., $\langle x|\mathcal{O}_k|x'\rangle = \delta_{x,x'}\mathcal{O}_k(x)$. Among the set of the operators $\{\mathcal{O}_k\}$, we include the identity $\mathcal{O}_{k=0} = \mathbb{I}$, thus $\alpha_0^R(t)$ allows us to fulfill the normalization condition of $\Psi(x,t)$ and $\alpha_0^I(t)$ to pick up an arbitrary phase factor during the real time dynamics.

The time evolution of this quantum state is governed by $\alpha_k(t)$, whose trajectories in time are fixed by a set of differential equations such to minimize the "distance" between the approximate and the exact states in the Hilbert space; equivalently, the same set of equations may be also obtained from the principle of stationary action as it will be described in the following.

7.2.1 Minimal Hilbert Space Distance

From the one hand, starting at a given time t, the *exact* infinitesimal real-time evolution of $\Psi(x,t)$ is given by:

$$\Phi(x,t+\epsilon) = \Psi(x,t)\left[1 - i\epsilon e_L(x,t)\right] + O(\epsilon^2), \tag{7.4}$$

where

$$e_L(x,t) = e_L^R(x,t) + ie_L^I(x,t) = \frac{\langle x|\mathcal{H}|\Psi(t)\rangle}{\langle x|\Psi(t)\rangle} \tag{7.5}$$

is the complex-valued local energy for a given set of variational parameters and for a given many-body configuration $|x\rangle$. On the other hand, an infinitesimal variation of the variational wave function due to the change of parameters is given by:

$$\Psi(x,t+\epsilon) = \Psi(x,t)\left[1 + \sum_k \delta\alpha_k(t)\mathcal{O}_k(x)\right] + O(\epsilon^2), \tag{7.6}$$

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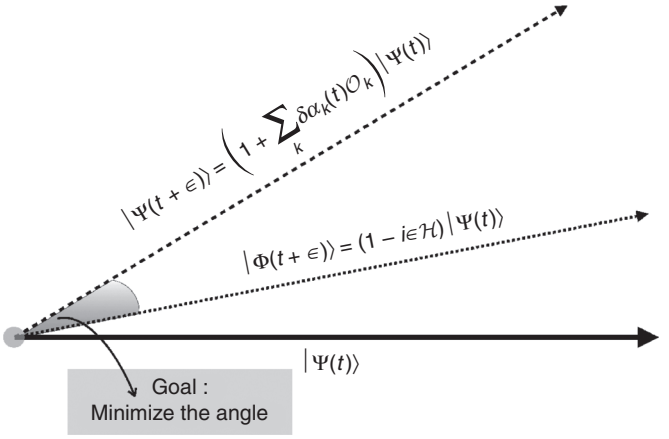

Figure 7.1 Pictorial representation of the infinitesimal real-time evolution of $|\Psi(t)\rangle$ (represented by a vector in the Hilbert space, solid arrow). The exact time evolved state is given by $|\Phi(t+\epsilon)\rangle$ (dotted arrow) and the approximated one is given by $|\Psi(t+\epsilon)\rangle$ (dashed arrow). The best "variational" state is obtained by minimizing the distance between these two states.

where $\delta\alpha_k(t)$ are small, i.e., $O(\epsilon)$, complex variables. Therefore, in order to obtain the optimal changes $\delta\alpha_k(t)$ of the variational parameters in the small-time interval considered, we can minimize the Euclidean distance $\Delta_\epsilon(t)$ between the exact time evolved state $\Phi(x, t+\epsilon)$ and our approximate *Ansatz* $\Psi(x, t+\epsilon)$, see Fig. 7.1:

$$\Delta_\epsilon^2(t) = \sum_x |\Psi(x, t+\epsilon) - \Phi(x, t+\epsilon)|^2 . \tag{7.7}$$

This quantity is conveniently written as an expectation value over the square-modulus of the wave function as:

$$\Delta_\epsilon^2(t) = \sum_x |\Psi(x,t)|^2 \left| i\epsilon e_L(x,t) + \sum_k \delta\alpha_k(t)\mathcal{O}_k(x) \right|^2 . \tag{7.8}$$

By using the Euler minimum condition:

$$\frac{d}{d\alpha_k^*(t)}\Delta_\epsilon^2(t) = 0, \tag{7.9}$$

we obtain:

$$\sum_{k'} \langle \mathcal{O}_{k'}\mathcal{O}_k\rangle_t \delta\alpha_{k'}(t) = -i\epsilon\langle \mathcal{O}_k e_L(t)\rangle_t, \tag{7.10}$$

which is correct up to $O(\epsilon^2)$; here, the symbol $\langle \dots \rangle_t$ indicates the average over square-modulus $|\Psi(x,t)|^2$:

$$\langle \mathcal{O}_k\mathcal{O}_{k'}\rangle_t = \sum_x |\Psi(x,t)|^2 \mathcal{O}_k(x)\mathcal{O}_{k'}(x) = \langle \Psi(t)|\mathcal{O}_k\mathcal{O}_{k'}|\Psi(t)\rangle, \tag{7.11}$$

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$$\langle \mathcal{O}_k e_L(t)\rangle_t = \sum_x |\Psi(x,t)|^2 \mathcal{O}_k(x) e_L(x,t) = \langle \Psi(t)|\mathcal{O}_k \mathcal{H}|\Psi(t)\rangle, \tag{7.12}$$

which can be easily implemented numerically by the standard variational Monte Carlo technique.

At this stage we can take the limit $\epsilon \to 0$ by introducing time derivatives of the variational parameters:

$$\dot{\alpha}_k(t) = \lim_{\epsilon \to 0} \frac{\delta\alpha_k(t)}{\epsilon}. \tag{7.13}$$

Furthermore, by taking the explicit dependence upon the real and imaginary parts of $\delta\alpha_k(t)$ in Eq. (7.10), we obtain closed differential equations for $\dot{\alpha}_k^R(t)$ and $\dot{\alpha}_k^I(t)$:

$$\sum_{k'} \langle \mathcal{O}_k \mathcal{O}_{k'}\rangle_t \dot{\alpha}_{k'}^R(t) = \langle \mathcal{O}_k e_L^I(t)\rangle_t, \tag{7.14}$$

$$\sum_{k'} \langle \mathcal{O}_k \mathcal{O}_{k'}\rangle_t \dot{\alpha}_{k'}^I(t) = -\langle \mathcal{O}_k e_L^R(t)\rangle_t; \tag{7.15}$$

these differential equations minimize $\Delta_\epsilon^2(t)$ in the limit $\epsilon \to 0$.

Numerically it is very important to be as close as possible to the continuous limit, because only in this case the linearized evolution in Eq. (7.4) becomes a proper propagation, and non-unitary terms consistently vanish for $\epsilon \to 0$. It should be noted that the solution of Eq. (7.10) also guarantees that in the short-time propagation the expectation values of the operators $\mathcal{O}_k$ remain close (i.e., up to $O(\epsilon^2)$) to the exact dynamics:

$$\langle \Psi(t+\epsilon)|\mathcal{O}_k|\Psi(t+\epsilon)\rangle \approx \langle \Phi(t+\epsilon)|\mathcal{O}_k|\Phi(t+\epsilon)\rangle. \tag{7.16}$$

We want to finish this part by showing a more explicit form of the differential equations (7.14) and (7.15) that highlights the part related to the norm and the global phase of the time-dependent wave function. Given that $\mathcal{O}_{k=0} = \mathbb{I}$, we can simplify Eqs. (7.14) and (7.15) and decouple the equations for $\alpha_0(t)$ from the others:

$$\sum_{k'>0} S_{k,k'} \dot{\alpha}_{k'}^R = \langle \mathcal{O}_k e_L^I(t)\rangle_t, \tag{7.17}$$

$$\sum_{k'>0} S_{k,k'} \dot{\alpha}_{k'}^I = -\langle \mathcal{O}_k e_L^R(t)\rangle_t + \langle e_L^R(t)\rangle_t \langle \mathcal{O}_k\rangle_t, \tag{7.18}$$

where $S_{k,k'} = \langle \mathcal{O}_k \mathcal{O}_{k'}\rangle_t - \langle \mathcal{O}_k\rangle_t \langle \mathcal{O}_{k'}\rangle_t$ and $\langle e_L^I(t)\rangle_t = 0$. In addition, the equations for $\alpha_0(t)$ read:

$$\dot{\alpha}_0^R(t) = -\sum_{k'>0} \langle \mathcal{O}_{k'}\rangle_t \dot{\alpha}_{k'}^R(t), \tag{7.19}$$

$$\dot{\alpha}_0^I(t) = -\langle e_L^R(t)\rangle_t - \sum_{k'>0} \langle \mathcal{O}_{k'}\rangle_t \dot{\alpha}_{k'}^I(t). \tag{7.20}$$

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7.2.2 Principle of Stationary Action

The equations of motion for the variational parameters can be also derived from an alternative approach, based on the principle of stationary action. In order to proceed, we introduce the action:

$$\mathcal{S} = \int dt \langle \Psi(t)| \left(i\frac{\partial}{\partial t} - \mathcal{H} \right) |\Psi(t)\rangle, \tag{7.21}$$

which is a functional of the variational parameters $\alpha_k(t)$. Notice that the assumption of a normalized wave function $\Psi(x,t)$ implies that the action $\mathcal{S}$ is real. As well known, the real exact dynamics can be obtained by taking the stationary solution of $\mathcal{S}$, namely:

$$\frac{\delta \mathcal{S}}{\delta \Psi^*(x,t)} = 0, \tag{7.22}$$

among all possible variations of $\Psi(x,t)$. In the following, we will show that the principle of stationary action can be extended to a variational *Ansatz* and allows the optimal choice for the time evolution of the variational parameters derived in the previous section. When the variational wave function is restricted to the form of Eq. (7.3), the action can be easily expressed in terms of $\dot{\alpha}_k(t)$ and reads:

$$\mathcal{S} = \int dt \langle \Psi(t)| \left(i \sum_{k'} \dot{\alpha}_{k'}(t) \mathcal{O}_{k'} - \mathcal{H} \right) |\Psi(t)\rangle. \tag{7.23}$$

The stationary condition for a normalized wave function parametrized by a set of complex parameters $\alpha_k(t)$ is given by:

$$\frac{\delta \mathcal{S}}{\delta \alpha_k^*(t)} = 0. \tag{7.24}$$

By using the definition of $|\Psi(t)\rangle$ given in Eq. (7.3), we notice that the dependence on $\alpha_k^*(t)$ in $\mathcal{S}$ is given only in $\langle \Psi(t)|$ and, therefore, we immediately get the stationary condition:

$$\langle \Psi(t)| \left(i \sum_{k'} \mathcal{O}_k \mathcal{O}_{k'} \dot{\alpha}_{k'} - \mathcal{O}_k \mathcal{H} \right) |\Psi(t)\rangle = 0, \tag{7.25}$$

which is clearly equivalent to Eq. (7.10) in the continuous limit $\epsilon \to 0$.

7.2.3 Norm and Energy Conservation

The differential equations (7.14) and (7.15) define a real-time dynamics of the variational states that preserves both the norm and the energy. As far as the norm of the wave function is concerned, we have that:

$$N(t) = \sum_x |\Psi(x,t)|^2, \tag{7.26}$$

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whose time-derivative is given by:

$$\dot{N}(t) = 2\left[\dot{\alpha}_0^R(t) + \sum_{k>0}\langle \mathcal{O}_k\rangle_t \dot{\alpha}_k^R(t)\right], \tag{7.27}$$

which vanishes, as a direct consequence of Eq. (7.19).

Moreover, the energy is given by:

$$E(t) = \sum_x |\Psi(x,t)|^2 e_L(x,t). \tag{7.28}$$

The time-derivative can be easily found:

$$\dot{E}(t) = 2\sum_k \left(\dot{\alpha}_k^R(t)\langle \mathcal{O}_k e_L^R\rangle_t + \dot{\alpha}_k^I(t)\langle \mathcal{O}_k e_L^I\rangle_t\right), \tag{7.29}$$

which also vanishes, given Eqs. (7.14) and (7.15).

7.2.4 Real-Time Variational Monte Carlo

Given the correlated nature of the variational wave function, a crucial point is to provide a reliable solution of the differential equations (7.14) and (7.15). The variational Monte Carlo method allows us for a numerically exact solution for the variational trajectories. Indeed, at each time t for a set of variational parameters $\{\alpha_k(t)\}$, the square modulus of the wave function $|\Psi(x,t)|^2$ can be straightforwardly interpreted as a probability distribution over the Hilbert space spanned by the configurations $|x\rangle$ and a Markov process can be devised, whose stationary equilibrium distribution coincides with the desired measure. All expectation values that enter into Eqs. (7.17) and (7.18) are computed as statistical averages over the random walk. Then, after a suitable number of Monte Carlo steps, the linear system of differential equations can be solved in order to obtain the first-order derivatives of the variational parameters, which can be in turn integrated by means of standard algorithms for first-order differential equations. To give the new set of parameters $\{\alpha_k(t+\epsilon)\}$. This procedure is iterated from the initial time until the final one is reached.

7.3 An Example for the Quantum Quench in One Dimension

Here, we would like to present a simple application of the time-dependent variational methodology that we have described in the previous sections. In particular, we show the spreading of density-density correlations in the Bose-Hubbard model after a sudden quench of the interaction strength U, from $U = U_{\text{init}}$ to $U = U_{\text{fin}}$. In particular, we consider the one-dimensional model defined by:

$$\mathcal{H} = -J\sum_i b_i^\dagger b_{i+1} + \text{h.c.} + \frac{U}{2}\sum_i n_i(n_i - 1), \tag{7.30}$$

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where $b_i^\dagger$ (b_i) creates (destroys) a boson on site i, and $n_i = b_i^\dagger b_i$ is the density of bosons on site i; periodic-boundary conditions are assumed on the chain with L sites, such that $b_{L+1}^\dagger \equiv b_1^\dagger$. Notice that, here, the hopping amplitude is denoted by J, in order not to confuse it with the time t.

The initial state at $t = 0$, is the best variational Jastrow wave function for $U = U_{\text{init}}$, then the real-time evolution of this state is performed according to the Hamiltonian (7.30) with $U = U_{\text{fin}}$, according to Eq. (7.10). In the numerical calculations, we use a sufficiently small time-step $\epsilon = 0.01$ and a fourth-order Runge-Kutta integration scheme, which conserves the energy with a very small systematic error of the order of one part in a thousand, for times up to $t = 100$ (Carleo et al., 2014). We consider the case with one boson per site in average, i.e., $\sum_i n_i = L$ and examine the evolution of the density-density correlation function:

$$N(r,t) = \frac{1}{L}\sum_i \left(\langle\Psi(t)|n_{i+r}n_i|\Psi(t)\rangle - \langle\Psi(0)|n_{i+r}n_i|\Psi(0)\rangle\right). \tag{7.31}$$

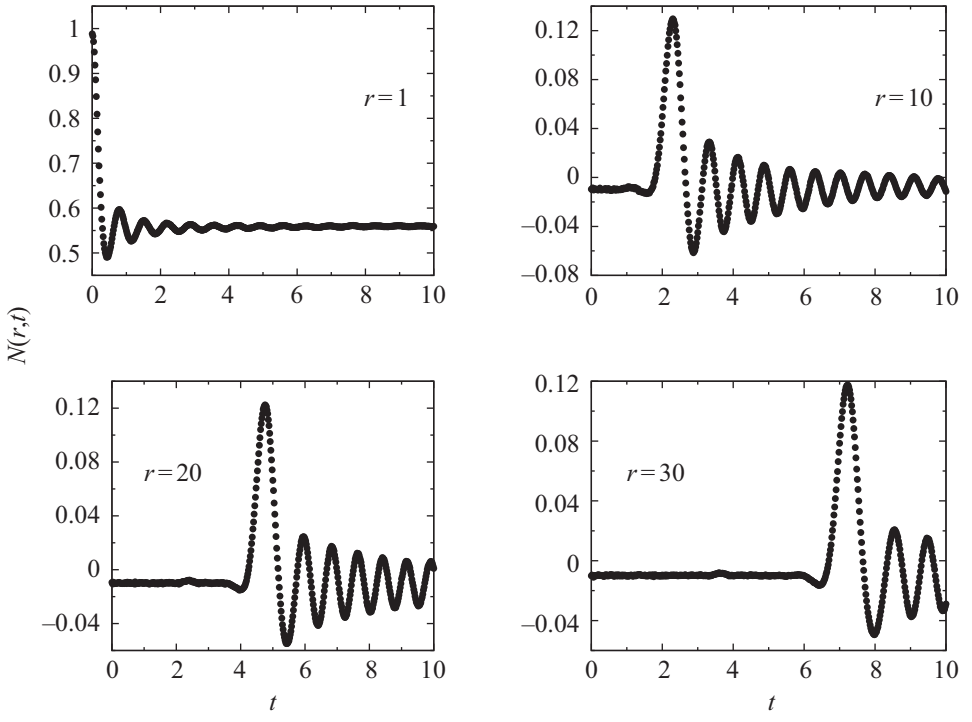

Figure 7.2 Time evolution of the density-density correlations $N(r,t)$, given by Eq. (7.31), for $r = 1$, 10, 20, and 30. The calculations are performed for the Bose-Hubbard model with $L = 100$ sites with periodic-boundary conditions with one boson per site in average. The initial state is the ground state for $U_{\text{init}} = 0$, the time evolution is done for $U_{\text{fin}}/J = 3$.

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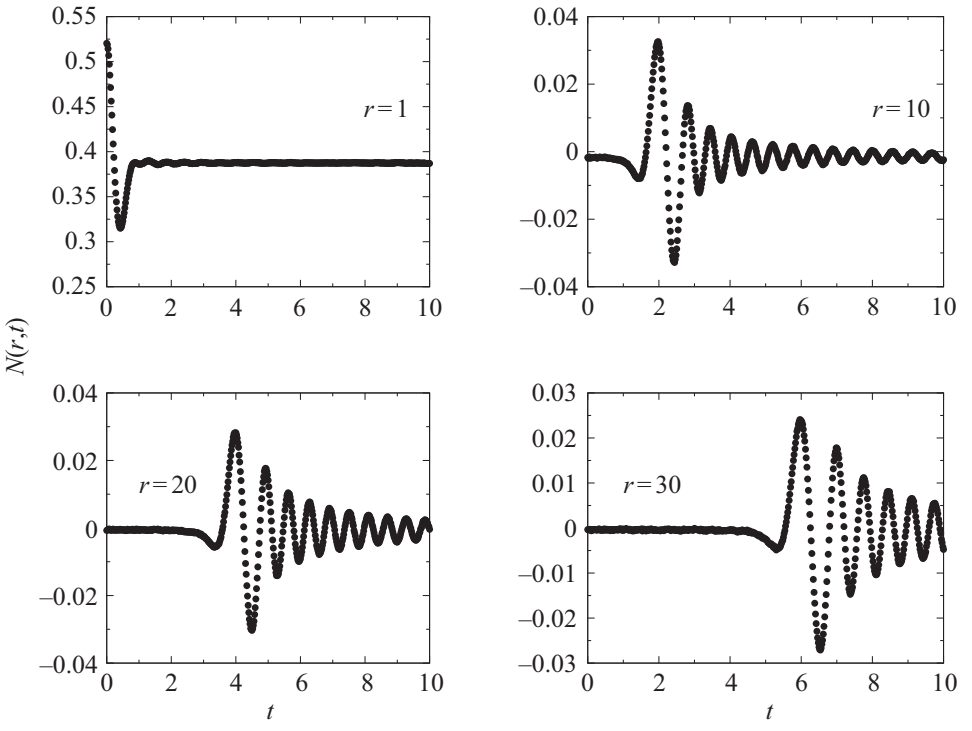

Figure 7.3 The same as in Fig. 7.2 for $U_{\rm init}/J = 2$ and $U_{\rm fin}/J = 4$. In this case, the initial state is given by the best Jastrow wave function for the initial interaction strength.

The results of the density-density correlation $N(r,t)$ for a chain with $L = 100$ are shown in Figs. 7.2 and 7.3 for $r = 1$, 10, 20, and 30. In the former case, we set $U_{\rm init} = 0$ and $U_{\rm fin}/J = 3$ (here, the initial state is the exact ground state of the non-interacting Bose-Hubbard Hamiltonian), while, in the latter one, we fixed $U_{\rm init}/J = 2$ and $U_{\rm fin}/J = 4$ (here, the initial state is just a variational *Ansatz* for the exact ground state). The existence of the so-called light cone is clearly visible: $N(r,t)$ is unaffected at short times, then develops a maximum at a finite time $t^\star(r)$ and finally undergoes damped oscillations. For large enough separation r, the activation time $t^\star(r)$ depends linearly on the separation, $t^\star(r) \approx v_{\rm lc} \times r$, which defines the light-cone velocity $v_{\rm lc}$. Remarkably, the time-dependent variational method allows us to simulate very long times in the ballistic regime without any instability. Indeed, we can easily reach times as large as $t \approx 100$, which are much larger than what is possible by using other numerical methods, as time-dependent density matrix renormalization group (White and Feiguin, 2004; Daley et al., 2004) and non-equilibrium dynamical mean-field theory (Aoki et al., 2014).

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