

1

Correlated Models and Wave Functions

1.1 Introduction

The aim of this chapter is to give a concise overview of the variational approach for strongly correlated systems on the lattice. In particular, we focus our attention on well-known wave functions that have been proven to describe a huge variety of stable phases of matter, e.g., metals, superconductors, band and topological insulators, and quantum Hall states. In the following (and throughout the entire book), we will assume that the reader is familiar with the second-quantization formalism; a simple and complete review of it can be found in the book by Fetter and Walecka (2003).

The use of variational wave functions is rooted in the early days of quantum mechanics. Indeed, soon after its development in 1925–26, Walter Heitler and Fritz London proposed a simplified treatment of the H_2 molecule and opened the way to a theoretical understanding of the chemical bond (Heitler and London, 1927). The Heitler-London *Ansatz* for the ground-state wave function of H_2 treats the two electrons as being highly correlated, since ionic configurations with both electrons on the same Hydrogen atom are excluded. By using the modern formalism of second quantization, the Heitler-London (singlet) state has the following form:

$$|\Psi_{\text{HL}}\rangle = \frac{1}{\sqrt{2}} \left(c_{1,\uparrow}^\dagger c_{2,\downarrow}^\dagger + c_{2,\uparrow}^\dagger c_{1,\downarrow}^\dagger \right) |0\rangle; \quad (1.1)$$

here $|0\rangle$ is the vacuum and $c_{i,\sigma}^\dagger$ creates an electron with spin $\sigma = \uparrow, \downarrow$ in a given orbital $\phi(\mathbf{r} - \mathbf{R}_i)$ centered around the atom $i = 1, 2$ at position \mathbf{R}_i :

$$c_{i,\sigma}^\dagger = \int d\mathbf{r} \phi(\mathbf{r} - \mathbf{R}_i) \psi_\sigma^\dagger(\mathbf{r}), \quad (1.2)$$

where $\psi_{\sigma}^{\dagger}(\mathbf{r})$ is the fermionic field operator. In the following, we consider the case in which the orbitals on different atoms are orthogonal:

$$\int d\mathbf{r} \phi^*(\mathbf{r} - \mathbf{R}_i) \phi(\mathbf{r} - \mathbf{R}_j) = \delta_{ij}, \quad (1.3)$$

thus leading to the anti-commutation relations among fermion operators:

$$\{c_{i,\sigma}, c_{j,\tau}^{\dagger}\} = \delta_{ij} \delta_{\sigma,\tau}, \quad (1.4)$$

$$\{c_{i,\sigma}^{\dagger}, c_{j,\tau}^{\dagger}\} = 0. \quad (1.5)$$

In the original work by Heitler and London, the orbitals were not taken to be orthogonal (e.g., they considered hydrogenic orbitals centered around the two atoms), implying a different normalization of $|\Psi_{\text{HL}}\rangle$. The wave function (1.1) becomes very accurate when the Hydrogen molecule is “stretched out,” namely when $|\mathbf{R}_1 - \mathbf{R}_2| \rightarrow \infty$, and becomes exact in the atomic limit, where the distance between the two atoms is infinite (here, $\phi(\mathbf{r})$ can be taken to be the 1s hydrogenic orbital). In fact, when their relative distance becomes very large, it is energetically favorable to have one electron “localized” on each atom, while the ionic configurations with both electrons on the same Hydrogen have a large energy originating from the electron-electron repulsion.

A distinctly different approach for the same problem was taken soon thereafter by Douglas Hartree, Vladimir Fock, and John Slater, who treated the electrons as being independent from each other (Slater, 1930). Within the independent-electron (Hartree-Fock) approximation, the ground-state wave function is given by a Slater determinant constructed from filling a molecular orbital with up and down spins:

$$|\Psi_{\text{HF}}\rangle = \Phi_{\uparrow}^{\dagger} \Phi_{\downarrow}^{\dagger} |0\rangle, \quad (1.6)$$

where Φ_{σ}^{\dagger} creates an electron on a given molecular orbital. The simplest case is obtained by taking a linear combination of orbitals localized around each atom:

$$\Phi_{\sigma}^{\dagger} = \frac{1}{\sqrt{2}} (c_{1,\sigma}^{\dagger} + c_{2,\sigma}^{\dagger}), \quad (1.7)$$

thus leading to a simple form of the Hartree-Fock wave function:

$$|\Psi_{\text{HF}}\rangle = \frac{1}{2} \left(c_{1,\uparrow}^{\dagger} c_{1,\downarrow}^{\dagger} + c_{1,\uparrow}^{\dagger} c_{2,\downarrow}^{\dagger} + c_{2,\uparrow}^{\dagger} c_{1,\downarrow}^{\dagger} + c_{2,\uparrow}^{\dagger} c_{2,\downarrow}^{\dagger} \right) |0\rangle. \quad (1.8)$$

Here, the ionic configurations $c_{1,\uparrow}^{\dagger} c_{1,\downarrow}^{\dagger} |0\rangle$ and $c_{2,\uparrow}^{\dagger} c_{2,\downarrow}^{\dagger} |0\rangle$ appear with the same weight of the non-ionic configurations $c_{1,\uparrow}^{\dagger} c_{2,\downarrow}^{\dagger} |0\rangle$ and $c_{2,\uparrow}^{\dagger} c_{1,\downarrow}^{\dagger} |0\rangle$. Therefore, when the two Hydrogen atoms are pulled apart, this variational wave function does not

reproduce the atomic limit. By contrast, this state becomes exact whenever the electron-electron repulsion is “switched off.”

Certainly, the exact result of the H_2 molecule lies in between these two extreme cases. However, the variational wave functions of Eqs. (1.1) and (1.6) represent the prototypes of many-body states that are considered in quantum chemistry and solid-state physics. They are the simplest examples to describe localized and delocalized electrons (i.e., Mott insulators and metals in solids). The molecular orbital approach had a great success in describing many diatomic and small molecules, since most of the chemical bonds are relatively weakly correlated.

From the one hand, in quantum chemistry, these two approaches have been pursued to obtain a quantitative understanding of the chemical bond. In particular, Linus Pauling developed the concept of *resonance* among different electronic configurations to describe the benzene molecule (Pauling, 1960), generalizing the Heitler-London picture for the Hydrogen molecule. Later, this approach has been extended by Patrick Fazekas and Philip Anderson, who introduced the concept of resonating valence-bond (RVB) insulator where localized spin-1/2 moments couple together to form singlet pairs; here, quantum fluctuations allow tunneling (i.e., a resonance) among a large number of singlet configurations (Fazekas and Anderson, 1974). The RVB theory had a real bloom with the discovery of high-temperature superconductors, when Anderson and collaborators (Anderson, 1987; Anderson et al., 1987; Baskaran and Anderson, 1988) proposed that an insulating RVB state, with “preformed” singlet pairs, may naturally lead to superconductivity upon electron or hole doping.

On the other hand, in solid-state theory, the Hartree-Fock approximation allowed an accurate description of several metals and band insulators. Moreover, the Hartree-Fock approach has introduced the concept of self-consistent field, in which each electron experiences the average field produced by the other electrons. The methods based upon a self-consistent field, leading to an independent-electron picture, have been widely developed in the last fifty years, mainly from the local-density approximation to the density functional theory (Martin, 2004). The failure of these approaches become evident in a number of materials where unfilled d or f shells are present, like in the so-called heavy-fermion systems (Stewart, 1984). The most celebrated examples are given by the Copper-based high-temperature superconductors (Lee et al., 2006); nowadays, there is a plethora of newly synthesized oxide materials that show strong deviations from what is predicted by using an independent-electron approximation (Imada et al., 1998), thus requiring alternative methods that may include electron-electron correlations. The definition of suitable variational wave functions represents a viable and promising tool to obtain an accurate description of several materials in which the role of interactions cannot be captured by simple mean-field approaches.

1.2 The Matrix Formulation

Once approaching many-body problems, it is always convenient to consider a *finite* basis set, by truncating the original (many-body) Hilbert space in some way. Then the low-energy states, including the ground state, may be approximately described within this truncated basis set. For example, in the Heitler-London wave function of Eq. (1.1), only two states are considered, where electrons with opposite spins occupy orbitals localized around different protons; instead, in the Hartree-Fock state of Eq. (1.8) there are four possible configurations, including the ionic ones with two electrons on the same proton. In these two examples, we did not really refer to any Hamiltonian, but we just construct *Ansätze* for the ground-state wave function.

From a different perspective, once a truncated basis with \mathcal{N} elements has been chosen, the Hamiltonian can be written as a $\mathcal{N} \times \mathcal{N}$ matrix. By indicating the generic state of the basis set by $|x\rangle$, the matrix element of the Hamiltonian \mathcal{H} is given by:

$$\mathcal{H}_{x,x'} \equiv \langle x | \mathcal{H} | x' \rangle, \quad (1.9)$$

which, in principle, can be computed from a given Hamiltonian \mathcal{H} and basis set $\{|x\rangle\}$. In the simplest approximation of the H_2 molecule, we can take only the four states with $S_z = 0$ that have been used in the Heitler-London and Hartree-Fock wave functions:

$$|1\rangle = c_{1,\uparrow}^\dagger c_{1,\downarrow}^\dagger |0\rangle, \quad (1.10)$$

$$|2\rangle = c_{1,\uparrow}^\dagger c_{2,\downarrow}^\dagger |0\rangle, \quad (1.11)$$

$$|3\rangle = c_{2,\uparrow}^\dagger c_{1,\downarrow}^\dagger |0\rangle, \quad (1.12)$$

$$|4\rangle = c_{2,\uparrow}^\dagger c_{2,\downarrow}^\dagger |0\rangle. \quad (1.13)$$

Within this truncated Hilbert space, the Hamiltonian reads as:

$$\mathcal{H} = -t \sum_{\sigma} \left(c_{1,\sigma}^\dagger c_{2,\sigma} + c_{2,\sigma}^\dagger c_{1,\sigma} \right) + U \sum_i n_{i,\uparrow} n_{i,\downarrow} + V \sum_{\sigma,\sigma'} n_{1,\sigma} n_{2,\sigma'}, \quad (1.14)$$

where $n_{i,\sigma} = c_{i,\sigma}^\dagger c_{i,\sigma}$ is the density per spin σ on the site $i = 1, 2$; t , U , and V are parameters that depend upon the overlap of orbitals $\phi(\mathbf{r} - \mathbf{R}_i)$ centered around the two atoms:

$$-t = \int d\mathbf{r} \phi^*(\mathbf{r} - \mathbf{R}_1) \left(-\frac{\hbar^2}{2m} \nabla^2 - \sum_{i=1,2} \frac{e^2}{|\mathbf{r} - \mathbf{R}_i|} \right) \phi(\mathbf{r} - \mathbf{R}_2), \quad (1.15)$$

$$U = \int \int d\mathbf{r} d\mathbf{r}' |\phi(\mathbf{r} - \mathbf{R}_1)|^2 \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} |\phi(\mathbf{r}' - \mathbf{R}_1)|^2, \quad (1.16)$$

$$V = \int \int d\mathbf{r} d\mathbf{r}' |\phi(\mathbf{r} - \mathbf{R}_1)|^2 \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} |\phi(\mathbf{r}' - \mathbf{R}_2)|^2. \quad (1.17)$$

In principle, the Hamiltonian (1.14) also contains the Coulomb interaction between the protons, however, this is a constant term, once their positions are fixed in \mathbf{R}_1 and \mathbf{R}_2 .

Therefore, within the truncated basis $\{|1\rangle, |2\rangle, |3\rangle, |4\rangle\}$, the solution of the problem corresponds to the diagonalization of the 4×4 matrix:

$$\mathbf{h} = \begin{pmatrix} U & -t & -t & 0 \\ -t & V & 0 & -t \\ -t & 0 & V & -t \\ 0 & -t & -t & U \end{pmatrix}. \quad (1.18)$$

The Hartree-Fock wave function is the exact ground state for $U = V = 0$, while the Heitler-London wave function is the ground state for $t = 0$ and $U > V$. In the generic case with finite t , U , and V , the exact ground state is a superposition of these two wave functions and gives the best variational wave function in this truncated Hilbert space.

Of course, the quality of the approximation can be improved by enlarging the Hilbert space, e.g., by including more orbitals in the truncated basis. The main issue comes from the fact that the problem becomes terribly complex as the dimension of the truncated Hilbert space, and consequently the size of the matrix, increases. At present, there are no exact methods that allow the solution of a general many-body Hamiltonian with a computational effort that scales polynomially with the system size. The complexity of the many-body problem is generally exponential, and this is the main reason why strong correlation is such a difficult task.

1.3 Effective Lattice Models

In this section, we would like to report a few examples of lattice models that represent important (and in most cases still *unsolved*) cases in which correlation effects show up, producing several unconventional quantum phases. A pedagogical introduction to the field of correlated systems can be found in the book by Fazekas (1999).

The simplest example has been independently conceived by John Hubbard (1963), Martin Gutzwiller (1963), and Junjiro Kanamori (1963) and is now universally known as the Hubbard model. Here, electrons on a lattice interact among each others through a simplified ‘‘Coulomb’’ potential that includes only the on-site term:

$$\mathcal{H} = -t \sum_{\langle ij \rangle, \sigma} c_{i, \sigma}^\dagger c_{j, \sigma} + \text{h.c.} + U \sum_i n_{i, \uparrow} n_{i, \downarrow}, \quad (1.19)$$

where $\langle \dots \rangle$ indicates neighboring sites on a given lattice in d spatial dimensions. For simplicity, in the following, we consider hyper-cubic (Bravais) lattices defined

by primitive vectors \mathbf{a}_μ , with $\mu = 1, \dots, d$; moreover, periodic boundary conditions are taken. However, the Hubbard model can be defined on any d -dimensional lattice. Then, $c_{j,\sigma}^\dagger$ ($c_{j,\sigma}$) creates (destroys) one electron with spin σ on a Wannier orbital residing on the site j :

$$\Xi_j(\mathbf{r}) = \frac{1}{\sqrt{L}} \sum_{\mathbf{k}} e^{-i\mathbf{k} \cdot \mathbf{R}_j} \Psi_{\mathbf{k}}(\mathbf{r}), \quad (1.20)$$

where L is the total number of sites and $\Psi_{\mathbf{k}}(\mathbf{r})$ are Bloch states constructed with the orbitals $\phi(\mathbf{r} - \mathbf{R}_i)$ centered around each site. Therefore, the operators at different sites create orthogonal states, thus satisfying the anti-commutation relation of Eqs. (1.4) and (1.5). The Hubbard model generalizes the H_2 Hamiltonian of Eq. (1.14) to a lattice of Hydrogen atoms (with $V = 0$) and is defined in the Hilbert space where each site can be empty, singly occupied (with either spin up or down), or doubly occupied. Moreover, the Hamiltonian (1.19) commutes with the total number of particles with up or down spin (i.e., N_\uparrow and N_\downarrow , $N_e = N_\uparrow + N_\downarrow$ being the total number of electrons), thus allowing us to consider sectors with different number of particles separately.

The first term of Eq. (1.19), proportional to t , describes the electron hopping, which favors delocalized states. Indeed, for $U = 0$, the Hamiltonian can be easily diagonalized in the Fourier space (i.e., by plane waves):

$$c_{k,\sigma}^\dagger = \frac{1}{\sqrt{L}} \sum_j e^{-i\mathbf{k} \cdot \mathbf{R}_j} c_{j,\sigma}^\dagger. \quad (1.21)$$

After performing this transformation, the non-interacting Hamiltonian becomes:

$$\mathcal{H}_t = \sum_{k,\sigma} \epsilon_k c_{k,\sigma}^\dagger c_{k,\sigma}, \quad (1.22)$$

where, for the case with nearest-neighbor hopping:

$$\epsilon_k = -2t \sum_{\mu=1}^d \cos(\mathbf{k} \cdot \mathbf{a}_\mu). \quad (1.23)$$

Any state constructed from filling k -vectors with up and/or down electrons is an eigenstate of \mathcal{H}_t :

$$|\Phi_t\rangle = \prod_{k,\sigma} \left(c_{k,\sigma}^\dagger \right)^{\eta_{k,\sigma}} |0\rangle, \quad (1.24)$$

where $\eta_{k,\sigma} = 1$ ($\eta_{k,\sigma} = 0$) indicates that the single-particle state with momentum k and spin σ is occupied (empty); this state has an energy:

$$E = \sum_{k,\sigma} \eta_{k,\sigma} \epsilon_k. \quad (1.25)$$

For $N_\uparrow = N_\downarrow = N_e/2$, the ground state of Eq. (1.22) is obtained by filling the $N_e/2$ lowest-energy levels with both up and down electrons, e.g., $\eta_{k\sigma} = 1$ for all the momenta such that $\epsilon_k \leq \epsilon_F$ (where ϵ_F denotes the Fermi energy) and $\eta_{k\sigma} = 0$ for all the momenta such that $\epsilon_k > \epsilon_F$. On a finite lattice, the ground state is unique if there is a (finite-size) gap between the highest-energy occupied level and the lowest-energy unoccupied one. In the thermodynamic limit, the gap goes to zero and, on the hyper-cubic lattice, this state describes a metal.

By contrast, whenever the hopping term vanishes, i.e., $U/t = \infty$, the Hubbard Hamiltonian is already diagonal in real space:

$$\mathcal{H}_U = U \sum_i n_{i,\uparrow} n_{i,\downarrow}. \quad (1.26)$$

In this case, any state constructed from putting electrons on sites of the lattice is an eigenstate of \mathcal{H}_U :

$$|\Phi_U\rangle = \prod_{i,\sigma} \left(c_{i,\sigma}^\dagger \right)^{\xi_{i,\sigma}} |0\rangle, \quad (1.27)$$

where $\xi_{i,\sigma} = 1$ ($\xi_{i,\sigma} = 0$) indicates that the site i is (not) occupied by an electron with spin σ . Its energy is given by:

$$E = U \sum_i \xi_{i,\uparrow} \xi_{i,\downarrow} = U N_d, \quad (1.28)$$

where N_d is the number of doubly occupied sites. The ground state is highly degenerate, with $E = 0$ for $N_e \leq L$ (corresponding to all states without doubly occupied sites) and $E = U(N_e - L)$ for $L < N_e \leq 2L$ (corresponding to all states with $N_e - L$ doubly occupied sites). In particular, for $N_e = L$ (half filling) the ground state has exactly one electron per site and degeneracy equal to 2^L , corresponding to all possible configurations with up or down spin on each site. This is an insulator that is stabilized by the strong electron-electron repulsion (i.e., $U/t = \infty$), which is called Mott insulator, after the pioneering work done by Nevill Mott (1949, 1990).

Besides these trivial limits, there are very few cases in which the Hubbard model can be exactly solved on large lattices (where exact diagonalizations cannot be performed). In one spatial dimension with nearest-neighbor hopping, the so-called Bethe *Ansatz* provides us with the exact results for the energy and other thermodynamic quantities, although correlation functions are difficult to compute (Lieb and Wu, 1968): here, the ground state is an insulator for $N_e = L$ and $U > 0$, while it is metallic for $N_e \neq L$. Notably, there is an exact solution in any dimension d for $U/t = \infty$ and $N_e = L - 1$ (e.g., one hole), where the ground state is a fully polarized ferromagnet (Nagaoka, 1966). More generally, it is possible to show

that the ground state is fully polarized on an arbitrary lattice whenever $t < 0$, $U/|t| = \infty$, and $N_e = L - 1$ (Tasaki, 1998). Otherwise, the exact ground-state properties of the Hubbard model with generic filling factor $n = N_e/L$ and interaction U/t are not known. Remarkably, a numerically exact Monte Carlo approach without sign problem (i.e., exact apart from statistical errors) can be performed in the half-filled case for any value of U/t in the square lattice; this approach will be discussed in Chapter 11.

From a general point of view, it is natural to expect that, in a generic d -dimensional lattice, a metal-insulator transition will appear for a given $U = U_c$ at half filling, i.e., $n = 1$ (for the exactly solvable model in one dimension, $U_c = 0$). This would be a *bona-fide* Mott transition, which is driven by the electron-electron interaction only, and not by a symmetry-breaking mechanism: in other words, electrons localize just because of the strong correlation. However, in most cases (when varying the dimensionality of the lattice and the coordination number) the metal-insulator transition comes together with the development of long-range order, most notably the formation of antiferromagnetic order. The existence of a super-exchange coupling, which favors antiferromagnetic order for large values of U/t , can be seen by performing a strong-coupling expansion with $U/t \gg 1$.

Whenever the interaction U is much larger than the hopping parameter t and $n = 1$, we can project out all the sub-spaces with one or more doubly occupied sites and obtain an effective low-energy model that describes the spin degrees of freedom. For $U/t = \infty$, the ground-state manifold is massively degenerate due to the fact that the spin of the electron can be either up or down on each site; the presence of a finite but small hopping lifts this degeneracy creating an antiferromagnetic super-exchange coupling $J = 4t^2/U$. Indeed, at the second-order of perturbation theory in t/U , two neighboring electrons with opposite spins may profit of a virtual hopping process that creates a doubly occupied site (see Fig. 1.1) while two electrons with parallel spins cannot gain any energy from that, because of the Pauli exclusion principle. As a result, the effective low-energy model that captures the spin dynamics is given by the Heisenberg Hamiltonian:

$$\mathcal{H} = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j, \quad (1.29)$$

where $\mathbf{S}_j = (S_j^x, S_j^y, S_j^z)$ is the spin-1/2 operator of electrons:

$$S_j^x = \frac{1}{2} (c_{j,\uparrow}^\dagger c_{j,\downarrow} + c_{j,\downarrow}^\dagger c_{j,\uparrow}), \quad (1.30)$$

$$S_j^y = \frac{1}{2i} (c_{j,\uparrow}^\dagger c_{j,\downarrow} - c_{j,\downarrow}^\dagger c_{j,\uparrow}), \quad (1.31)$$

$$S_j^z = \frac{1}{2} (c_{j,\uparrow}^\dagger c_{j,\uparrow} - c_{j,\downarrow}^\dagger c_{j,\downarrow}). \quad (1.32)$$

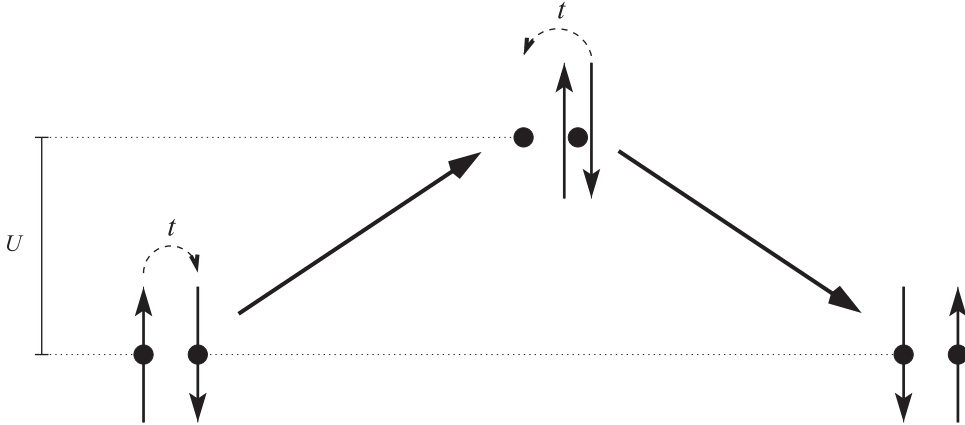


Figure 1.1 In second-order perturbation theory in t/U , if the spins of neighboring sites are antiparallel, they gain energy by a virtual process creating a double occupation.

The Heisenberg model is defined in the Hilbert space where each site is singly occupied. Again, the exact solution of the Heisenberg model can be obtained in one spatial dimension, by the *Bethe Ansatz* (Bethe, 1931): here, the ground state is not magnetically ordered and the excitation spectrum is gapless (implying power-law spin-spin correlations). The absence of a true magnetic order in the ground-state of one-dimensional systems is due to an extension of the Mermin-Wagner theorem (Pitaevskii and Stringari, 1991). In more than one spatial dimension, for bipartite lattices (i.e., where the sites can be partitioned in two sub-lattices and the super-exchange term only couples sites on different sub-lattices) there are Monte Carlo methods that provide us with numerically exact results (see Chapter 8). These stochastic approaches have been crucial to definitively show that the ground state of the Heisenberg model on the two-dimensional square lattice has long-range magnetic (Néel) order (Reger and Young, 1988). The Heisenberg model can be generalized to have an arbitrary value of the spin S (also in this case, for bipartite lattices, Monte Carlo approaches allow us to get numerically exact results).

Mobile holes can be injected in the Heisenberg model of Eq. (1.29), leading to the so-called t – J model (Fazekas, 1999):

$$\mathcal{H} = -t \sum_{\langle i,j \rangle, \sigma} c_{i,\sigma}^\dagger c_{j,\sigma} + \text{h.c.} + J \sum_{\langle i,j \rangle} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j \right), \quad (1.33)$$

where all the operators act on the restricted Hilbert space without doubly occupied sites. The t – J model captures the strong-coupling limit of the Hubbard model for $n < 1$ and is usually considered to give the minimal description of Cuprate

superconductors (Lee et al., 2006). Moreover, the t – J model can be also obtained from the strong-coupling expansion of a three-band Hubbard model, which includes both Copper and Oxygen atoms (Zhang and Rice, 1988). There are no exact solutions of the t – J model for generic values of the ratio J/t and electron doping n , both in one and two spatial dimensions, except in one dimension for the super-symmetric point $J/t = 2$ (Sutherland, 1975).

We would like to mention that the Hubbard model with a *negative* interaction U can be considered to describe the case where an effective attractive electron-electron interaction is present (for example, for a non-retarded electron-phonon coupling, leading to superconductivity). Therefore, the Hubbard model with $U < 0$ can be seen as the simplest model to capture the stabilization of a superconducting phase. Also in this case, there are Monte Carlo methods that allow a numerically exact solution of the model (see Chapter 11).

Finally, the case of bosonic particles can be also considered, which is relevant for various physical systems, like for interacting ^4He atoms, or to represent tightly coupled pairs of fermions that may undergo a superconductor-insulator transition. The bosonic Hubbard model is defined by:

$$\mathcal{H} = -t \sum_{\langle i,j \rangle} b_i^\dagger b_j + \text{h.c.} + \frac{U}{2} \sum_i n_i(n_i - 1), \quad (1.34)$$

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 ; these creation and annihilation operators satisfy commutation relations:

$$[b_i, b_j^\dagger] = \delta_{ij}, \quad (1.35)$$

$$[b_i^\dagger, b_j^\dagger] = 0. \quad (1.36)$$

Again the Hamiltonian (1.34) commutes with the total number of bosons N_b , so that any sector with different number of particles can be considered separately. Notice that the Hilbert space of the bosonic Hubbard model is much larger than the fermionic one, since any number of bosons is allowed on each site. The bosonic Hubbard model is only defined for repulsive interactions, since bosons are thermodynamically unstable in presence of attractive interactions.

For $U = 0$, the non-interacting ground state is easily obtained by condensing all bosons in the lowest-energy single-particle state:

$$|\Phi_0\rangle = \frac{1}{\sqrt{N_b!}} \left(b_{k=0}^\dagger \right)^{N_b} |0\rangle. \quad (1.37)$$

By contrast, for $t = 0$, the ground state is given by placing bosons on sites and minimizing the number of multiply occupied sites (as done for the fermionic case):

for example, for $N_b \leq L$ the ground state has only empty or singly occupied sites. In contrast to the fermionic case, for $N_b = L$, the ground state, with one boson per site, is unique.

For this lattice model, there are no exact solutions (in the sense of the Bethe *Ansatz*) for generic values of the bosonic density $n = N_b/L$ and interaction U . Nevertheless, it is possible to obtain numerically exact results by using Monte Carlo techniques for any values of n and U/t ; see Chapter 8.

1.4 The Variational Principle

Instead of exactly solving the truncated Hamiltonian, which is an exponentially hard problem, we can define, in analogy to Heitler-London and Hartree-Fock approaches, variational wave functions that may capture the correct low-energy properties of correlated systems. Indeed, the *variational principle* represents one important pillar when searching for reliable approximations of strongly correlated electronic or bosonic systems. Here, we discuss the basic aspects of the variational approach.

Given any approximate state $|\Psi_{\text{var}}\rangle$ for the exact ground state $|\Upsilon_0\rangle$ of a given Hamiltonian, we can define its variational energy as:

$$E_{\text{var}} = \frac{\langle \Psi_{\text{var}} | \mathcal{H} | \Psi_{\text{var}} \rangle}{\langle \Psi_{\text{var}} | \Psi_{\text{var}} \rangle}. \quad (1.38)$$

Any state in the Hilbert space can be expanded in terms of the eigenfunctions $|\Upsilon_i\rangle$ of the Hamiltonian (with energies E_i), so that the variational state can be written as:

$$|\Psi_{\text{var}}\rangle = \sum_i a_i |\Upsilon_i\rangle, \quad (1.39)$$

with $a_i = \langle \Upsilon_i | \Psi_{\text{var}} \rangle$. The normalization condition reads as:

$$\langle \Psi_{\text{var}} | \Psi_{\text{var}} \rangle = \sum_i |a_i|^2 = 1. \quad (1.40)$$

By using the expansion of Eq. (1.39), we easily obtain that:

$$\epsilon \equiv E_{\text{var}} - E_0 = \sum_{i \neq 0} |a_i|^2 (E_i - E_0) \geq 0, \quad (1.41)$$

which implies that any trial state $|\Psi_{\text{var}}\rangle$ provides an *upper bound* of the exact energy and represents the basis of controlled approximate techniques. In practice, given any approximation $|\Psi_{\text{var}}\rangle$, all computational efforts are devoted to minimizing the variational energy E_{var} .

Let us now analyze in what sense an approximate wave function, with given “distance” in energy ϵ from the exact ground state, can be considered as a good

approximation of the many-body ground state $|\Upsilon_0\rangle$. A crucial role is played by the gap to the first excited state, which is always finite in a system with N particles (apart from accidental degeneracies that occur for very particular models and boundary conditions), i.e., $\Delta = E_1 - E_0 > 0$. From Eq. (1.41) and the fact that $E_i \geq E_0 + \Delta$, it follows that:

$$\epsilon \geq \Delta \sum_{i \neq 0} |a_i|^2; \quad (1.42)$$

then, by using the normalization condition (1.40), we finally have that:

$$\eta = 1 - |a_0|^2 \leq \frac{\epsilon}{\Delta}. \quad (1.43)$$

This relation tells us that, in order to have an accurate approximation of the exact ground state (i.e., $\eta \ll 1$), a sufficient condition is that the error ϵ in the variational energy has to be much smaller than the gap Δ to the first excited state.

The accuracy of correlation functions (i.e., expectation values of Hermitian operators, which do not commute with the Hamiltonian, over $|\Psi_{\text{var}}\rangle$) is usually worse than the one on the ground-state energy. Let us consider a generic operator \mathcal{O} and express the variational wave function as:

$$|\Psi_{\text{var}}\rangle = a_0|\Upsilon_0\rangle + \sqrt{\eta}|\Upsilon'\rangle, \quad (1.44)$$

where $|\Upsilon'\rangle$ is orthogonal to the ground state $|\Upsilon_0\rangle$ and $\eta = 1 - |a_0|^2$. Then, the difference between the expectation value calculated with the variational state and the exact one is given by:

$$|\langle \Psi_{\text{var}} | \mathcal{O} | \Psi_{\text{var}} \rangle - \mathcal{O}_0| = |2a_0\sqrt{\eta}\langle \Upsilon_0 | \mathcal{O} | \Upsilon' \rangle + \eta\langle \Upsilon' | \mathcal{O} | \Upsilon' \rangle - \eta\mathcal{O}_0|, \quad (1.45)$$

where we have denoted $\mathcal{O}_0 = \langle \Upsilon_0 | \mathcal{O} | \Upsilon_0 \rangle$ and assumed, for simplicity, real wave functions. Whenever the variational state is close to the exact ground state, $\eta \ll \sqrt{\eta}$, and we can neglect all the terms that are proportional to η :

$$|\langle \Psi_{\text{var}} | \mathcal{O} | \Psi_{\text{var}} \rangle - \mathcal{O}_0| \approx \sqrt{\eta}|\langle \Upsilon_0 | \mathcal{O} | \Upsilon' \rangle|, \quad (1.46)$$

which shows that the accuracy in correlation functions is more problematic than the one on the ground-state energy, with a term proportional to $\sqrt{\eta}$.

1.5 Variational Wave Functions

Since no exact solutions of the fermionic and the bosonic Hubbard models are known for generic values of the coupling constants in two or higher spatial dimensions, it may be profitable to define suitable variational wave functions that may capture the main aspects of the ground-state properties. In the following, we will describe few many-body states that represent important examples in condensed-matter physics.

1.5.1 Hartree-Fock Wave Functions

For fermionic models, the simplest example is given by the Hartree-Fock approximation, where the many-body wave function is taken to be a product state of suitably optimized single-particle orbitals:

$$|\Psi_{\text{HF}}\rangle = \prod_{\alpha=1}^{N_e} \Phi_{\alpha}^{\dagger} |0\rangle; \quad (1.47)$$

here, Φ_{α}^{\dagger} can be expressed in terms of the original fermionic operators as:

$$\Phi_{\alpha}^{\dagger} = \sum_i W_{\uparrow,\alpha,i}^* c_{i,\uparrow}^{\dagger} + \sum_i W_{\downarrow,\alpha,i}^* c_{i,\downarrow}^{\dagger}, \quad (1.48)$$

where $\{W_{\sigma,\alpha,i}\}$ are complex coefficients that can be optimized to get the best variational state. The condition that orbitals are normalized and orthogonal to each other implies that:

$$\sum_i (W_{\uparrow,\alpha,i} W_{\uparrow,\beta,i}^* + W_{\downarrow,\alpha,i} W_{\downarrow,\beta,i}^*) = \delta_{\alpha,\beta}. \quad (1.49)$$

In turn, the original fermionic operators can be written as:

$$c_{i,\uparrow}^{\dagger} = \sum_{\alpha} W_{\uparrow,\alpha,i} \Phi_{\alpha}^{\dagger}, \quad (1.50)$$

$$c_{i,\downarrow}^{\dagger} = \sum_{\alpha} W_{\downarrow,\alpha,i} \Phi_{\alpha}^{\dagger}. \quad (1.51)$$

The expectation value of any Hamiltonian can be easily evaluated analytically. For example, for the Hubbard model of Eq. (1.19), the variational energy is given by:

$$\begin{aligned} E_{\text{HF}} &= \frac{\langle \Psi_{\text{HF}} | \mathcal{H} | \Psi_{\text{HF}} \rangle}{\langle \Psi_{\text{HF}} | \Psi_{\text{HF}} \rangle} = -t \sum_{\langle i,j \rangle, \sigma} \sum_{\alpha=1}^{N_e} W_{\sigma,\alpha,i} W_{\sigma,\alpha,j}^* + \text{h.c.} \\ &+ U \sum_i \sum_{\alpha=1}^{N_e} \sum_{\beta=1}^{N_e} (|W_{\uparrow,\alpha,i}|^2 |W_{\downarrow,\beta,i}|^2 - W_{\uparrow,\alpha,i} W_{\uparrow,\beta,i}^* W_{\downarrow,\beta,i} W_{\downarrow,\alpha,i}^*), \end{aligned} \quad (1.52)$$

where we have used the fact that $\langle \Psi_{\text{HF}} | \Psi_{\text{HF}} \rangle = 1$. The optimal many-body state is obtained by minimizing the variational energy with respect to all possible amplitudes $W_{\sigma,\alpha,i}^*$:

$$\frac{\partial E_{\text{HF}}}{\partial W_{\sigma,\alpha,i}^*} = -t \sum_{\langle j \rangle_i} W_{\sigma,\alpha,j} + U \sum_{\beta=1}^{N_e} (|W_{-\sigma,\beta,i}|^2 W_{\sigma,\alpha,i} - W_{\sigma,\beta,i} W_{-\sigma,\beta,i}^* W_{-\sigma,\alpha,i}), \quad (1.53)$$

where $\langle j \rangle_i$ indicates all the sites j that are neighbors of the site i . Here, the electronic orbitals define self-consistent fields: the first term proportional to U

(i.e., $\sum_{\beta=1}^{N_e} |W_{-\sigma,\beta,i}|^2$) is a “direct” Coulomb term, while the second one (i.e., $\sum_{\beta=1}^{N_e} W_{\sigma,\beta,i} W_{-\sigma,\beta,i}^*$) is an “exchange” term, which is due to the anti-symmetry of the many-body wave function. The best amplitudes can be obtained by the steepest-descent procedure:

$$W_{\sigma,\alpha,i} \rightarrow W_{\sigma,\alpha,i} - \frac{\partial E_{\text{HF}}}{\partial W_{\sigma,\alpha,i}^*} \delta\tau, \quad (1.54)$$

where $\delta\tau$ is an *ad hoc* parameter that ensures to lower the energy at every iterative step. The updated orbitals are no longer orthogonal to each other; however, the variational energy does not change by taking any linear combination of the occupied orbitals and, therefore, we can obtain a new set of orthogonal states by using the Gram-Schmidt method. In this way, we can iterate the procedure until convergence.

An alternative approach is to define the Hartree-Fock wave function $|\Psi_{\text{HF}}\rangle$ as the ground state of an uncorrelated (auxiliary) Hamiltonian:

$$\mathcal{H}_0 = \sum_{i,j,\sigma,\tau} h_{ij}^{\sigma,\tau} c_{i,\sigma}^\dagger c_{j,\tau}, \quad (1.55)$$

where $h_{ij}^{\sigma,\tau}$ are variational parameters that must be optimized to minimize the variational energy of $|\Psi_{\text{HF}}\rangle$. The advantage of this approach with respect to the previous one is that selected symmetries can be easily imposed in the wave function, by taking a particular *Ansatz* for the $h_{ij}^{\sigma,\tau}$'s (e.g., translational symmetry is imposed by choosing a translational invariant \mathcal{H}_0). By defining:

$$\Delta_{ij}^{\sigma,\tau} = \frac{\langle \Psi_{\text{HF}} | c_{i,\sigma}^\dagger c_{j,\tau} | \Psi_{\text{HF}} \rangle}{\langle \Psi_{\text{HF}} | \Psi_{\text{HF}} \rangle}, \quad (1.56)$$

the Hartree-Fock equations for the Hubbard model of Eq. (1.19) are given by:

$$h_{ij}^{\sigma,\tau} = -t_{ij} \delta_{\sigma,\tau} + U \delta_{ij} (\delta_{\sigma,\tau} \Delta_{ii}^{-\sigma,-\sigma} - \delta_{\sigma,-\tau} \Delta_{ii}^{\tau,\sigma}), \quad (1.57)$$

where $t_{ij} = t$ for nearest-neighbor sites and 0 otherwise. These are also self-consistent equations, since the set of parameters $\{h_{ij}^{\sigma,\tau}\}$ defines the many-body wave function, which in turn determines the values of the $\Delta_{ij}^{\sigma,\tau}$'s by Eq. (1.56).

On the lattice, it is relatively simple to obtain a solution for the Hartree-Fock equations by using iterative methods; instead, it is much more difficult to reach the solution corresponding to the lowest energy, since, in the general case, there are several solutions that correspond to local minima in the variational energy. Most importantly, while the Hartree-Fock approximation may give reasonable results in the weak-coupling regime, its accuracy becomes questionable for moderate and strong interactions. For example, a Mott insulator, with no symmetry breaking, cannot be described within this approximation; moreover, it is also not possible to stabilize superconducting phases in purely repulsive Hamiltonians, thus excluding

the RVB physics (Fazekas, 1999). Therefore, a step forward is needed, in order to reach a better characterization of highly correlated systems.

1.5.2 The Gutzwiller Wave Function

The simplest example of a correlated state, which goes beyond the Hartree-Fock approximation, has been conceived by Gutzwiller (1963) to describe the effect of the Hubbard U interaction in reducing the weight of configurations with multiply occupied sites. The Gutzwiller wave function is constructed by starting from the non-interacting ground state $|\Phi_0\rangle$ (either fermionic or bosonic) and then applying an operator \mathcal{P}_G that suppresses the weight of configurations with multiply occupied sites:

$$|\Psi_G\rangle = \mathcal{P}_G|\Phi_0\rangle; \quad (1.58)$$

here, \mathcal{P}_G is the so-called Gutzwiller factor that depends upon a single variational parameter g (e.g., $g > 0$ for the repulsive Hubbard model):

$$\mathcal{P}_G = \exp \left[-\frac{g}{2} \sum_i (n_i - n)^2 \right], \quad (1.59)$$

where n is the average density. Generalizations in which $|\Phi_0\rangle$ is a generic, non-interacting (i.e., Hartree-Fock) state are often considered.

The effect of the Gutzwiller factor becomes clear once the variational state is expanded in a basis set whose elements $\{|x\rangle\}$ represent configurations with particles sitting on the lattice sites. Indeed, since the Gutzwiller factor is diagonal in this basis (it contains the density operator on each site n_i), we have that:

$$\langle x|\Psi_G\rangle = \mathcal{P}_G(x)\langle x|\Phi_0\rangle, \quad (1.60)$$

where $\mathcal{P}_G(x) \leq 1$ is a number that depends on how many doubly occupied (or multi-occupied) sites are present in the configuration $|x\rangle$. Therefore, the amplitude of the non-interacting state $\langle x|\Phi_0\rangle$ is renormalized by $\mathcal{P}_G(x)$. In the simple example of the Hydrogen molecule, we can take the Hartree-Fock wave function (1.8) as the non-interacting state $|\Phi_0\rangle$, such that, apart from a normalization constant:

$$|\Psi_G\rangle \propto \left(e^{-g} c_{1,\uparrow}^\dagger c_{1,\downarrow}^\dagger + c_{1,\uparrow}^\dagger c_{2,\downarrow}^\dagger + c_{2,\uparrow}^\dagger c_{1,\downarrow}^\dagger + e^{-g} c_{2,\uparrow}^\dagger c_{2,\downarrow}^\dagger \right) |0\rangle. \quad (1.61)$$

Therefore, within this approach, it is possible to interpolate between the Hartree-Fock approximation, which is obtained for $g = 0$, and the Heitler-London one, which is recovered in the limit of $g = \infty$.

Let us now discuss the case of an arbitrary number of lattice sites. For the Hubbard model, when the particle density is $n = 1$, we argued that a metal-insulator (for fermions) or superfluid-insulator (for bosons) transition is expected

at finite values of U/t . However, a simple argument suggests that the Gutzwiller wave function can describe such a transition only when the variational parameter g tends to infinity. Indeed, for $n = 1$, on average, there is one particle per site and density excitations are represented by doublons (doubly occupied sites) and holons (empty sites). In the non-interacting state $|\Phi_0\rangle$, these objects are free to move and then responsible for the conductivity (for example, in the fermionic model, a doublon is negatively charged with respect to the average background, while the holon is positively charged). The effect of the Gutzwiller factor is to penalize the formation of such objects; however, once created, doublons and holons are no longer correlated, thus being free to move independently. Only when the energetic penalty is infinite, an insulator is obtained; here, all the density degrees of freedom are frozen and no transport is possible, implying an oversimplified description of a true insulator, where instead density fluctuations are always present. Extensive calculations have shown that the superfluid-insulator transition in bosonic systems takes place at a finite value of U/t , i.e., the optimal parameter g diverges for a finite value of U/t , (Rokhsar and Kotliar, 1991; Krauth et al., 1992); instead, for fermions, g is finite for all values of U/t and diverges only for $U/t = \infty$ (Yokoyama and Shiba, 1987a,b, 1990).

Finally, let us briefly discuss the case of $n = 1$ in the limit of $g = \infty$. In the bosonic system, only one configuration with exactly one boson per site survives after the application of the Gutzwiller factor with $g = \infty$, implying that the fully projected state is trivial. Instead, in the fermionic case, there is still an exponentially large number of states with singly occupied sites, which differ by the spin configurations. Therefore, non-trivial spin fluctuations are still allowed, possibly leading to the RVB insulator that is obtained by taking the fully projected wave function:

$$|\Psi_\infty\rangle = \mathcal{P}_\infty |\Phi_0\rangle, \quad (1.62)$$

where the full Gutzwiller projector (i.e., with $g = \infty$) is given by:

$$\mathcal{P}_\infty = \prod_i (n_{i,\uparrow} - n_{i,\downarrow})^2. \quad (1.63)$$

Below, we will discuss few examples of RVB states that are obtained by Gutzwiller projecting particular non-interacting wave functions.

1.5.3 The Density-Density Jastrow Wave Function

As we have discussed in the previous section, the variational description of an insulator with density fluctuations is not captured by the simple Gutzwiller wave function (1.58) and requires a modification of the correlation term that is applied to the non-interacting wave function. An alternative approach is to start from a wave

function that describes the localized $U/t = \infty$ limit and then includes a term that delocalizes the electrons (Eichenberger and Baeriswyl, 2007). In the following, we will pursue the former approach.

A straightforward generalization of the Gutzwiller wave function is given by the inclusion of long-range terms in the correlator:

$$|\Psi_J\rangle = \mathcal{J}|\Phi_0\rangle, \quad (1.64)$$

where \mathcal{J} is the so-called Jastrow factor (Jastrow, 1955) that has been introduced in continuum models much before the Gutzwiller wave function. On the lattice, \mathcal{J} takes a simple form:

$$\mathcal{J} = \exp \left[-\frac{1}{2} \sum_{i,j} v_{i,j} (n_i - n)(n_j - n) \right], \quad (1.65)$$

where $v_{i,j}$ is a pseudo-potential for density-density correlations in the variational state. For translationally invariant models, like the Hubbard Hamiltonian (1.19), $v_{i,j}$ only depends upon the relative distance of the two sites i and j , i.e., $|\mathbf{R}_i - \mathbf{R}_j|$; moreover, the on-site term $v_{i,i}$ corresponds to the Gutzwiller parameter g . The Jastrow pseudo-potential can be either parametrized in some way, in order to reduce the number of variational parameters, or optimized for all possible distances, which are $O(L)$ in translationally invariant systems; in Chapter 6, we will discuss an efficient algorithm to find the optimal Jastrow parameters $v_{i,j}$. The role of the long-range tail of the Jastrow factor is to create a bound state between holons and doublons, possibly impeding conduction, but still allowing local density fluctuations. Indeed, we have shown that such Jastrow terms may turn a non-interacting metallic state $|\Phi_0\rangle$ into an insulator in both fermionic and bosonic systems (Capello et al., 2005, 2006, 2007, 2008). In particular, by denoting the Fourier transform of the (translationally invariant) pseudo-potential $v_{i,j}$ by v_q , the gapless (i.e., metallic) phase is described by having $v_q \approx 1/|\mathbf{q}|$ for $|\mathbf{q}| \rightarrow 0$, in any spatial dimension d ; by contrast, a fully gapped (i.e., insulating) phase is obtained in one-dimension with $v_q \approx 1/|\mathbf{q}|^2$ for $|\mathbf{q}| \rightarrow 0$ (Capello et al., 2005, 2008). This singular behavior of the pseudo-potential induces an exponential decay of the density-density correlations. In two and three spatial dimensions, a holon-doublon bound-state is generated by $v_q \approx \beta/|\mathbf{q}|^d$ for a sufficiently large value of β (Capello et al., 2006, 2007). However, these behaviors of the pseudo-potential, which are obtained by an energy minimization, are not sufficient to have a fully gapped phase, since a residual power-law behavior in the density-density correlations is still present.

As we mentioned above, the Jastrow wave function of Eq. (1.64) has been introduced to study continuum models (Jastrow, 1955) and has been employed to perform the first quantum Monte Carlo calculation in a many-body system

(McMillan, 1965). More precisely, a system of interacting bosons has been considered to model the ground-state properties of ^4He in three spatial dimensions with Lennard-Jones interactions. Here, in a first-quantization notation, the wave function with N_b bosons reads:

$$\Psi_J(\mathbf{r}_1, \dots, \mathbf{r}_{N_b}) = \prod_{i < j} f(r_{ij}) = \exp \left[- \sum_{i < j} u(r_{ij}) \right], \quad (1.66)$$

where $\{\mathbf{r}_i\}$ are the coordinates of the bosons and $f(r_{ij}) = \exp[-u(r_{ij})]$ is a function that depends upon the relative distance between two bosons $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$. Notice that the wave function of Eq. (1.66) is totally symmetric when exchanging two particles, thus having the correct symmetry for a bosonic wave function.

A suitable correlated wave function for N_e fermions can be obtained by applying the symmetric Jastrow factor $\prod_{i < j} f(r_{ij})$ to a (anti-symmetric) Slater determinant, which, by using first-quantization notations, reads as:

$$\Psi_{\text{HF}}(\mathbf{r}_1, \dots, \mathbf{r}_{N_e}) = \det\{\phi_\alpha(\mathbf{r}_j)\}, \quad (1.67)$$

where $\{\phi_\alpha(\mathbf{r}_j)\}$ is a set of one-particle orbitals. Then the Jastrow-Slater wave function is given by:

$$\Psi_{\text{JS}}(\mathbf{r}_1, \dots, \mathbf{r}_{N_e}) = \prod_{i < j} f(r_{ij}) \times \Psi_{\text{HF}}(\mathbf{r}_1, \dots, \mathbf{r}_{N_e}). \quad (1.68)$$

In total, this wave function is anti-symmetric when exchanging two particles and, therefore, has the correct symmetry for a fermionic state.

1.5.4 The Backflow Wave Function

Besides the inclusion of Jastrow factors, a different way to improve the non-interacting wave function is to construct a multi-determinant (variational) wave function that is written in terms of a linear combination of different quantum states. For example, within the configuration-interaction scheme (Szabo and Ostlund, 1996), we have:

$$|\Psi_{\text{CI}}\rangle = A_0 |\Psi_{\text{HF}}\rangle + \sum_{\alpha=1}^{N_c} A_\alpha |\Psi_{\text{HF},\alpha}\rangle, \quad (1.69)$$

where $|\Psi_{\text{HF}}\rangle$ is a given Hartree-Fock wave function, which is the ground-state of a suitable non-interacting Hamiltonian, and $\{|\Psi_{\text{HF},\alpha}\rangle\}$ is a set of states obtained by considering particle-hole excitations on top of $|\Psi_{\text{HF}}\rangle$; $\{A_\alpha\}$ denotes the set of variational parameters. By considering all possible virtual excitations, the approach

becomes exact. Indeed, this method is equivalent to computing the best state within the basis set of the above-mentioned wave functions. In practice, this technique is suitable to describe atoms and small molecules, for which N_c can be kept sufficiently small, but not extended systems, like solids, since in the latter case an exponentially large number of states is necessary to reach an accurate approximation of correlated systems.

An alternative and more practical way to include some correlation inside the original variational state is to introduce a parametrization that allows the orbitals to depend upon the positions of the other particles, leading to the concept of *backflow* correlations. In quantum systems, a particle that moves is surrounded by a counter-flow generated by all the other particles; the existence of this flow pattern pushes away the particles, thus preventing a significant overlap among them. This idea has been originally introduced by Wigner and Seitz (1934) and then developed by Feynman (1954) and Feynman and Cohen (1956) in the context of excitations in ^4He and the effective mass of a ^3He impurity in liquid ^4He . In the fermionic case, the Slater determinant is not constructed with the actual positions of the electrons $(\mathbf{r}_1, \dots, \mathbf{r}_{N_c})$, see Eq. (1.67), but with new “coordinates” given by:

$$\mathbf{r}_i^b = \mathbf{r}_i + \sum_{j \neq i} \eta(|\mathbf{r}_i - \mathbf{r}_j|)(\mathbf{r}_j - \mathbf{r}_i), \quad (1.70)$$

where $\eta(|\mathbf{r}_i - \mathbf{r}_j|)$ is a suitable function that describes the effective displacement of the i -th particle due to the j -th one. The simplest wave function is built by taking plane-waves with positions given by $\{\mathbf{r}_i^b\}$. The effect of backflow correlations introduces many-body effects inside the Slater determinant, since, when the i -th electron is moved, all the new “coordinates” are modified, such that all particles respond to the movement of the single electron, adapting their positions accordingly.

Wave functions including both Jastrow factors and backflow correlations have been used to study Helium systems within the so-called hyper-netted chain approximation (Pandharipande and Itoh, 1973; Schmidt and Pandharipande, 1979). Then, they have also been used in Monte Carlo calculations to compute the properties of the homogeneous electron gas in two and three spatial dimensions (Kwon et al., 1993, 1998). The advantage of the backflow wave function is that a single Slater determinant is used, allowing us to perform calculations with a large number of particles.

More recently, the same idea of modifying the single-electron orbitals to improve variational wave functions has been extended for lattice models (Tocchio et al., 2008, 2011). Here, the transformation (1.70) cannot be applied, since electrons live on the lattice sites. Nevertheless, we can imagine that the amplitudes of the Hartree-Fock orbitals (1.48) are changed according to the many-body configuration:

$$W_{\sigma,i,\alpha}^b = \eta_0 W_{\sigma,i,\alpha} + \sum_{j \neq i} \eta_j \mathcal{O}_{ij} W_{\sigma,j,\alpha}, \quad (1.71)$$

where $\{\eta_j\}$ is a set of variational parameters and \mathcal{O}_{ij} is a generic many-body operator that acts on the sites i and j . For example, within the repulsive Hubbard model, the formation of holon-doublon pairs is energetically expensive for large values of U/t ; therefore, these objects tend to recombine into singly occupied sites. In this case, we can consider a many-body operator $\mathcal{O}_{ij} = D_i H_j$, where D_i (H_i) is the operator that gives 1 if the site i is doubly occupied (empty) and 0 otherwise. Then, the many-body state, which is constructed by taking the Slater determinant of these new “orbitals,” will contain terms with single occupation, thus releasing the energy. More complicated expressions of the new “orbital” can be considered, as described by Tocchio et al. (2008, 2011).

1.5.5 The Haldane-Shastry Wave Function

As we have seen in the previous sections, Slater determinants describe non-interacting fermions, being constructed from single-particle orbitals, while Jastrow factors, parametrized by the pseudo-potential $f(r_{ij})$ that depends upon the relative positions of two particles, introduce a two-body correlation in the wave function. Remarkably, there are examples in which a Slater determinant is equivalent to a Jastrow factor. This is the case when the Slater determinant is constructed from the so-called Vandermonde matrix:

$$\mathbf{V} = \begin{pmatrix} 1 & \alpha_1 & \alpha_1^2 & \dots & \alpha_1^{N-1} \\ 1 & \alpha_2 & \alpha_2^2 & \dots & \alpha_2^{N-1} \\ 1 & \alpha_3 & \alpha_3^2 & \dots & \alpha_3^{N-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \alpha_N & \alpha_N^2 & \dots & \alpha_N^{N-1} \end{pmatrix}, \quad (1.72)$$

where α_i is a generic (complex) number. More concisely $V_{ij} = \alpha_i^{j-1}$. The determinant of this matrix is given by:

$$\det\{V_{ij}\} = \prod_{i < j} (\alpha_j - \alpha_i). \quad (1.73)$$

The equivalence between the determinant and a Jastrow factor is obtained once we can interpret $\{\alpha_i\}$ as the coordinates of the particles, as in Eq. (1.66). The simplest example of this correspondence is given by non-interacting spin-less fermions on a one-dimensional lattice (with L sites and periodic-boundary conditions):

$$\mathcal{H} = -t \sum_i c_i^\dagger c_{i+1} + \text{h.c.}; \quad (1.74)$$

then, the single-particle orbitals are given by plane waves, labeled by the momentum $k = 2\pi n/L$, with $n = 0, \dots, L-1$:

$$c_k^\dagger = \frac{1}{\sqrt{L}} \sum_j e^{-ikX_j} c_j^\dagger. \quad (1.75)$$

For an odd number of electrons, the many-body ground-state is unique and is obtained by filling the N_e lowest-energy levels:

$$\Psi_{\text{SF}}(X_1, \dots, X_{N_e}) = \det \begin{pmatrix} \alpha_1^{-L_e} & \alpha_1^{-(L_e-1)} & \dots & \alpha_1^{L_e} \\ \alpha_2^{-L_e} & \alpha_2^{-(L_e-1)} & \dots & \alpha_2^{L_e} \\ \vdots & \vdots & \ddots & \vdots \\ \alpha_{N_e}^{-L_e} & \alpha_{N_e}^{-(L_e-1)} & \dots & \alpha_{N_e}^{L_e} \end{pmatrix}, \quad (1.76)$$

where we have defined $\alpha_j \equiv \exp(-2\pi i X_j/L)$ and $L_e \equiv (N_e - 1)/2$. Then, the previous determinant can be recast in the following form:

$$\Psi_{\text{SF}}(X_1, \dots, X_{N_e}) = \prod_i \alpha_i^{-L_e} \det \begin{pmatrix} 1 & \alpha_1 & \dots & \alpha_1^{N_e-1} \\ 1 & \alpha_2 & \dots & \alpha_2^{N_e-1} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & \alpha_{N_e} & \dots & \alpha_{N_e}^{N_e-1} \end{pmatrix}, \quad (1.77)$$

which, apart from a phase factor, is a Vandermonde determinant:

$$\Psi_{\text{SF}}(X_1, \dots, X_{N_e}) = \prod_i \alpha_i^{-L_e} \prod_{i < j} (\alpha_j - \alpha_i). \quad (1.78)$$

Finally, by using the definition of the α_j 's, we obtain (apart from a normalization factor):

$$\Psi_{\text{SF}}(X_1, \dots, X_{N_e}) \propto \prod_{i < j} \sin \left(\frac{\pi(X_j - X_i)}{L} \right). \quad (1.79)$$

A much less trivial example in which an exact ground-state wave function can be written in terms of Vandermonde determinants is given by a Heisenberg model with long-range interactions in one dimension, namely the so-called Haldane-Shastry model (Haldane, 1988; Shastry, 1988):

$$\mathcal{H} = \sum_{i,j} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j, \quad (1.80)$$

where \mathbf{S}_i is the spin-1/2 operator on the site i and the super-exchange coupling is $J_{ij} = J/d_{ij}^2$, which depends upon the chord distance between two sites (i, j) :

$$d_{ij} = \frac{L}{\pi} \left| \sin \left[\frac{\pi(i-j)}{L} \right] \right|. \quad (1.81)$$

Here, the ground state is written as:

$$\Psi_{\text{HS}}(X_1, \dots, X_{N_e}) = \prod_i e^{\pi i X_i} \prod_{i < j} \left[\sin \left(\frac{\pi(X_j - X_i)}{L} \right) \right]^2, \quad (1.82)$$

where $\{X_i\}$ indicate the positions of the up spins. In second-quantization notation, the Haldane-Shastry wave function can be written as a Gutzwiller projected state of spinful electrons:

$$|\Psi_{\text{HS}}\rangle = \mathcal{P}_{\infty} \prod_{|k| < k_F} c_{k,\uparrow}^{\dagger} c_{k,\downarrow}^{\dagger} |0\rangle, \quad (1.83)$$

where $k_F = \pi/2$, i.e., $N_e = L/2$.

The elementary excitations of the Haldane-Shastry model are *fractional* $S = 1/2$ objects, called *spinons*, like in the Heisenberg model with nearest-neighbor interactions (Bethe, 1931; Faddeev and Takhtajan, 1981). However, the unique feature of the model with long-range interactions of Eq. (1.81) is that the spinon excitations are free and that the $S = 1$ spectrum is exhausted by two-spinon excitations (Haldane, 1991).

We finally mention that the Haldane-Shastry model has been motivated by a previous exact solution for a one-dimensional system with long-range interactions on the continuum (Sutherland, 1971):

$$\mathcal{H} = - \sum_i \frac{\partial^2}{\partial X_i^2} + \frac{g\pi^2}{L^2} \sum_{i < j} \left[\sin \left(\frac{\pi(X_j - X_i)}{L} \right) \right]^{-2}, \quad (1.84)$$

where g defines the coupling strength of the potential. Also in this case, the ground-state wave function has a Jastrow-like form, which depends upon a real number λ that is fixed by the value of g , i.e., $g = 2\lambda(\lambda - 1)$:

$$\Psi_{\text{Sutherland}}(X_1, \dots, X_{N_e}) = \prod_{i < j} \left[\sin \left(\frac{\pi(X_j - X_i)}{L} \right) \right]^{\lambda}. \quad (1.85)$$

1.5.6 The Laughlin Wave Function

Another example in which a Vandermonde determinant provides the exact ground-state wave function is when electrons on the continuum are confined in two spatial dimensions in the presence of an external magnetic field B . In particular, by using

the symmetric gauge and a disk geometry, the single-particle orbitals in the lowest Landau level are given by (Jain, 2012):

$$\psi_k(z_j) = C_k z_j^k e^{-\frac{eB}{4\hbar c} |z_j|^2}, \quad (1.86)$$

where k is a non-negative integer, C_k is the normalization factor, and $z_j = X_j - iY_j$ is a complex representation of the coordinates (X_j, Y_j) of the j -th particle in the plane. Therefore, the unique many-body state describing the filled lowest Landau level is given by the Vandermonde determinant with $V_{j,k} = z_j^{k-1}$ (apart from irrelevant terms):

$$\Psi_{\text{LLL}}(z_1, \dots, z_{N_e}) = \prod_{i < j} (z_j - z_i) = \det \begin{pmatrix} 1 & z_1 & \dots & z_1^{N_e-1} \\ 1 & z_2 & \dots & z_2^{N_e-1} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & z_{N_e} & \dots & z_{N_e}^{N_e-1} \end{pmatrix}. \quad (1.87)$$

Robert Laughlin had a very simple and accurate description of the incompressible quantum fluid that is obtained at fractional filling factors $\nu = 1/m$ (Laughlin, 1983). He was influenced by the form of the non-interacting wave function of the lowest Landau level (1.87) and the success of the Jastrow wave function of Eq. (1.66) to describe the superfluid ^4He . The Laughlin wave functions, apart from irrelevant constant terms, are given by:

$$\Psi_{\text{Laughlin}}(z_1, \dots, z_{N_e}) = \prod_{i < j} (z_j - z_i)^m. \quad (1.88)$$

Here, the correct symmetry properties when exchanging two electrons are obtained by odd integer values of m , corresponding to a filling factor $\nu = 1/m$ in the lowest Landau level. Remarkably, the Laughlin wave functions are the exact ground states of Hamiltonians with contact interactions (Haldane, 1983); moreover, they give an excellent description of the microscopic Hamiltonian with the full Coulomb interaction (Fano et al., 1986). On the one hand, the Laughlin wave function can be written as a Jastrow factor applied to the Vandermonde determinant of Eq. (1.87); indeed, by taking $m = 2p + 1$, we have that:

$$\Psi_{\text{Laughlin}}(z_1, \dots, z_{N_e}) = \prod_{i < j} (z_j - z_i)^{2p} \prod_{i < j} (z_j - z_i); \quad (1.89)$$

here, the first term (that is symmetric under particle exchange) can be seen as a Jastrow factor, which is applied to the second term (which is anti-symmetric). On the other hand, we can use the fact that $\prod_{i < j} (z_j - z_i)^{2p} = (-1)^{pm} \prod_i \prod_{j \neq i} (z_j - z_i)^p \propto \prod_i F(z_i)$, where $m = N_e(N_e - 1)/2$, such that:

$$\Psi_{\text{Laughlin}}(z_1, \dots, z_{N_e}) \propto \prod_i F(z_i) \prod_{i < j} (z_j - z_i) = \det \begin{pmatrix} F(z_1) & z_1 F(z_1) & \dots & z_1^{N_e-1} F(z_1) \\ F(z_2) & z_2 F(z_2) & \dots & z_2^{N_e-1} F(z_2) \\ \vdots & \vdots & \ddots & \vdots \\ F(z_{N_e}) & z_{N_e} F(z_{N_e}) & \dots & z_{N_e}^{N_e-1} F(z_{N_e}) \end{pmatrix}. \quad (1.90)$$

In this way, the Laughlin state can be expressed as a single determinant, with “renormalized” orbitals, in the spirit of backflow corrections.

The very surprising prediction of the Laughlin wave functions is that by creating a “hole” at position z_0 , an overall electric charge of e/m is lost, thus implying the existence of excitations with *fractional* quantum numbers and *fractional* (anyon) statistics (Arovas et al., 1984). Furthermore, the ground-state degeneracy, in the thermodynamic limit, depends on the topology of the space (Haldane, 1983; Haldane and Rezayi, 1985). The Laughlin state for $\nu = 1/m$ has a m^g degenerate ground state on a surface with genus g (e.g., $g = 0$ for a sphere and $g = 1$ for a torus). This degeneracy is not a consequence of a spontaneous symmetry breaking (or a symmetry of the Hamiltonian), but has a topological origin and, therefore, is robust against perturbations (Wen and Niu, 1990; Wen, 1991).

The Laughlin state (1.88) represents a suitable variational wave function also for bosonic systems, whenever m is an even integer. In particular, for $m = 2$ it represents the simplest case of an incompressible bosonic fluid. The latter state is the two-dimensional generalization of the Haldane-Shastry wave function (1.82) that has been defined in spin models.

Several other variational wave functions have been introduced in the context of the quantum Hall effect, to describe different filling factors. Among them, a particularly important one is given by the so-called Pfaffian state introduced by Moore and Read (1991), which should describe the $\nu = 5/2$ fraction (i.e., $\nu = 1/2$ in the second Landau level). The Moore-Read state has $p + ip$ pairing correlations and non-Abelian excitations with charge of $e/4$. Like the vortices in a p -wave superfluid, these quasiparticles are Majorana-fermion states at zero energy. Later, non-Abelian anyons have been further established in other quantum Hall states, e.g., the ones described by the Read-Rezayi states (Read and Rezayi, 1999).

1.5.7 The Bardeen-Cooper-Schrieffer Wave Function

One of the most celebrated variational wave functions in condensed matter physics is given by the Bardeen-Cooper-Schrieffer (BCS) approach that has been proposed to explain superconductivity originating from electron-phonon coupling (Bardeen et al., 1957; Schrieffer, 1964). In several metals, the coupling between electrons

and lattice vibrations (phonons) induces an effective attraction between electrons, thus creating a bound state of particles with opposite momenta (\mathbf{k} , $-\mathbf{k}$) and opposite spins. For a translational invariant system, the BCS wave function reads as:

$$|\Psi_{\text{BCS}}\rangle = \exp\left(\sum_k f_k c_{k,\uparrow}^\dagger c_{-k,\downarrow}^\dagger\right) |0\rangle, \quad (1.91)$$

where f_k is the *pairing function*. We would like to emphasize that the BCS wave function has not a fixed number of particles, being a superposition of states with all possible (even) number of particles; therefore, it breaks the global $U(1)$ symmetry related to charge conservation.

The BCS wave function is the ground state of the non-interacting BCS Hamiltonian, which will be used often in the following as a starting point to define correlated wave functions:

$$\mathcal{H} = \sum_{k,\sigma} (\epsilon_k - \mu_0) c_{k,\sigma}^\dagger c_{k,\sigma} + \sum_k \Delta_k c_{k,\uparrow}^\dagger c_{-k,\downarrow}^\dagger + \text{h.c.}, \quad (1.92)$$

where ϵ_k gives the band structure, e.g., the one of Eq. (1.23), μ_0 is the chemical potential, and $\Delta_k = \Delta_{-k}$ is a (for simplicity, real) singlet pairing amplitude. The BCS Hamiltonian can be cast in a simple 2×2 matrix form (apart from constant terms):

$$\mathcal{H} = \sum_{k,\sigma} \begin{pmatrix} c_{k,\uparrow}^\dagger & c_{-k,\downarrow} \end{pmatrix} \begin{pmatrix} \epsilon_k - \mu_0 & \Delta_k \\ \Delta_k & -\epsilon_k + \mu_0 \end{pmatrix} \begin{pmatrix} c_{k,\uparrow} \\ c_{-k,\downarrow}^\dagger \end{pmatrix}. \quad (1.93)$$

The 2×2 matrix can be diagonalized by a unitary transformation:

$$\begin{pmatrix} \beta_k \\ \gamma_k \end{pmatrix} = \begin{pmatrix} u_k & -v_k \\ v_k & u_k \end{pmatrix} \begin{pmatrix} c_{k,\uparrow} \\ c_{-k,\downarrow}^\dagger \end{pmatrix}, \quad (1.94)$$

where $u_k^2 + v_k^2 = 1$ preserves the anti-commutation relations. Then, denoting the BCS spectrum by:

$$E_k = \sqrt{(\epsilon_k - \mu_0)^2 + \Delta_k^2}, \quad (1.95)$$

we obtain (apart from constant terms):

$$\mathcal{H} = \sum_k E_k \left(\beta_k^\dagger \beta_k + \gamma_k^\dagger \gamma_k \right). \quad (1.96)$$

The ground state $|\Psi_{\text{BCS}}\rangle$ is obtained by imposing that:

$$\beta_k |\Psi_{\text{BCS}}\rangle = 0, \quad (1.97)$$

$$\gamma_k |\Psi_{\text{BCS}}\rangle = 0, \quad (1.98)$$

which directly lead to the form of Eq. (1.91) with $f_k = v_k/u_k$.

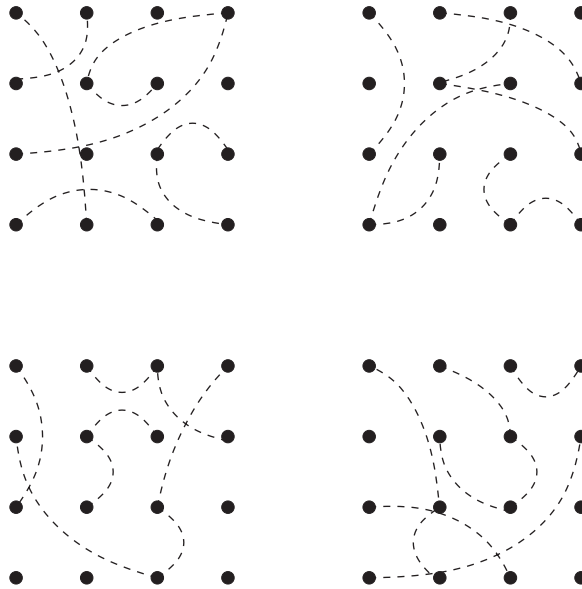


Figure 1.2 In a 4×4 cluster, we show four singlet-pair patterns of the BCS wave function. The dashed lines denote the singlet pairing among sites (i, j) . The case with 8 singlets, i.e., 16 electrons, is shown. Notice that the BCS wave function allows configurations with doubly occupied sites, namely cases where two dashed lines joint in a single site.

At this point, it is useful to rewrite the BCS state in real space:

$$|\Psi_{\text{BCS}}\rangle = \exp \left(\sum_{ij} f_{ij} c_{i,\uparrow}^\dagger c_{j,\downarrow}^\dagger \right) |0\rangle = \sum_{N_p} \frac{1}{N_p!} \left(\sum_{ij} f_{ij} c_{i,\uparrow}^\dagger c_{j,\downarrow}^\dagger \right)^{N_p} |0\rangle, \quad (1.99)$$

where the pairing function in real space $f_{ij} = f_{ji}$ depends on $\mathbf{R}_i - \mathbf{R}_j$. Therefore, for each sector with $N_e = 2N_p$ electrons, the wave function is a linear combination of all possible singlet-pair patterns on the lattice (see Fig. 1.2).

Within the BCS theory, superconductivity is an instability of the metallic phase, which is described by a Fermi liquid (Nozieres, 1964); here, the direct electron-electron repulsion is efficiently screened and turns out to be treated as a small perturbation that does not drastically change the non-interacting picture. However, the presence of phonons induces an attraction among electrons, leading to an instability towards the formation of a liquid of electron pairs. In many superconducting materials, it is well established that the BCS pairing is originated by the electron-phonon coupling; in this case, the BCS theory and its further refinements give an accurate description (Schrieffer, 1964). Instead, there are several compounds in which it is less clear whether the origin of the electron attraction is mediated by

phonons or by other modes (e.g., charge and/or spin fluctuations). For example, in various transition-metal oxides, there are two important aspects that have been considered crucial: the incipient presence of an insulating phase and the lack of screening effects, leading to a strong electron-electron repulsion. In a seminal paper, Anderson (1987) suggested an alternative approach, based upon a Gutzwiller projected BCS wave function, which we describe in the following section.

1.5.8 The Resonating-Valence Bond Wave Function

The RVB theory of high-temperature superconductivity is based upon the work done by Anderson and collaborators (Anderson, 1987; Anderson et al., 1987; Baskaran and Anderson, 1988), who suggested that a superconducting phase may emerge when doping a Mott insulator with “preformed” singlet pairs. In fact, the RVB state describes a liquid of spin singlets, and was proposed originally as a variational ground state of the $S = 1/2$ Heisenberg model on the triangular lattice. The key feature is that the singlets of the RVB insulator become mobile when the system is doped and thus they form real superconducting pairs. A suitable and elegant representation of the RVB state is given by Gutzwiller projecting the BCS state:

$$|\Psi_{\text{RVB}}\rangle = \mathcal{P}_{\infty}|\Psi_{\text{BCS}}\rangle. \quad (1.100)$$

Since the Gutzwiller projector imposes to have one electron per site, the RVB wave function is clearly insulating, with no density fluctuations. Anderson (1987) suggested that the RVB state could be very close in energy to the Néel state for undoped materials. However, for a generic (translational invariant) pairing function f_k , $|\Psi_{\text{RVB}}\rangle$ does not possess long-range magnetic order, being described by a linear combination of an exponentially large number of singlet coverings of the lattice. In fact, starting from the BCS state, which contains all possible coverings of singlets (including the ones in which two electrons with opposite spins occupy the same site – see Fig. 1.2), the Gutzwiller projector annihilates the configurations with these overlapping singlets and leaves untouched all the others (Gros, 1989), as shown in Fig. 1.3. The simplest case in which $f_{i,j} \neq 0$ only for nearest-neighbor sites is called short-range RVB state and represents an important example of a gapped insulator with *fractional* spin excitations (spinons) and topological degeneracy. Indeed, the lowest-energy spin excitation of the short-range RVB is obtained by “breaking” a singlet pair to form a triplet, which costs an energy $E = O(J)$ for the Heisenberg Hamiltonian with super-exchange coupling J . Moreover, the two spin-1/2 objects (spinons) that are created in this process are not bound together, since they can be separated without any further energy cost by rearranging the other singlets around them (see Fig. 1.4). In addition to spinons, a short-range RVB sustains also gapped excitations that do not carry spin, the so-called *visons*

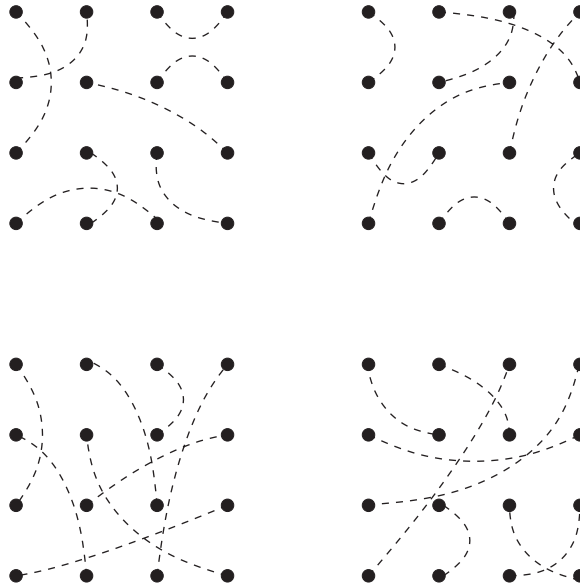


Figure 1.3 In a 4×4 cluster, we show four singlet-pair patterns of the projected BCS wave function, i.e., the RVB state. The dashed lines denote the singlet pairing among sites (i, j) . The case with 8 singlets, i.e., 16 electrons, is shown. Here, in contrast to Fig. 1.2, all the configurations have singly occupied sites, namely there is always one dashed line coming out from each site.

(Kivelson et al., 1987; Read and Chakraborty, 1989; Senthil and Fisher, 2000). In the thermodynamic limit, the ground state has a degeneracy 4^g that depends upon the genus g of the surface on which the short-range RVB state is defined (Read and Chakraborty, 1989). As for the fractional quantum Hall effect, this degeneracy is not related to any spontaneous symmetry breaking, but it has a topological origin. The connection between the existence of excitations with fractional quantum numbers (and statistics) and the presence of topological order has been discussed by Oshikawa and Senthil (2006).

The generic long-range RVB wave function is obtained by allowing long-range singlets, i.e., considering $f_{i,j} \neq 0$ also for distant couples of sites (i, j) . Equivalently, we can consider a generic BCS Hamiltonian and construct its ground state. The physical properties of the Gutzwiller projected state should reflect those of the BCS wave function. In particular, the BCS Hamiltonian may lead either to a gapped or to a gapless excitation spectrum, which is expected to be related to the spin excitations of the RVB state. While a gapped spectrum should imply gapped spin excitations (as for the short-range RVB), for a gapless spectrum, “breaking” very long-range singlets may have a negligible cost for a short-range Hamiltonian, thus leading to a gapless RVB state. Whether there exist two-dimensional models with

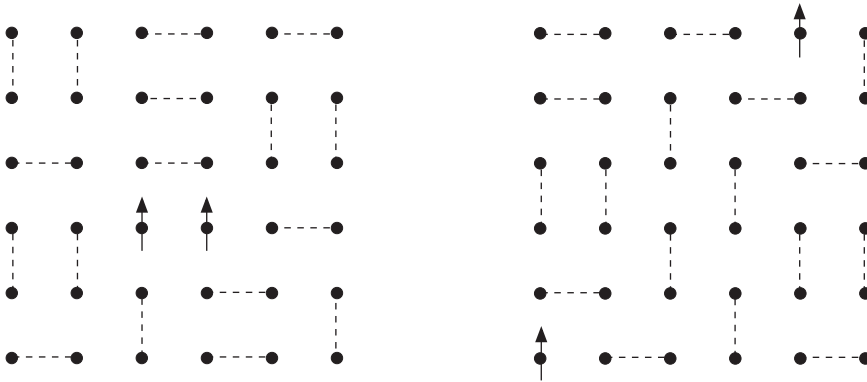


Figure 1.4 In a 6×6 cluster, a singlet pair is “broken” into a triplet, with two spinons with up spins (left). Singlets (only at nearest-neighbor sites) are shown as dashed lines. The spinons can separate themselves without any energetic cost, since the singlet background may rearrange around them (right). Therefore, they represent elementary excitations with spin $S = 1/2$ (and no charge).

an RVB ground state is still an open question; however, in various frustrated Heisenberg models, (long-range) RVB states provide very accurate variational energies (Capriotti et al., 2001; Iqbal et al., 2011).

We would like to emphasize that the definition of Eq. (1.100) is rather general and allows an efficient Monte Carlo sampling on any lattice geometry. An alternative definition of the RVB wave function is given by Liang et al. (1988); however, in this case, an efficient sampling is possible only for bipartite lattices, while for other geometries the variational Monte Carlo approach has the sign problem that usually is so serious to prevent us from obtaining reliable results on large clusters.

When mobile holes are considered, e.g., within the t – J model of Eq. (1.33), the RVB wave function describes a superconducting state, as shown by using variational Monte Carlo techniques (Gros et al., 1987; Gros, 1988). Notice that, in this case, the Gutzwiller projector must allow empty sites, e.g., $\mathcal{P}_\infty \rightarrow \tilde{\mathcal{P}}_\infty = \prod_i (1 - n_{i,\uparrow} n_{i,\downarrow})$. Indeed, it has been shown that the RVB state represents an accurate variational *Ansatz* for describing the ground state of the t – J model in a wide range of parameters (Sorella et al., 2002; Hu et al., 2012), even though states with charge and spin modulations also give competitive energies (White and Scalapino, 1998; Corboz et al., 2014).

1.6 Size Extensivity

In the definition of a variational wave function for a macroscopic system, i.e., a system defined by a Hamiltonian with a fixed density in the thermodynamic limit $L \rightarrow \infty$, an important concept is given by the so-called size extensivity. This term

is borrowed from thermodynamics, where extensive properties are the ones that are proportional to the size of the system (Bartlett, 1981). Loosely speaking, a wave function is size extensive if the coupling between small, but macroscopic, sub-systems can be neglected; then, the wave function is written (apart from boundary corrections) as a product of independent factors, each one defined in a given sub-system:

$$|\Psi\rangle \approx \prod_{\text{sub-system}} |\Psi_{\text{sub-system}}\rangle. \quad (1.101)$$

In this way, for local Hamiltonians $\mathcal{H} \approx \sum_{\text{sub-system}} \mathcal{H}_{\text{sub-system}}$ (i.e., the coupling between different sub-systems can be neglected on a macroscopic scale), the total energy is explicitly given by the sum of the energies in each sub-system:

$$\frac{\langle \Psi | \mathcal{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle} \approx \sum_{\text{sub-system}} \frac{\langle \Psi_{\text{sub-system}} | \mathcal{H}_{\text{sub-system}} | \Psi_{\text{sub-system}} \rangle}{\langle \Psi_{\text{sub-system}} | \Psi_{\text{sub-system}} \rangle}, \quad (1.102)$$

namely, an extensive quantity that is linear in the volume and the number of particles. This definition is very similar to standard concepts in classical thermodynamics, where, for example, the canonical distribution is given by the Boltzmann distribution, $\mathcal{P}(E) \propto \exp(-\beta E)$, where β is the inverse temperature. Size extensivity tells us that the entanglement between different macroscopic sub-systems is negligible in the thermodynamic limit; from this point of view, it represents a necessary condition for satisfying the so-called *area law*, a celebrated property of the low-energy spectrum of Hamiltonians with a gap (Eisert et al., 2010). With this definition, it turns out that size-extensive wave functions can be written in an exponential form (like for example Jastrow or BCS wave functions), where the exponent contains a size-extensive operator that can allow the factorization of the total wave function in the various sub-systems.

1.6.1 A Simple Model for Size Extensivity

Consider a simple model for phonons in a lattice with L sites, described by the following Hamiltonian:

$$\mathcal{H} = \omega \sum_i a_i^\dagger a_i + g \sum_i (a_i^\dagger + a_i), \quad (1.103)$$

where a_i^\dagger (a_i) creates (destroys) a phonon on the site i . Here, exciting a phonon on each site costs an energy ω and g defines the stress tension that determines the equilibrium positions of the nuclei. The Hamiltonian is just the sum of non-interacting Hamiltonians acting on each site, which can be considered a sub-system in Eq. (1.101). The ground state is given by:

$$|\Upsilon_0\rangle = \prod_i e^{-\gamma a_i^\dagger} |0\rangle, \quad (1.104)$$

where $\gamma = g/\omega$. Its energy $E_0 = -Lg^2/\omega$ is correctly extensive, which is consistent with the fact that the wave function is a product of exponential factors. Therefore, the exact solution of this model is clearly size extensive, since any sub-system has no interaction with the other ones.

In order to emphasize the importance of having an exponential form of the wave function, let us consider a much simpler variational *Ansatz* given by:

$$|\Psi_{\text{lin}}\rangle = \left(1 + \alpha \sum_i a_i^\dagger\right) |0\rangle. \quad (1.105)$$

A simple calculation shows that:

$$E_{\text{lin}}(\alpha) = \frac{\langle \Psi_{\text{lin}} | \mathcal{H} | \Psi_{\text{lin}} \rangle}{\langle \Psi_{\text{lin}} | \Psi_{\text{lin}} \rangle} = \frac{\omega \alpha^2 L + 2g\alpha L}{1 + L\alpha^2}. \quad (1.106)$$

In the thermodynamic limit ($L \rightarrow \infty$), the minimization of $E_{\text{lin}}(\alpha)$ does not lead to an extensive energy:

$$E_{\text{lin}}(\alpha) \propto -\sqrt{L}, \quad (1.107)$$

which implies that the linear *Ansatz* of Eq. (1.105) is not size extensive.

1.6.2 The Classical Mapping

In this section, we discuss some general aspects of the variational wave functions. In particular, whenever we are focusing on *diagonal* operators (in the chosen basis set $\{|x\rangle\}$), the quantum expectation values over a wave function $|\Psi_{\text{var}}\rangle$ can be expressed in terms of a classical partition function at finite temperature, in the same spatial dimensions (Capello et al., 2006; Kaneko et al., 2016). This correspondence is very useful to show that quantum phase transitions are possible within the variational picture and enables us to make some general statements on the size extensivity of the wave function. To prove the mapping between quantum expectation values and classical partition functions, let us consider a basis set $\{|x\rangle\}$ in which particles have definite positions in the lattice. Then, the quantum average of any operator \mathcal{O} , which is diagonal in this basis, can be written in terms of the *classical* distribution:

$$\frac{\langle \Psi_{\text{var}} | \mathcal{O} | \Psi_{\text{var}} \rangle}{\langle \Psi_{\text{var}} | \Psi_{\text{var}} \rangle} = \sum_x \mathcal{P}(x) \langle x | \mathcal{O} | x \rangle, \quad (1.108)$$

where $\mathcal{P}(x)$ is given by:

$$\mathcal{P}(x) = \frac{|\langle x | \Psi_{\text{var}} \rangle|^2}{\langle \Psi_{\text{var}} | \Psi_{\text{var}} \rangle}. \quad (1.109)$$

Since $\mathcal{P}(x) \geq 0$ and $\sum_x \mathcal{P}(x) = 1$, there is a precise correspondence between the wave function and an effective classical potential $V_{\text{cl}}(x)$:

$$\mathcal{P}(x) \equiv \frac{1}{\mathcal{Z}} e^{-V_{\text{cl}}(x)}. \quad (1.110)$$

The explicit form of the potential $V_{\text{cl}}(x) = -2 \ln |\langle x | \Psi_{\text{var}} \rangle|$ depends upon the choice of the variational wave function. In particular, it is interesting to consider a Jastrow or Jastrow-Slater state $|\Psi_{\text{var}}\rangle = \mathcal{J}|\Phi_0\rangle$ of Eq. (1.64). In this case, we have that:

$$V_{\text{cl}}(x) = \sum_{i,j} v_{ij} [n_i(x) - n] [n_j(x) - n] - 2 \ln |\Phi_0(x)|, \quad (1.111)$$

where $n_i(x)$ is the electron density at site i for the configuration $|x\rangle$, i.e., $n_i|x\rangle = n_i(x)|x\rangle$ and $\Phi_0(x) = \langle x | \Phi_0 \rangle$ is the amplitude of the non-interacting state over the configuration $|x\rangle$. The first term of Eq. (1.111) is a two-body potential, which describes a classical model of charged particles (e.g., in the fermionic case, $n_i(x) = 1$ represents the “background” charge, while holons and doublons carry charge $+1$ and -1 , respectively) mutually interacting through a given potential. The second term in Eq. (1.111) gives a generic potential, which includes multi-body effects. However, when density fluctuations are suppressed (for example, in presence of a large Gutzwiller factor), the quadratic term gives the most relevant contribution. In this case, we can explicitly consider the overall scale of the pseudo-potential β , i.e., $v_{ij} = \beta \bar{v}_{ij}$, as an inverse *classical* temperature. By using this kind of Jastrow-Slater wave functions, Kaneko et al. (2016) have shown that spontaneous symmetry breaking phenomena are possible within the variational approach when varying the strength of the Jastrow factor β . More precisely, even when both the non-interacting state $|\Phi_0\rangle$ and the Jastrow factor \mathcal{J} preserve all the lattice and spin symmetries, clear signatures of order can be obtained. We would like to emphasize the fact that Jastrow wave functions are size extensive whenever the pseudo-potential v_{ij} gives rise to a stable classical model.

1.7 Projection Techniques

Variational wave functions can be improved by using the so-called *projection techniques*, which filter out the high-energy components of the “initial” (or trial) variational state. The main idea is very simple and relies on the fact that the exact ground state can be obtained by applying the so-called *power method*; let us take an initial wave function $|\Psi_0\rangle$ that may be chosen to be the best variational state $|\Psi_{\text{var}}\rangle$. Whenever the initial state $|\Psi_0\rangle$ has a finite overlap with the exact ground state $|\Upsilon_0\rangle$, we have that:

$$\lim_{n \rightarrow \infty} (\Lambda - \mathcal{H})^n |\Psi_0\rangle \propto |\Upsilon_0\rangle, \quad (1.112)$$

where Λ is a diagonal operator with $\Lambda_{x,x} = \lambda$, where λ is a real number to be specified later. In fact, Eq. (1.112) can be implemented iteratively by defining:

$$|\Psi_{n+1}\rangle = (\Lambda - \mathcal{H})|\Psi_n\rangle. \quad (1.113)$$

Then, by using the expansion of Eq. (1.39) for the initial state, we have that:

$$\begin{aligned} (\Lambda - \mathcal{H})^n |\Psi_0\rangle &= \sum_i a_i (\lambda - E_i)^n |\Upsilon_i\rangle = \\ &= (\lambda - E_0)^n \left[a_0 |\Upsilon_0\rangle + \sum_{i \neq 0} a_i \left(\frac{\lambda - E_i}{\lambda - E_0} \right)^n |\Upsilon_i\rangle \right]. \end{aligned} \quad (1.114)$$

By choosing λ such that:

$$\text{Max}_i |\lambda - E_i| = |\lambda - E_0|, \quad (1.115)$$

namely for $\lambda > (E_{\max} + E_0)/2$, where E_{\max} is the maximum eigenvalue of \mathcal{H} , the ground-state component in the expansion (1.114) grows much faster than all the other ones for $n \rightarrow \infty$, leading to the ground state $|\Upsilon_0\rangle$, apart from an irrelevant normalization factor $a_0(\lambda - E_0)^n$. Notice that the convergence of $|\Psi_n\rangle$ to $|\Upsilon_0\rangle$ is obtained with an exponentially increasing accuracy in n , namely with an error that is proportional to δ^n , where $\delta = (\lambda - E_1)/(\lambda - E_0)$.

The iterative procedure of Eq. (1.113) is computationally affordable when the Hamiltonian is *sparse*, which is the case of *local* Hamiltonians that contain non-diagonal processes involving only few electrons at relatively short distances. Here, although the number of possible configurations $|x\rangle$ grows exponentially with the number of particles, whenever the Hamiltonian acts on a single configuration, it generates only a relatively small number of configurations. Therefore, the $\mathcal{N} \times \mathcal{N}$ matrix $H_{x,x'}$ has only $O(L \times \mathcal{N})$ non-zero elements over \mathcal{N}^2 total entries. Due to the sparseness of the matrix, each iteration (1.113) is relatively easy to perform, as only the knowledge of the non-vanishing matrix elements are required:

$$\Psi_{n+1}(x') = \sum_x (\lambda \delta_{x',x} - \mathcal{H}_{x',x}) \Psi_n(x), \quad (1.116)$$

where $\Psi_n(x) = \langle x | \Psi_n \rangle$. This iterative step can be performed *exactly* whenever the whole Hilbert space can be kept in the computer memory, by using two vectors of dimension \mathcal{N} , i.e., $\Psi_{n+1}(x)$ and $\Psi_n(x)$. On the other hand, when the dimension of the Hilbert space is too large to be stored, the iterative procedure can be implemented stochastically, as we will describe in Chapter 8.

Finally, we mention that an alternative approach to filter out the high-energy components of the trial wave function is to consider an imaginary-time propagation:

$$\lim_{\tau \rightarrow \infty} e^{-\tau \mathcal{H}} |\Psi_0\rangle \propto |\Upsilon_0\rangle. \quad (1.117)$$

Indeed, as before, by using the expansion of Eq. (1.39) for the initial state, we have that:

$$e^{-\tau\mathcal{H}}|\Psi_0\rangle = \sum_i a_i e^{-\tau E_i} |\Upsilon_i\rangle = e^{-\tau E_0} \left[a_0 |\Upsilon_0\rangle + \sum_{i \neq 0} a_i e^{-\tau(E_i - E_0)} |\Upsilon_i\rangle \right], \quad (1.118)$$

which shows that all the components with $i \neq 0$ are exponentially suppressed with respect to the ground state for $\tau \rightarrow \infty$; therefore, this procedure leads to the ground state $|\Upsilon_0\rangle$, apart from an irrelevant normalization factor $a_0 \exp(-\tau E_0)$. Notice that, whenever the energy spectrum is not bounded from above (i.e., $E_{\max} = \infty$), it is necessary to consider this approach, since the condition $\lambda > (E_{\max} + E_0)/2$ cannot be satisfied. The imaginary-time propagation is often implemented, with a Trotter approximation, in stochastic approaches, as we will discuss in Chapter 11.