Chapter 9

Many–Particle Systems

In this chapter we develop the quantummechanical description of non-relativistic many–particle-systems. Systems to which this chapter applies appear in many disguises, as electrons in crystals, molecules and atoms, as photons in the electromagmetic field, as vibrations and combination of electrons and phonons in crystals, as protons and neutrons in nuclei and, finally, as quarks in mesons and baryons. The latter systems require, however, relativistic descriptions.
The interaction among many identical particles gives rise to a host of fascinating phenomena, e.g., collective excitations in nuclei, atoms and molecules, superconductivity, the quantum Hall effect. A description of the mentioned phenomena requires a sufficient account of the interactions among the particles and of the associated many–particle motions. In the following we will introduce the rudimentary tools, mainly those tools which are connected with effective single–particle descriptions.

9.1 Permutation Symmetry of Bosons and Fermions

We seek to determine the stationary states of systems of many *identical* particles as described through the stationary Schrödinger equation

$$H\,|\Psi\rangle \;=\; E\,|\Psi\rangle\;. \tag{9.1}$$

Here $|\Psi\rangle$ represents the state of the system which in the following will be considered in a representation defined by *space–spin–coordinates* $\vec{x}_j \;=\; (\vec{r}_j, \sigma_j)$. $\vec{r}_j$ and σ_j denote position and spin, respectively, of the j-th particle. The spin variable for electrons, for example, is $\sigma_j \;=\; \pm\frac{1}{2}$. We will assume systems composed of N particles, i.e., the particle index j runs from 1 to N. The wave function in the space–spin representation is then

$$\Psi(\vec{x}_1, \vec{x}_2, \ldots \vec{x}_N) \;=\; \langle \vec{x}_1, \vec{x}_2, \ldots \vec{x}_N\,|\Psi\rangle\;. \tag{9.2}$$

Permutations

The essential aspect of the systems described is that the particles are assumed to be identical. This has the consequence that one cannot distinguish between states which differ only in a permutation of particles. In fact, quantum theory dictates that all such states are identical, i.e., are not counted

repeatedly like degenerate states. However, not any state can be chosen as to represent the many–particle system, rather only states which obey a certain transformation property under permutations are acceptable. This property will be established now. In the following sections we will then introduce the *operators of second quantization* which provide a means to ascertain that manipulation of wave functions always leave the transformation property under permutations uncompromised.

The permutations we need to consider for a system of N particles are the elements of the group S_N, the set of all permutations of N objects. The elements $P \in S_N$ can be represented conveniently as $2 \times N$ matrices, the top row representing the numbers 1 to N labelling the N particles under consideration, and the second row showing the numbers 1 to N again, but in a different order, number k under the entry j of the first row indicating that particle j is switched with particle k. Examples for an eight particle system are

$$P_1 = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\ 1 & 2 & 4 & 5 & 6 & 3 & 8 & 7 \end{pmatrix}; \; P_2 = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\ 1 & 2 & 3 & 5 & 4 & 6 & 7 & 8 \end{pmatrix}. \tag{9.3}$$

P_2 which affects only two particles, i.e., particles 4 and 5, leaving all other particles unchanged, is called a transposition. Transpositions denoted by $T(j,k)$ are characterized by the two indices (j,k) of the two particles transposed, i.e., $(j,k) = (4,5)$ in case of P_2. We can then state $P_2 = T(4,5)$.

We will not discuss here at any depth the properties of the permutation groups S_N, even though these properties, in particular, the representations in the space of N–particle wave functions are extremely useful in dealing with N–particle systems. A reader interested in the quantum mechanical description of N particle systems is strongly encouraged to study these representations. For the following we will require only two properties of S_N, namely implicitly the group property, and explicitly the fact that any $P \in S_N$ can be given as a product of transpositions $T(j,k)$. The latter factorization has the essential property that the number of factors is either even or odd, i.e., a given P can either only be presented by even numbers of transpositions or by odd numbers of transpositions. One calls permutations of the first type *even permutations* and permutations of the second type *odd permutations*. The group S_N is then composed of two disjunct classes of even and of odd permutations. For the permutations P_1 and P_2 given above holds

$$P_1 \; = \; T(3,4)\,T(4,5)\,T(5,6)\,T(6,3)\,T(7,8)\;; \quad P_2 \; = \; T(4,5) \tag{9.4}$$

both permutations being obviously odd. The product $P_1 P_2$ of even and odd permutations P_1 and P_2 obey the following multiplication table:

$P_2 \setminus P_1$	even	odd
even	even	odd
odd	odd	even

We finally determine the action of permutations P on the wave functions (9.2). Denoting by $P(j)$ the image of j, i.e., in notation (9.3) the j-th index in the second row, one can state

$$P\,\Psi(\vec{x}_1, \vec{x}_2, \ldots, \vec{x}_j, \ldots, \vec{x}_N) \; = \; \Psi(\vec{x}_{P(1)}, \vec{x}_{P(2)}, \ldots, \ldots, \vec{x}_{P(j)}, \ldots, \vec{x}_{P(N)})\,. \tag{9.5}$$

Permutation Symmetry

A second consequence of the identical character of the particles under consideration is that the Hamiltonian must reflect the permutation symmetry. In fact, the Hamiltonian must be of the type

$$H \;=\; \sum_{j=1}^{N} F(\vec{x}_j) \;+\; \frac{1}{2}\sum_{j,k=1}^{N} G(\vec{x}_j, \vec{x}_k) \tag{9.6}$$

which describes one–particle interactions and two–particle interactions of the system. $G(\vec{x}_j, \vec{x}_k)$ is symmetric in its two arguments. The terms of the Hamiltonian will be discussed further below. Presently, it is essential that the functions $F(\,)$ and $G(\,,\,)$ are the same for all particles and for all pairs of particles, all particles being governed by the same interactions. From this property follows that H is independent of any specific assignment of indices to the particles (note that (9.5) implies that a permutation effectively changes the indices of the particles) and, hence, the Hamiltonian for permuted indices PHP^{-1} is identical to H. From the latter results

$$[H, P] \;=\; 0\,. \tag{9.7}$$

This property, in turn, implies that the permutation operators can be chosen in a diagonal representation. In fact, it is a postulate of quantum mechanics that for any description of many–particle systems the permutation operators must be diagonal. Since permutations do not necessarily commute, a diagonal representation can only berealized in a simpler group. In fact, the representation is either isomorphic to the group composed of only the '1', i.e., 1 together with multiplication, or the corresponding group of two elements $1, -1$. The first case applies to bosons, i.e. particles with integer spin values, the second group to fermions, i.e., particles with half–integer spin values. In the latter case all even permutations are represented by '1' and all odd permutations by '-1'. Obviously, both groups, i.e., {1} (trivial) and {1,-1}, provide a representation of the group structure represented by the multiplication table of even and odd permutations given above.
The boson and fermion property stated implies that for a system of N *bosons* holds

$$P\,|\Psi\rangle \;=\; |\Psi\rangle \quad \forall P \in S_N\,. \tag{9.8}$$

For *fermions* holds

$$P\,|\Psi\rangle \;=\; \epsilon_P\,|\Psi\rangle \quad \forall P \in S_N \tag{9.9}$$

where

$$\epsilon_P \;=\; \begin{cases} 1 & \text{for } P \text{ even} \\ -1 & \text{for } P \text{ odd} \end{cases}\,. \tag{9.10}$$

We will construct now wave functions which exhibit the appropriate properties.

Fock-Space

Our derivation will start by placing each particle in a set of S *orthonormal* single particle states $\langle\vec{x}|k\rangle \;=\; \phi_k(\vec{x})$, $k = 1, 2, \ldots S$ where S denotes the number of available single particle states, usually a very large number. The single particle states are assumed to be orthonormal, i.e., for the scalar product holds

$$\langle j|k\rangle \;=\; \delta_{j\,k}\,. \tag{9.11}$$

The scalar product involves spin as well as space coordinates and is explicitly given by

$$\langle j|k\rangle \;=\; \int d^3r\, \phi_j^*(\vec{r})\, \phi_k(\vec{r}) \;\cdot\; \langle \sigma_j|\sigma_k\rangle \tag{9.12}$$

where the second factor represents the scalar product between spin states. We first consider orthonormal many–particle wave functions, the so-called Fock-states, which do not yet obey the symmetries (9.8, 9.9). In a second step we form linear combinations of Fock states with the desired symmetries.
The Fock states represent N particles which are placed into S states $|\lambda_1\rangle, |\lambda_2\rangle, \ldots, |\lambda_N\rangle$, $\lambda_j \in \{1, 2, \ldots S\}$ of the type (9.11, 9.12), each particle j into a specific state $|\lambda_j\rangle$, i.e.,

$$\langle \vec{x}_1, \vec{x}_2, \ldots \vec{x}_N|\Psi^{\mathrm{Fock}}(\lambda_1, \lambda_2, \ldots, \lambda_N)\rangle \;=\; \prod_{j=1}^{N} \phi_{\lambda_j}(\vec{x}_j)\;. \tag{9.13}$$

These states form an orthonormal basis of N-particle states. It holds

$$\langle \Psi^{\mathrm{Fock}}(\lambda_1', \lambda_2', \ldots, \lambda_N')|\Psi^{\mathrm{Fock}}(\lambda_1, \lambda_2, \ldots, \lambda_N)\rangle \;=\; \prod_{j=1}^{N} \delta_{\lambda_j' \lambda_j}\;. \tag{9.14}$$

Obviously, the states $|\Psi^{\mathrm{Fock}}(\lambda_1, \lambda_2, \ldots, \lambda_N)\rangle$ do not exhibit the symmetries dictated by (9.8, 9.9).

Wave Functions with Boson Symmetry in the Occupation Number Representation

Wave functions with the proper symmetries can be obtained as linear combinations of Fock states. A wave function which obeys the boson symmetry (9.8) is

$$\langle \vec{x}_1, \vec{x}_2, \ldots \vec{x}_N|\Psi^{\mathrm{B}}(n_1, n_2, \ldots, n_S)\rangle \;= \tag{9.15}$$

$$\left[\frac{\prod_{j=1}^{S}(n_j!)}{N!}\right]^{\frac{1}{2}} \sum\nolimits_{P\in\Lambda(\lambda_1,\ldots\lambda_N)} P\,\langle \vec{x}_1, \vec{x}_2, \ldots \vec{x}_N|\Psi^{\mathrm{Fock}}(\lambda_1, \lambda_2, \ldots\; .\lambda_N)\rangle$$

Here the states $(\lambda_1, \lambda_2, \ldots\; .\lambda_N)$ on the rhs. is a particular choice of placing N particles consistent with the occupation numbers $(n_1, n_2, \ldots, n_S)$. $\Lambda(\lambda_1, \ldots, \lambda_N) \subset S_N$ is the set of all permutations involving only particles j with *different* λ_j, e.g., $T(j,k) \in \Lambda(\lambda_1, \ldots, \lambda_N)$ only if $\lambda_j \neq \lambda_k$. The integers n_j are equal to the number of λ_k in (9.15) with $\lambda_k = j$, i.e. the n_j specify how often a single particle state $|j\rangle$ is occupied. The numbers n_j, referred to as the occupation numbers, characterize the wave function (9.15) completely and, therefore, are essential. The reader is well advised to pause and grasp the definition of the n_j.
An important detail of the definition (9.15) is that the sum over permutations does not involve permutations among indices $j, k, \ldots$ with $\lambda_j = \lambda_k = \ldots$. This detail is connected with the fact that a two–particle state of the type $\Psi^{\mathrm{Fock}}(\lambda, \lambda)$ in which two particles occupy the *same* single–particle state $|\lambda\rangle$ does not allow transposition of particles; the reason is that such transposition duplicates the state which would, hence, appear severalfold in (9.15).

The wave functions (9.15) describe, for example, the photons of the electromagnetic field or the phonons in a crystal. These states form an orthonormal basis, i.e., for two sets of occupation numbers $\mathcal{N} = (n_1, n_2, \ldots, n_S)$ and $\mathcal{N}' = (n'_1, n'_2, \ldots, n'_S)$ holds

$$\langle \Psi^{\mathrm{B}}(\mathcal{N}') | \Psi^{\mathrm{B}}(\mathcal{N}) \rangle \;=\; \prod_{j=1}^{S} \delta_{n_j\, n'_j} \; . \tag{9.16}$$

Exercise 9.1.1:
(a) Show that the states (9.15) obey the boson symmetry (9.8).
(b) Show that for the states (9.15) holds (9.16).

Wave Functions with Fermion Symmetry in the Occupation Number Representation

One can construct similarly a wave function which obeys the fermion symmetry property (9.9). Such wave function is

$$\langle \vec{x}_1, \vec{x}_2, \ldots \vec{x}_N | \Psi^{\mathrm{F}}(n_1, n_2, \ldots, n_S) \rangle \;=$$

$$\tfrac{1}{\sqrt{N!}} \textstyle\sum_{P \in S_N} \epsilon_P \, P \, \langle \vec{x}_1, \vec{x}_2, \ldots \vec{x}_N | \Psi^{\mathrm{Fock}}(\lambda_1, \lambda_2, \ldots \, . \lambda_N) \rangle \tag{9.17}$$

Here the states $(\lambda_1, \lambda_2, \ldots \, . \lambda_N)$ on the rhs. correspond to a particular choice of placing N particles consistent with the occupation numbers $(n_1, n_2, \ldots, n_S)$. Using the identity governing the determinant of $N \times N$–matrices $\mathbf{A}$

$$det(\mathbf{A}) \;=\; \sum_{P \in S_N} \epsilon_P \prod_{j=1}^{N} A_{j\, P(j)} \tag{9.18}$$

this wave function can also be expressed through the so-called *Slater determinant*

$$\langle \vec{x}_1, \vec{x}_2, \ldots \vec{x}_N | \Psi^{\mathrm{F}}(n_1, n_2, \ldots, n_S) \rangle \;=$$

$$\tfrac{1}{\sqrt{N!}} \begin{vmatrix} \phi_{\lambda_1}(\vec{x}_1) & \phi_{\lambda_2}(\vec{x}_1) & \ldots & \phi_{\lambda_N}(\vec{x}_1) \\ \phi_{\lambda_1}(\vec{x}_2) & \phi_{\lambda_2}(\vec{x}_2) & \ldots & \phi_{\lambda_N}(\vec{x}_2) \\ \vdots & \vdots & \vdots & \vdots \\ \phi_{\lambda_1}(\vec{x}_N) & \phi_{\lambda_2}(\vec{x}_N) & \ldots & \phi_{\lambda_N}(\vec{x}_N) \end{vmatrix} \tag{9.19}$$

Here, the integers n_j denote the occupancy of the single–particle state $|j\rangle$. The important property holds that n_j can only assume the two values $n_j = 0$ or $n_j = 1$. For any value $n_j > 1$ two or more of the columns of the Slater matrix are identical and the wave function vanishes.
The fermion states (9.17) describe, for example, electrons in an atom, a molecule or a crystal. These states form an orthonormal basis, i.e., for two sets of occupation numbers $\mathcal{N} = (n_1, n_2, \ldots, n_S)$ and $\mathcal{N}' = (n'_1, n'_2, \ldots, n'_S)$ holds

$$\langle \Psi^{\mathrm{F}}(\mathcal{N}') | \Psi^{\mathrm{F}}(\mathcal{N}) \rangle \;=\; \prod_{j=1}^{S} \delta_{n_j\, n'_j} \; . \tag{9.20}$$

The representation of wave functions (9.15) and (9.17) is commonly referred to as the *occupation number representation* since the wave functions are uniquely specified by the set of occupation numbers $\mathcal{N} = (n_1, n_2, \ldots, n_S)$.

Exercise 9.1.2:
(a) Show that the states (9.17) obey the fermion symmetry (9.9).
(b) Show that the states (9.17) obey the orthonormality property (9.20).

9.2 Operators of 2nd Quantization

An important tool to describe mathematically systems of many bosons or fermions, guaranteeing the correct permutation properties of the many–particle states, are the so-called operators of 2nd quantization. These operators allow one to construct and manipulate many–particle wave functions while preserving permutation symmetry.

Creation and Annihilation Operators for Bosons

We consider the operator a_j defined through

$$a_j \, \Psi^{\mathrm{B}}(n_1, \ldots, n_j, \ldots, n_S) = \begin{cases} \sqrt{n_j} \, \Psi^{\mathrm{B}}(n_1, \ldots, n_j - 1, \ldots, n_S) & n_j \geq 1 \\ 0 & n_j = 0 \end{cases} . \tag{9.21}$$

The factor $\sqrt{n_j}$ appears here on the rhs. since both the N-particle wave function $\Psi^{\mathrm{B}}(n_1, \ldots, n_j, \ldots, n_S)$ and the $N-1$-particle wave function $\Psi^{\mathrm{B}}(n_1, \ldots, n_j - 1, \ldots, n_S)$ are normalized according to (9.15). For the adjoint operator $a_j^\dagger$ holds

$$a_j^\dagger \Psi^{\mathrm{B}}(n_1, \ldots, n_j, \ldots, n_S) = \sqrt{n_j + 1} \; \Psi^{\mathrm{B}}(n_1, \ldots, n_j + 1, \ldots, n_S) . \tag{9.22}$$

The operators a_j and $a_j^\dagger$ obey the commutation properties

$$[a_j, a_k] = 0 , \quad [a_j^\dagger, a_k^\dagger] = 0 \tag{9.23}$$

$$[a_j, a_k^\dagger] = \delta_{j\,k} . \tag{9.24}$$

The operators $a_j^\dagger$ and a_j are referred to as the creation and annihilation operators of bosons for the orthonormal single–particle states $|j\rangle$.
To prove that (9.22) follows from (9.21) we consider the matrix $\mathbb{A}_j$ corresponding to a_j in the basis of many–particle states (9.15). Employing the superindices $\mathcal{N}'$ and $\mathcal{N}$ introduced above and using the orthonormality property (9.16) one obtains

$$(\mathbb{A}_j)_{\mathcal{N}'\mathcal{N}} = \langle \Psi^{\mathrm{B}}(\mathcal{N}') | \, a_j \, | \Psi^{\mathrm{B}}(\mathcal{N}) \rangle = \sqrt{n_j} \, \delta_{n'_j \, n_j - 1} \prod_{\substack{k=1 \\ k \neq j}}^{S} \delta_{n'_k n_k} . \tag{9.25}$$

Let $\mathbb{A}_j^\dagger$ be the matrix adjoint to $\mathbb{A}_j$. One obtains for its matrix elements

$$\begin{aligned}\left(\mathbb{A}_j^\dagger\right)_{\mathcal{N}'\mathcal{N}} &= \langle\Psi^{\mathrm{B}}(\mathcal{N}')|\, a_j^\dagger\,|\Psi^{\mathrm{B}}(\mathcal{N})\rangle \;=\; \overline{(\mathbb{A}_j)_{\mathcal{N}\mathcal{N}'}} \\ \sqrt{n_j'}\,\delta_{n_j\,n_j'-1}\prod_{\substack{k=1\\k\neq j}}^{S}\delta_{n_k n_k'} &= \sqrt{n_j+1}\,\delta_{n_j'\,n_j+1}\prod_{\substack{k=1\\k\neq j}}^{S}\delta_{n_k' n_k}\;. \end{aligned} \tag{9.26}$$

From this result one can immediately conclude that (9.22) follows from (9.21) and *vice versa*.
We will prove the commutation properties (9.24), the properties (9.23) follow in an analogous way. It holds for $j = k$

$$(a_j a_j^\dagger \;-\; a_j^\dagger a_j)|\Psi(\mathcal{N})\rangle \;=\; (n_j + 1 \;-\; n_j)|\Psi(\mathcal{N})\rangle \;=\; |\Psi(\mathcal{N})\rangle\;. \tag{9.27}$$

Since this holds for any $|\Psi(\mathcal{N})\rangle$ it follows $[a_j, a_j^\dagger] = \mathbb{1}$. For $j \neq k$ follows similarly

$$\begin{aligned}(a_j a_k^\dagger \;-\; a_k^\dagger a_j)|\Psi(\mathcal{N})\rangle \;=\; \\ (\sqrt{n_j(n_k+1)} \;-\; \sqrt{(n_k+1)n_j})|\Psi(n_1,\ldots n_j-1\ldots n_k+1\ldots n_S)\rangle \;=\; 0\;.\end{aligned} \tag{9.28}$$

Equations (9.27, 9.29) yield the commutation relationship (9.24).
The creation operators $a_j^\dagger$ allow one to construct boson states $\Psi^{\mathrm{B}}(\mathcal{N})\rangle$ from the vacuum state

$$|0\rangle \;=\; |\Psi^{\mathrm{B}}(n_1 = 0, n_2 = 0, \ldots, n_S = 0)\rangle \tag{9.29}$$

as follows

$$|\Psi^{\mathrm{B}}(n_1, n_2, \ldots, n_S)\rangle \;=\; \prod_{j=1}^{S}\frac{\left(a_j^\dagger\right)^{n_j}}{\sqrt{n_j!}}\,|0\rangle\;. \tag{9.30}$$

Of particular interest is the operator

$$\hat{N}_j \;=\; a_j^\dagger a_j\;. \tag{9.31}$$

This operator is diagonal in the occupation number representation, i.e., for basis states $|\Psi^{\mathrm{B}}(n_1, n_2, \ldots, n_S)\rangle = |\Psi^{\mathrm{B}}(\mathcal{N})\rangle$. One can readily show using (9.21, 9.22)

$$\hat{N}_j\,|\Psi^{\mathrm{B}}(\mathcal{N})\rangle \;=\; n_j\,|\Psi^{\mathrm{B}}(\mathcal{N})\rangle\;, \tag{9.32}$$

i.e., the eigenvalues of $\hat{N}_j$ are the occupation numbers n_j. One refers to $\hat{N}_j$ as the *occupation number operator*. The related operator

$$\hat{N} \;=\; \sum_{j=1}^{S}\hat{N}_j \tag{9.33}$$

is called the *particle number operator* since, obviously,

$$\begin{aligned}\hat{N}\,|\Psi^{\mathrm{B}}(n_1, n_2, \ldots, n_S)\rangle \;&=\; \sum_{j=1}^{S} n_j\,|\Psi^{\mathrm{B}}(n_1, n_2, \ldots, n_S)\rangle \\ &=\; N\,|\Psi^{\mathrm{B}}(n_1, n_2, \ldots, n_S)\rangle\;.\end{aligned} \tag{9.34}$$

In using the boson creation and annihilation operators, in general, one needs to apply only the commutation propertes (9.23, 9.24) and the property $a_j|0\rangle = 0$. As long as one starts from a wave function with the proper boson symmetry, e.g., from the vacuum state $|0\rangle$ or states $|\Psi^{\rm B}(\mathcal{N})\rangle$, one does not need to worry ever about proper symmetries of wave functions, since they are induced through the algebra of $a_j^\dagger$ and a_j.

Exercise 9.2.1: The commutation relationships (9.23, 9.24) and $a_j|0\rangle = 0$ imply that the the properties (9.21, 9.22, 9.23) hold for the state defined through (9.29, 9.30). Prove this by induction, showing that the property holds for $n_j = 0$ and, in case it holds for n_j, it also holds for $n_j + 1$.

Exercise 9.2.2: Show that the boson operators $a_j^\dagger$ and a_j satisfy

$$\begin{aligned}[a_j, f(a_j^\dagger)] &= \frac{\partial f(a_j^\dagger)}{\partial a_j^\dagger} \\ [a_j^\dagger, f(a_j)] &= -\frac{\partial f(a_j)}{\partial a_j}\end{aligned}$$

where the operator function is assumed to have a convergent Taylor expansion

$$f(A) \;=\; \sum_{n=0}^{\infty} \frac{1}{n!}\, f^{(n)}(0)\, A^n \tag{9.35}$$

and where the derivative operation is defined through

$$\frac{\partial f(A)}{\partial A} \;=\; \sum_{n=1}^{\infty} \frac{1}{(n-1)!}\, f^{(n)}(0)\, A^{n-1}\,. \tag{9.36}$$

Creation and Annihilation Operators for Fermions

We want to consider now creation and annihilation operators for fermions, i.e., operators which can alter the occupancy of the wave function (9.17, 9.19) without affecting the fermion symmetry (9.9). Before proceeding in this respect we need to account for the following property of the fermion wave function which applies in the case $n_j, n_{j+1} = 1$, i.e., in case that the single particle states $|j\rangle$ and $|j+1\rangle$ are both occupied,

$$\langle \vec{x}_1, \vec{x}_2, \ldots \vec{x}_N | \Psi^{\rm F}(n_1, \ldots n_j, n_{j+1} \ldots n_S)\rangle \;= \tag{9.37}$$

$$-\langle \vec{x}_1, \vec{x}_2, \ldots \vec{x}_N | \Psi^{\rm F}(n_1, \ldots, n_{j+1}, n_j \ldots n_S)\rangle\,. \tag{9.38}$$

Obviously, the fermion wave function changes sign when one exchanges the order of the occupancy. To prove this property we notice that the l.h.s. of (9.38) corresponds to

$$\langle \vec{x}_1, \vec{x}_2, \ldots \vec{x}_N | \Psi^{\rm F}(n_1, \ldots n_j, n_{j+1} \ldots n_S)\rangle \;=$$

$$\frac{1}{\sqrt{N!}} \begin{vmatrix} \ldots & \phi_j(\vec{x}_1) & \phi_{j+1}(\vec{x}_1) & \ldots \\ \ldots & \phi_j(\vec{x}_2) & \phi_{j+1}(\vec{x}_2) & \ldots \\ \vdots & \vdots & \vdots & \vdots \\ \ldots & \phi_j(\vec{x}_N) & \phi_{j+1}(\vec{x}_N) & \ldots \end{vmatrix}\,. \tag{9.39}$$

The r.h.s. of (9.38) reads

$$-\langle\vec{x}_1,\vec{x}_2,\ldots\vec{x}_N|\Psi^{\rm F}(n_1,\ldots,n_{j+1},n_j\ldots n_S)\rangle \;=$$

$$-\tfrac{1}{\sqrt{N!}}\begin{vmatrix} \ldots & \phi_{j+1}(\vec{x}_1) & \phi_j(\vec{x}_1) & \ldots \\ \ldots & \phi_{j+1}(\vec{x}_2) & \phi_j(\vec{x}_2) & \ldots \\ \vdots & \vdots & \vdots & \vdots \\ \ldots & \phi_{j+1}(\vec{x}_N) & \phi_j(\vec{x}_N) & \ldots \end{vmatrix} . \tag{9.40}$$

Because of the property of the determinant to change sign when two columns are interchanged, the expressions (9.39) and (9.40) are identical.
Obviously, it is necessary to specify for a fermion wave function the order in which the single–particle states $|\lambda_j\rangle$ are occupied. For this purpose one must adhere to a strict convention: the labelling of single–particle states by indices $j = 1, 2, \ldots$ must be chosen once and for all at the beginning of a calculation and these states must be occupied always in the order of increasing indices. A proper example is the two particle fermion wave function

$$\begin{aligned}&\langle\vec{x}_1,\vec{x}_2|\Psi^{\rm F}(n_1=0,n_2=1,n_3=0,n_4=0,n_5=1,n_6=n_7=\ldots n_S=0)\rangle \\ &= \tfrac{1}{\sqrt{2}}\begin{vmatrix}\phi_2(\vec{x}_1) & \phi_5(\vec{x}_1)\\ \phi_2(\vec{x}_2) & \phi_5(\vec{x}_2)\end{vmatrix} = \tfrac{1}{\sqrt{2}}\left[\phi_2(\vec{x}_1)\phi_5(\vec{x}_2) - \phi_5(\vec{x}_1)\phi_2(\vec{x}_2)\right] .\end{aligned} \tag{9.41}$$

Before we consider the definition of fermion creation and annihilation operators we need to take notice of the fact that one also needs to define at which position in the wave function, i.e., at which column of the Slater determinant (9.19), particles are being created or annihilated. *One adopts the convention that particles are created and annihilated by these operators always at the first position of the wave function,* i.e., at the first column of the Slater determinant (9.19). This requires one, however, in order to be consistent with this convention, that occupancies are always ordered according to a monotonous increase of the single–particle state index, to move the particle to the first position (to be annihilated there) or to move it from the first position to its canonical position (after it had been created at the first position). This change of position is connected with a possible sign change $(-1)^{q_j}$ where q_j is defined for a given $\mathcal{N} = (n_1, n_2, \ldots n_S)$ as follows:

$$q_j \;=\; \sum_{k=1}^{j-1} n_k \;, \tag{9.42}$$

i.e., q_j is the number of states $|k\rangle$ with $k < j$ which are occupied in a fermion wave function. We will be adopting below the notational convention that q'_j corresponds to occupancies $\mathcal{N}' = (n'_1, n'_2, \ldots n'_S)$.
We are now ready to define the annihilation operator c_j for fermions in the single–particle state $|j\rangle$ as follows

$$\begin{aligned} c_j\,|\Psi^{\rm F}(n_1,n_2,\ldots n_j\ldots n_S)\rangle \;=\; \\ n_j\,(-1)^{q_j}\,|\Psi^{\rm F}(\underbrace{n_1,n_2,n_3\ldots n_{j-1}}_{q_j\text{ states occupied}},n_j\to 0,n_{j+1}\ldots n_S)\rangle\end{aligned} \tag{9.43}$$

In case that the single particle state $|j\rangle$ is not occupied, i.e., $n_j = 0$, the rhs. vanishes.

The operator $c_j^\dagger$ adjoint to c_j exhibits the following property

$$\begin{aligned} c_j^\dagger \,|\Psi^{\rm F}(n_1, n_2, \ldots n_j \ldots n_S)\rangle \;=\; \\ (-1)^{q_j}(1 \,-\, n_j)\,|\Psi^{\rm F}(\underbrace{n_1, n_2, n_3 \ldots n_{j-1}}_{q_j \text{ states occupied}}, n_j \to 1, n_{j+1} \ldots n_S)\rangle \end{aligned} \tag{9.44}$$

The operators thus defined obey the commutation properties

$$[c_j, c_k]_+ \;=\; 0\,; \quad [c_j^\dagger, c_k^\dagger]_+ \;=\; 0 \tag{9.45}$$

$$[c_j, c_k^\dagger]_+ \;= \delta_{j\,k} \tag{9.46}$$

where we have used the definition of the so-called *anti-commutators* $[A, B]_+ \,=\, AB \,+\, BA$.
We first show that (9.44) follows from the definition (9.43). Let $\mathbb{C}_j$ be the matrix corresponding to the operator c_j in the basis of fermion states (9.17, 9.19). The elements of $\mathbb{C}_j$ are then (note that n_j only assumes values 0 or 1)

$$(\mathbb{C}_j)_{\mathcal{N}'\mathcal{N}} \;=\; \langle \Psi^{\rm F}(\mathcal{N}')|\; c_j\,|\Psi^{\rm F}(\mathcal{N})\rangle \;=\; n_j\,(-1)^{q_j}\,\delta_{n'_j\,n_j-1}\prod_{\substack{k=1\\k\neq j}}^{S}\delta_{n'_k n_k}\,. \tag{9.47}$$

Let $\mathbb{C}_j^\dagger$ be the matrix adjoint to $\mathbb{C}_j$. One obtains for its matrix elements

$$\begin{aligned} \left(\mathbb{C}_j^\dagger\right)_{\mathcal{N}\mathcal{N}'} \;&=\; \langle \Psi^{\rm F}(\mathcal{N}')|\; c_j^\dagger\,|\Psi^{\rm F}(\mathcal{N})\rangle \;=\; \overline{(\mathbb{C}_j)_{\mathcal{N}'\mathcal{N}}} \\ &=\; n'_j\,(-1)^{q'_j}\,\delta_{n_j\,n'_j-1}\prod_{\substack{k=1\\k\neq j}}^{S}\delta_{n_k n'_k} \\ &=\; (-1)^{q_j}(1-n_j)\,\delta_{n'_j\,n_j+1}\prod_{\substack{k=1\\k\neq j}}^{S}\delta_{n'_k n_k}\,. \end{aligned} \tag{9.48}$$

From this follows (9.44). We have used here the definition $q'_j \;=\; \sum_{k<j} n'_k$ along with $q'_j \;=\; q_j$, otherwise, the last factor on the rhs. of (9.48) vanishes.
We will prove now the anti-commutation property (9.46). The anti-commutation properties (9.45) follow in an analogous way and will not be derived here. We consider (9.46) first for the case $j = k$. It holds

$$\begin{aligned} c_j^\dagger c_j|\Psi^{\rm F}(\mathcal{N})\rangle \;&=\; c_j^\dagger(-1)^{q_j}n_j\,|\Psi^{\rm F}(n_1 \ldots n_j \to 0 \ldots n_S)\rangle \;= \\ (-1)^{q_j}(1-n_j+1)(-1)^{q_j}n_j\,|\Psi^{\rm F}(\mathcal{N})\rangle \;&=\; n_j\Psi^{\rm F}(\mathcal{N})\rangle \end{aligned} \tag{9.49}$$

The derivation involves realization of the fact that a non-zero result is obtained only in case $n_j = 1$. Similarly one obtains

$$\begin{aligned} c_j c_j^\dagger|\Psi^{\rm F}(\mathcal{N})\rangle \;&=\; c_j(-1)^{q_j}(1-n_j)\,|\Psi^{\rm F}(n_1 \ldots n_j \to 1 \ldots n_S)\rangle \;= \\ (-1)^{q_j}(n_j+1))(-1)^{q_j}(1-n_j)\,|\Psi^{\rm F}(\mathcal{N})\rangle \;&=\; (1-n_j)\,|\Psi^{\rm F}(\mathcal{N})\rangle \end{aligned} \tag{9.50}$$

(9.49) and (9.50) yield

$$(c_j c_j^\dagger \, + \, c_j^\dagger c_j \,) \, |\Psi^{\rm F}(\mathcal{N})\rangle \; = \; |\Psi^{\rm F}(\mathcal{N})\rangle \; . \tag{9.51}$$

For $j < k$ one obtains

$$\begin{aligned} c_j c_k^\dagger |\Psi^{\rm F}(\mathcal{N})\rangle \; &= \; (-1)^{q_j+q_k} n_j (1-n_k) |\Psi^{\rm F}(n_1 \ldots n_j = 0 \ldots n_k = 1 \ldots n_S)\rangle \\ c_k^\dagger c_j |\Psi^{\rm F}(\mathcal{N})\rangle \; &= \; (-1)^{q_j+q_k-1} n_j (1-n_k) |\Psi^{\rm F}(n_1 \ldots n_j = 0 \ldots n_k = 1 \ldots n_S)\rangle \end{aligned}$$

and, hence,

$$(c_j c_k^\dagger \, + \, c_k^\dagger c_j \,) \, |\Psi^{\rm F}(\mathcal{N})\rangle \; = \; 0 \; . \tag{9.52}$$

One can obtain similarly the same relationship in the case $j > k$. Since (9.51, 9.52) hold for any $|\Psi^{\rm F}(\mathcal{N})\rangle$ one can conclude (9.46).
Equation (9.49) shows that the operator

$$\hat{N}_j \; = \; c_j^\dagger c_j \tag{9.53}$$

is diagonal in the occupation number representation, i.e., in the basis $|\Psi^{\rm F}(\mathcal{N})\rangle$, with eigenvalues equal to the occupation numbers n_j

$$\hat{N}_j \, |\Psi^{\rm F}(\mathcal{N})\rangle \; = \; n_j \, |\Psi^{\rm F}(\mathcal{N})\rangle \tag{9.54}$$

$\hat{N}_j$, hence, is referred to as the *occupation number operator*. Correspondingly,

$$\hat{N} \; = \; \sum_{j=1}^{S} \hat{N}_j \tag{9.55}$$

is called the *particle number operator*.
It is an interesting exercise to demonstrate that $\hat{N}_j$ only has eigenvalues 0 or 1, for which purpose one needs to envoke only the algebraic (anti-commutation) properties (9.46). The stated property follows from the idempotence of $\hat{N}_j$ which can be derived as follows

$$\hat{N}_j^2 \; = \; c_j^\dagger c_j c_j^\dagger c_j \; = \; c_j^\dagger \, (1 - c_j^\dagger c_j) c_j \; = \; c_j^\dagger c_j \; - \; c_j^\dagger c_j^\dagger c_j c_j \; = \; c_j^\dagger c_j \; = \; \hat{N}_j \; . \tag{9.56}$$

Here we have made use of $c_j c_j = 0$ and $c_j^\dagger c_j^\dagger = 0$ which follows from $n_j \in \{0, 1\}$.
We finally note that the creation operators $c_j^\dagger$ allow one to construct any fermion state $|\Psi^{\rm F}(\mathcal{N})\rangle$ from the vacuum state $|0\rangle$ defined as above (see (9.29))

$$|\Psi^{\rm F}(\ldots n_{\lambda_1} \ldots n_{\lambda_2} \ldots n_{\lambda_N} \ldots)\rangle \; = \; c_{\lambda_1}^\dagger c_{\lambda_2}^\dagger \cdots c_{\lambda_N}^\dagger \, |0\rangle \; . \tag{9.57}$$

On the l.h.s. of this equation we meant to indicate only those N occupation numbers n_{λ_j} which are non-vanishing. On the r.h.s. the creation operators must operate in the proper order, i.e., an operator c_j must be on the left of an operator c_k for $j < k$.
In the following we will apply fermion operators $c_j^\dagger$ and c_j only to electrons which carry spin $\frac{1}{2}$. We will often separate the states $|j\rangle$, coordinates $\vec{x}$ and index j into a space part and a spin part, i.e.,

$$j \to j, \sigma \quad (\sigma = \pm \tfrac{1}{2}) \; ; \qquad \langle \vec{x} | j \rangle \; \to \; \phi_j(\vec{r}) \, |\tfrac{1}{2}\sigma\rangle \; . \tag{9.58}$$

9.3 One– and Two–Particle Operators

Definition

Operators acting on N particle systems of the type

$$\hat{F} \;=\; \sum_{j=1}^{N} \hat{f}(\vec{x}_j) \tag{9.59}$$

are called *single–particle operators*. The operators $\hat{f}(\vec{x})$ which constitute $\hat{F}$ are called the *associated generic single–particle operators*[1]. Operators of the type

$$\hat{G} \;=\; \frac{1}{2} \sum_{\substack{j,k=1 \\ j\neq k}}^{N} \hat{g}(\vec{x}_j, \vec{x}_k) \tag{9.60}$$

correspondingly are called *two–particle operators*. The operators $\hat{g}(\vec{x}, \vec{x}')$ which constitute $\hat{G}$ are called the *associated generic two–particle operators*. These operators had been introduced already in Eq. (9.6) above. The essential aspect of definition (9.59, 9.60) is that the sum over particles in (9.59) and over pairs of particles in (9.60) involves generic operators – acting on $\vec{x}_j$ and on $\vec{x}_j, \vec{x}_k$, respectively – which are all identical. An operator

$$\hat{R} \;=\; \sum_{j=1}^{N} \hat{r}_j(\vec{x}_j) \tag{9.61}$$

is not a one particle operator as long as the N operators $\hat{r}_j(\vec{x})$, $j = 1, 2, \ldots, N$ are not all identical. We seek to determine now how one–particle operators $\hat{F}$ and two–particle operators $\hat{G}$ act on many–boson and many–fermion states $|\Psi^{\mathrm{B}}(\mathcal{N})\rangle$ and $|\Psi^{\mathrm{F}}(\mathcal{N})\rangle$, respectively. The action of the operators is obviously described through the *many–particle state* matrix elements

$$\langle \Psi^{\mathrm{B,F}}(\mathcal{N}')|\hat{F}|\Psi^{\mathrm{B,F}}(\mathcal{N})\rangle \;; \qquad \langle \Psi^{\mathrm{B,F}}(\mathcal{N}')|\hat{G}|\Psi^{\mathrm{B,F}}(\mathcal{N})\rangle \;. \tag{9.62}$$

These matrix elements can be obtained by chosing the operators and many-particle states in the position representation, i.e., (9.59, 9.59) and (9.15, 9.17) and integrating over all particle space-spin coordinates $\vec{x}_1, \vec{x}_2, \ldots \vec{x}_N$. This procedure is most tedious and becomes essentially impossible in the general case that many-particle basis functions are linear combinations of wave functions of the type (9.15, 9.17).

Since the many–particle states are built-up from a basis $|r\rangle$, $r = 1, 2, \ldots S$ of single–particle spin-orbital states (see page 243) and the operators are specified through the associated generic operators $\hat{f}$ and $\hat{g}$, one expects that the matrix elements can actually be expressed in terms of matrix elements involving solely the generic operators and the single–particle states, namely,

$$\langle r|\hat{f}|s\rangle \;=\; \int d^3r\, \psi_r^*(\vec{r}, \sigma_r)\, \hat{f}(\vec{x})\, \psi_s(\vec{r}, \sigma_s) \tag{9.63}$$

[1]This expression has been specified for the purpose of these notes to distinguish $\hat{F}$ and $\hat{f}$ and is not common terminology. We adopt a similar expression to distinguish two–particle operators $\hat{G}$ and $\hat{g}$.

$$\langle r,s|\hat{g}|t,u\rangle \;=\; \int d^3r \int d^3r'\, \psi_r^*(\vec{r},\sigma_r)\psi_s^*(\vec{r}\,',\sigma_s)\, \hat{g}(\vec{x},\vec{x}\,')\, \psi_t(\vec{r},\sigma_t)\psi_u(\vec{r}\,',\sigma_u)\;. \tag{9.64}$$

We like to note an important symmetry of the matrix element $\langle r,s|\hat{g}|t,u\rangle$ which follows directly from the definition (9.64)

$$\langle r,s|\hat{g}|t,u\rangle \;=\; \langle s,r|\hat{g}|u,t\rangle\;. \tag{9.65}$$

This symmetry will be exploited repeatedly below. Notice, that the symmetry implies that one can switch *simultaneously* the pairs of indices r,s and t,u, *one cannot switch the indices of one pair individually.*

The aim of the present section is to express the matrix elements of single– and two–particle operators in a basis of many–particle states (9.62) in terms of the matrix elements of single–particle states (9.63, 9.64). We will show that the boson and fermion creation and annihilation operators serve this purpose.

Examples of One– and Two–Particle Operators

An example for a single–particle operator is the *kinetic energy operator*

$$\hat{T} \;=\; \sum_{j=1}^{N} \left(-\frac{\hbar^2}{2m}\right) \frac{\partial^2}{\partial \vec{r}_j^{\,2}}\;. \tag{9.66}$$

Here we adopt the notation for the Laplacian

$$\frac{\partial^2}{\partial \vec{r}^{\,2}} \;=\; \frac{\partial^2}{\partial x_1^2} \;+\; \frac{\partial^2}{\partial x_2^2} \;+\; \frac{\partial^2}{\partial x_3^2}\;. \tag{9.67}$$

In this case the generic single–particle operator, according to (9.59), is $\hat{t}(\vec{x}) \;=\; (-\hbar^2/2m)(\partial^2/\partial\vec{r}^{\,2})$. The matrix elements of this operator in a single–particle basis are

$$\langle r\sigma|\hat{t}|s\sigma'\rangle \;=\; \delta_{\sigma\sigma'} \int d^3r\, \phi_r^*(\vec{r}) \left(-\frac{\hbar^2}{2m}\right) \frac{\partial^2}{\partial \vec{r}^{\,2}}\, \phi_s(\vec{r})\;. \tag{9.68}$$

Another single–particle operator is the *one–particle density operator*

$$\hat{\rho}(\vec{\vec{r}}\,') \;=\; \sum_{j=1}^{N} \delta(\vec{\vec{r}} \;-\; \vec{r}_j)\;. \tag{9.69}$$

In this case the generic operator is $\hat{f}(\vec{x}) \;=\; \delta(\vec{\vec{r}} \;-\; \vec{r})$. The matrix elements of the generic operator in the one–particle basis are

$$\langle r\sigma|\hat{f}|s\sigma'\rangle \;=\; \delta_{\sigma\sigma'} \int d^3r\, \phi_r^*(\vec{r})\, \delta(\vec{\vec{r}} \;-\; \vec{r})\, \phi_s(\vec{r}) \;=\; \delta_{\sigma\sigma'}\; \phi_r^*(\vec{\vec{r}})\, \phi_s(\vec{\vec{r}})\, \delta_{\sigma\sigma'} \tag{9.70}$$

Both operators, i.e., (9.66) and (9.69), are spin-independent as is evident from the factor $\delta_{\sigma\sigma'}$.

An example for a two–particle operator is the *Coulomb repulsion operator*

$$\hat{V} \;=\; \frac{1}{2} \sum_{\substack{j,k=1 \\ j\neq k}}^{N} \frac{q^2}{|\vec{r}_j \;-\; \vec{r}_k|} \tag{9.71}$$

which is also spin-independent. In this case the generic operator is $\hat{v}(\vec{x},\vec{x}') = q^2/|\vec{r}_1 - \vec{r}_2|$. The matrix elements of the generic operator in terms of single–particle states are

$$\langle r,\sigma;\, s,\sigma'|\,\hat{t}\,|t,\sigma'';\, u,\sigma'''\rangle \;= \\ \int d^3r_1 \int d^3r_2\, \phi_r^*(\vec{r}_1)\phi_s^*(\vec{r}_2)\,\frac{q^2}{|\vec{r}_1-\vec{r}_2|}\,\phi_t(\vec{r}_1)\phi_u(\vec{r}_2)\,\delta_{\sigma\sigma''}\delta_{\sigma'\sigma'''} \tag{9.72}$$

As a final example of one– and two–particle operators we consider operators of total spin. The operator

$$\vec{S} \;=\; \sum_{j=1}^{N} \vec{S}_j \tag{9.73}$$

is a one-particle operator. Here, $\vec{S}_j$ is the spin operator for particle j with components (in the spherical representation) $S_{j,+}$, $S_{j,-}$, $S_{j,3}$. The generic operator is given through the Pauli matrices, i.e., $\vec{\hat{s}} = \frac{1}{2}\vec{\sigma}$. The *non-vanishing* matrix elements of the spherical components of $\vec{s}$ are ($\alpha = +\frac{1}{2}, \beta = -\frac{1}{2}$)

$$\begin{aligned} \langle r,\alpha|\hat{s}_+|s,\beta\rangle &= \delta_{rs} \\ \langle r,\beta|\hat{s}_-|s,\alpha\rangle &= \delta_{rs} \\ \langle r,\alpha|\hat{s}_3|s,\alpha\rangle &= +\tfrac{1}{2}\,\delta_{rs} \\ \langle r,\beta|\hat{s}_3|s,\beta\rangle &= -\tfrac{1}{2}\,\delta_{rs} \end{aligned} \tag{9.74}$$

The operator

$$S^2 \;=\; \left(\sum_{j=1}^{N}\vec{S}_j\right)^2 \;=\; \sum_{j,k=1}^{N}\vec{S}_j\cdot\vec{S}_k \tag{9.75}$$

is a two–particle operator, however, not in the strict sense of our definition above since the restriction $j \neq k$ does not apply in the summation. However, one can obviously extract the term $\sum_j S_j^2$ to be left with a two–particle operator in the strict sense of our definition. The generic operator is

$$\hat{s}_{12} \;=\; \vec{S}_1\cdot\vec{S}_2 \;=\; \frac{1}{2}S_{1,+}S_{2,-} \;+\; \frac{1}{2}S_{1,-}S_{2,+} \;+\; S_{1,3}S_{2,3} \tag{9.76}$$

the single–particle state matrix elements of which are

$$\langle r,\sigma;\, s,\sigma'|\,\hat{s}_{12}\,|t,\sigma'';\, u,\sigma'''\rangle \;=\; \delta_{rt}\,\delta_{su}\left(\tfrac{1}{2}\delta_{\frac{1}{2}\sigma}\delta_{-\frac{1}{2}\sigma''}\delta_{-\frac{1}{2}\sigma'}\delta_{\frac{1}{2}\sigma'''} \;+ \right. \\ \left. +\;\tfrac{1}{2}\delta_{-\frac{1}{2}\sigma}\delta_{\frac{1}{2}\sigma''}\delta_{\frac{1}{2}\sigma'}\delta_{-\frac{1}{2}\sigma'''} \;+\; \tfrac{1}{4}\,\delta_{\sigma\sigma''}\delta_{\sigma'\sigma'''}\,(\,\delta_{\sigma\sigma'} \;-\; \delta_{-\sigma\sigma'}\,)\right). \tag{9.77}$$

The operators (9.74) and (9.77) are orbital-independent as evidenced by the factors δ_{rs} and $\delta_{rt}\delta_{su}$ in the respective formulas.

Definition in Terms of Creation and Annihilation Operators

In order to express many–particle state matrix elements (9.62) through single–particle state matrix elements (9.63, 9.64) one replaces the operators $\hat{F}$ in (9.59) and $\hat{G}$ in (9.60) as follows

$$\sum_{j=1}^{N} \hat{f}(\vec{x}_j) \;\rightarrow\; \begin{cases} \sum_{r,s=1}^{S} \langle r|\hat{f}|s\rangle \, a_r^\dagger a_s & \text{bosons} \\ \sum_{r,s=1}^{S} \langle r|\hat{f}|s\rangle \, c_r^\dagger c_s & \text{fermions} \end{cases} \tag{9.78}$$

$$\frac{1}{2} \sum_{\substack{j,k=1 \\ j\neq k}}^{N} \hat{g}(\vec{x}_j, \vec{x}_k) \;\rightarrow\; \begin{cases} \frac{1}{2} \sum_{r,s,t,u=1}^{S} \langle r,s|\hat{g}|t,u\rangle \, a_r^\dagger a_s^\dagger a_t a_u & \text{bosons} \\ \frac{1}{2} \sum_{r,s,t,u=1}^{S} \langle r,s|\hat{g}|t,u\rangle \, c_r^\dagger c_s^\dagger c_u c_t & \text{fermions} \end{cases} \tag{9.79}$$

It is crucial to notice in the expression for the fermion two–particle operator that the order of the annihilation operators in (9.79) is opposite to that in the matrix element $\langle r,s|\hat{g}|t,u\rangle$, namely $c_u c_t$, and **not** $c_t c_u$.

Expressions (9.78) and (9.79) have the following implication: The operators (9.78, 9.79) in the basis of many–particle states $|\Psi^{\mathrm{B,F}}(\mathcal{N})\rangle$ have the same values as the respective matrix elements (9.62). In order to determine these matrix elements one needs to evaluate first the matrix elements of the generic operators $\langle r|\hat{f}|s\rangle$ $\langle r,s|\hat{g}|t,u\rangle$ as defined in (9.63) and (9.64), respectively, and then in a second step the matrix elements

$$\langle \Psi^{\mathrm{B}}(\mathcal{N}')|a_r^\dagger a_s|\Psi^{\mathrm{B}}(\mathcal{N})\rangle \;, \quad \langle \Psi^{\mathrm{B}}(\mathcal{N}')|a_r^\dagger a_s^\dagger a_t a_u|\Psi^{\mathrm{B}}(\mathcal{N})\rangle \quad \text{bosons} \tag{9.80}$$

$$\langle \Psi^{\mathrm{F}}(\mathcal{N}')|c_r^\dagger c_s|\Psi^{\mathrm{F}}(\mathcal{N})\rangle \;, \quad \langle \Psi^{\mathrm{F}}(\mathcal{N}')|c_r^\dagger c_s^\dagger c_t c_u|\Psi^{\mathrm{F}}(\mathcal{N})\rangle \quad \text{fermions} \tag{9.81}$$

For the latter matrix elements simple rules can be derived from the algebraic properties of the boson and fermion operators (9.23, 9.24) and (9.45, 9.46), respectively. These rules will be provided below only for the case of fermions. To show that the resulting values of the matrix elements (9.62) are correct one needs to compare the result derived with conventional derivations of the matrix elements[2].

The Matrix Elements $\langle \Psi^{\mathrm{F}}(\mathcal{N}')|c_r^\dagger c_s|\Psi^{\mathrm{F}}(\mathcal{N})\rangle$

We consider first the case $r = s$. The matrix elements are then actually those of the number operator $c_r^\dagger c_r$ which is diagonal in the occupation number representation, i.e.,

$$\langle \Psi^{\mathrm{F}}(\mathcal{N}')|c_r^\dagger c_r|\Psi^{\mathrm{F}}(\mathcal{N})\rangle \;=\; n_r \prod_{r=1}^{S} \delta_{n'_r\, n_r} \;. \tag{9.82}$$

In case of $r \neq s$ one obtains

$$\begin{aligned} &\langle \Psi^{\mathrm{F}}(\mathcal{N}')|c_r^\dagger c_s|\Psi^{\mathrm{F}}(\mathcal{N})\rangle \;= \\ &\langle c_r\, \Psi^{\mathrm{F}}(\mathcal{N}')|c_s\, \Psi^{\mathrm{F}}(\mathcal{N})\rangle \;=\; n'_r(-1)^{q'_r}\, n_s(-1)^{q_s}\, \delta_{n'_r-1\, n_r} \delta_{n'_s\, n_s-1} \prod_{\substack{t=1 \\ t\neq r,s}} \delta_{n'_t\, n_t} \end{aligned} \tag{9.83}$$

[2]We refer the reader to Condon and Shortley's 'Theory of Atomic Spectra', pp.171 and pp.176 where the matrix elements of fermion states can be found.

From (9.82, 9.84) we can conclude that for *diagonal elements* holds

$$\langle \Psi^{\mathrm{F}}(\mathcal{N})|\hat{F}|\Psi^{\mathrm{F}}(\mathcal{N})\rangle \;=\; \sum_{r=1}^{S} n_r \,\langle r|\hat{f}|r\rangle \tag{9.84}$$

The *off-diagonal elements* with $n'_r = n_r$ except for $r = s,t$, in which case $n'_s = n_s + 1$ and $n'_t = n_t - 1$ holds, are

$$\langle \Psi^{\mathrm{F}}(\mathcal{N}')|\hat{F}|\Psi^{\mathrm{F}}(\mathcal{N})\rangle \;=\; (1-n_s)(-1)^{q'_s}\, n_t (-1)^{q_t}\,\langle s|\hat{f}|t\rangle \tag{9.85}$$

All other matrix elements vanish, i.e., those for which $\mathcal{N}'$ and $\mathcal{N}$ differ in more than two occupation numbers. Comparision with the results in Condon&Shortley (pp. 171) shows that the operator defined in (9.78) does yield the same results as the operator defined in (9.59) when the matrix elements are determined between Slater determinant wave functions.

The Matrix Elements $\langle \Psi^{\mathrm{F}}(\mathcal{N}')|c_r^\dagger c_s^\dagger c_t c_u|\Psi^{\mathrm{F}}(\mathcal{N})\rangle$

Before we determine these matrix elements we will investigate which possible combination of indices r,s,t,u need to be considered. Starting from the definition (9.79) and using $\left(c_r^\dagger\right)^2 = 0$, $c_r^2 = 0$ we can write

$$\hat{G} \;=\; \frac{1}{2} \sum_{\substack{r,s,t,u \\ r\neq s,\, t\neq u}}^{S} \langle rs|\hat{g}|tu\rangle c_r^\dagger c_s^\dagger c_u c_t \tag{9.86}$$

For the combination of indices r,s,t,u in this sum three possibilities exist

Case 0 two of the four indices are different;

Case 1 three of the four indices are different;

Case 2 all four indices are different.

Accordingly, we split the sum in (9.86) into three contributions, namely, $\hat{G} = \hat{G}_0 + \hat{G}_1 + \hat{G}_2$, where each contribution corresponds to one of the three cases mentioned.
The first contribution $\hat{G}_0$ is

$$\hat{G}_0 \;=\; \frac{1}{2} \sum_{\substack{r,s=1 \\ \text{a.i.d.}}}^{S} \langle r\, s|\hat{g}|r\, s\rangle c_r^\dagger c_s^\dagger c_s c_r \;+\; \frac{1}{2} \sum_{\substack{r,s=1 \\ \text{a.i.d.}}}^{S} \langle r\, s|\hat{g}|s\, r\rangle c_r^\dagger c_s^\dagger c_r c_s \;. \tag{9.87}$$

Here and in the following we denote by 'a.i.d.' (*all indices different*) that only tuples (r,s), (r,s,t), (r,s,t,u) are included in the summation for which all indices are different, i.e., for which holds $r \neq s$, $r \neq t$ etc. The anti-commutation property (9.45) yields together with the definition of the occupation number operator (9.53)

$$\hat{G}_0 \;=\; \frac{1}{2} \sum_{\substack{r,s=1 \\ \text{a.i.d.}}}^{S} \Big(\langle r\, s|\hat{g}|r\, s\rangle \;-\; \langle r\, s|\hat{g}|s\, r\rangle \Big)\, \hat{N}_r\, \hat{N}_s \;. \tag{9.88}$$

Obviously, this contribution to the two–particle operator is diagonal in the occupation number representation. As we will find, this part accounts for all diagonal contributions to $\hat{G}$.
The second contribution $\hat{G}_1$ is

$$\begin{aligned}\hat{G}_1 &= \tfrac{1}{2}\sum_{\substack{r,s,t=1\\ \text{a.i.d.}}}^{S}\langle r\,s|\hat{g}|r\,t\rangle c_r^\dagger c_s^\dagger c_t c_r \\ &+ \tfrac{1}{2}\sum_{\substack{r,s,t=1\\ \text{a.i.d.}}}^{S}\langle r\,s|\hat{g}|t\,s\rangle c_r^\dagger c_s^\dagger c_s c_t \\ &+ \tfrac{1}{2}\sum_{\substack{r,s,t=1\\ \text{a.i.d.}}}^{S}\langle r\,s|\hat{g}|s\,t\rangle c_r^\dagger c_s^\dagger c_t c_s \\ &+ \tfrac{1}{2}\sum_{\substack{r,s,t=1\\ \text{a.i.d.}}}^{S}\langle r\,s|\hat{g}|t\,r\rangle c_r^\dagger c_s^\dagger c_r c_t\ . \end{aligned} \tag{9.89}$$

Commutation of $c_t c_u$ according to (9.45), employing the symmetry property (9.65), relabelling summation indices and using $c_r^\dagger c_s^\dagger c_t c_r = c_s^\dagger c_r^\dagger c_r c_t = c_s^\dagger c_t \hat{N}_r$ yields

$$\hat{G}_1 = \sum_{\substack{r,s,t=1\\ \text{a.i.d.}}}^{S}\Big(\langle r\,s|\hat{g}|r\,t\rangle - \langle r\,s|\hat{g}|t\,r\rangle\Big) c_s^\dagger c_t \hat{N}_r\ . \tag{9.90}$$

Since $\hat{N}_r$ is diagonal, this contribution obviously behaves similarly to the off-diagonal part (9.84) of the one–particle operator $\hat{F}$.
A similar series of transformations allows one to express $\hat{G}_2$ which can be written

$$\begin{aligned}\hat{G}_2 &= \tfrac{1}{2}\sum_{\substack{r,s,t,u\\ r>s,t>u}}^{S}\langle r\,s|\hat{g}|t\,u\rangle c_r^\dagger c_s^\dagger c_u c_t \\ &+ \tfrac{1}{2}\sum_{\substack{r,s,t,u\\ r>s,t<u}}^{S}\langle r\,s|\hat{g}|t\,u\rangle c_r^\dagger c_s^\dagger c_u c_t \\ &+ \tfrac{1}{2}\sum_{\substack{r,s,t,u\\ r<s,t>u}}^{S}\langle r\,s|\hat{g}|t\,u\rangle c_r^\dagger c_s^\dagger c_u c_t \\ &+ \tfrac{1}{2}\sum_{\substack{r,s,t,u\\ r<s,t<u}}^{S}\langle r\,s|\hat{g}|t\,u\rangle c_r^\dagger c_s^\dagger c_u c_t \end{aligned} \tag{9.91}$$

as follows

$$\hat{G}_2 = \sum_{\substack{r,s,t,u\\ r>s,t>u}}^{S}\Big(\langle r\,s|\hat{g}|t\,u\rangle - \langle r\,s|\hat{g}|u\,t\rangle\Big) c_r^\dagger c_s^\dagger c_u c_t\ . \tag{9.92}$$

This contribution to $\hat{G}$ has non-vanishing matrix elements only when $\mathcal{N}'$ differs from $\mathcal{N}$ in *four* occupation numbers n_r, n_s, n_t, n_u. A similar contribution does not arise for $\hat{F}$.
We can state now the matrix elements $\langle\Psi^{\mathrm{F}}(\mathcal{N}')|\hat{G}|\Psi^{\mathrm{F}}(\mathcal{N})\rangle$. For this purpose we consider three cases which actually correspond to the three cases considered below Eq. (9.86).

Case 0 This case covers diagonal matrix elements, i.e., $\mathcal{N}' = \mathcal{N}$ or $n_r' = n_r$ for all r. Only $\hat{G}_0$, given in (9.88), contributes in this case. One obtains

$$\langle\Psi^{\mathrm{F}}(\mathcal{N})|\hat{G}|\Psi^{\mathrm{F}}(\mathcal{N})\rangle = \frac{1}{2}\sum_{r,s}^{S} n_r n_s\Big(\langle r,\,s|\hat{g}|r,\,s\rangle - \langle r,\,s|\hat{g}|s,\,r\rangle\Big)\ . \tag{9.93}$$

Case 1 This case covers off-diagonal elements with $n'_r = n_r$ except for $r = s, t$ for which holds $n'_s = n_s + 1$ and $n'_t = n_t - 1$. Only $\hat{G}_1$, given in (9.90), contributes in this case. One obtains

$$\begin{aligned} &\langle \Psi^{\mathrm{F}}(\mathcal{N}')|\hat{G}|\Psi^{\mathrm{F}}(\mathcal{N})\rangle \;= \\ &(-1)^{q'_s+q_t}(1-n_s)n_t \sum\nolimits_{\substack{r \\ r\neq s,t}} n_r \left(\langle r,s|\hat{g}|r,t\rangle \;-\; \langle r,s|\hat{g}|t,r\rangle \right) \end{aligned} \tag{9.94}$$

Case 2 This case covers off-diagonal elements with $n'_r = n_r$ except for $r = s, t, u, v$ for which holds $n'_s = n_s + 1$, $n'_t = n_t + 1$, $n'_u = n_u - 1$, $n'_v = n_v - 1$. Only $\hat{G}_2$, given in (9.92), contributes in this case. One obtains

$$\begin{aligned} &\langle \Psi^{\mathrm{F}}(\mathcal{N}')|\hat{G}|\Psi^{\mathrm{F}}(\mathcal{N})\rangle \;= \\ &\pm (-1)^{q'_s+q'_r+q_u+q_v}(1-n_s)(1-n_r)n_u n_v \left(\langle r,s|\hat{g}|u,v\rangle \;-\; \langle r,s|\hat{g}|v,u\rangle \right) \end{aligned} \tag{9.95}$$

In the latter formula the '+'-sign applies for $s < r$, $u < v$ or $s > r$, $u > v$, the '−'-sign applies for $s < r$, $u > v$ or $s > r$, $u < v$.

All matrix elements which are not covered by the three cases above vanish. In particular, for *non-vanishing* matrix elements $\langle \Psi^{\mathrm{F}}(\mathcal{N}')|\hat{G}|\Psi^{\mathrm{F}}(\mathcal{N})\rangle$ *at most four occupation numbers* n'_r and n_r *can differ*. Furthermore, *particle number is conserved*, i.e., it holds $\sum_{r=1}^{S} n'_r = \sum_{r=1}^{S} n_r$.

Exercise 9.3.1: Derive (9.90) from (9.89).
Exercise 9.3.2: Derive (9.92) from (9.91).
Exercise 9.3.3: Derive (9.95) from (9.92).
Exercise 9.3.4: Show that the matrix elements of $\hat{F}$ and of $\hat{G}$ conserve particle number.
Exercise 9.3.5: Derive the non-vanishing matrix elements (9.62) for bosons.

Spin Operators

In this section we will briefly consider the spin operators $\vec{\hat{S}}$ given in (9.73) and $\hat{S}^2$ given in (9.75) which are, respectively, one–particle and two–particle operators. The matrix elements of the corresponding generic operators are (9.74) and (9.76). We like to express these operators through fermion creation and annihilation operators. One obtains for the three components of $\vec{\hat{S}}$

$$\begin{aligned} \hat{S}_3 &= \frac{1}{2}\sum_{r=1}^{S} \left(\hat{N}_{r\alpha} \;-\; \hat{N}_{r\beta} \right) \\ \hat{S}_+ &= \sum_{r=1}^{S} c^\dagger_{r\alpha} c_{r\beta} \\ \hat{S}_- &= \sum_{r=1}^{S} c^\dagger_{r\beta} c_{r\alpha} \end{aligned} \tag{9.96}$$

For $\hat{S}^2$ one obtains

$$\hat{S}^2 \;=\; \frac{1}{2}\hat{N} \;+\; \frac{1}{4}\sum_{r,s=1}^{S}(\hat{N}_{r\alpha} \;-\; \hat{N}_{r\beta})(\hat{N}_{s\alpha} \;-\; \hat{N}_{s\beta}) \;-\; \sum_{r,s=1}^{S} c^{\dagger}_{r\alpha}c^{\dagger}_{s\beta}c_{r\beta}c_{s\alpha}\;. \tag{9.97}$$

The summation in (9.96, 9.97) is over the orbital states, the spin part of the single–particle states is represented by $\alpha = \frac{1}{2}$ and $\beta = -\frac{1}{2}$.

Exercise 9.3.6: Derive (9.96) and (9.97).

9.4 Independent-Particle Models

In the remaining part of this chapter we will apply the technique of operators of 2nd quantization to the description of many–fermion systems as they arise, e.g., in crystals, molecules, atoms and nuclei. In all these systems the *Hamiltonian* is a sum of one– and two–particle operators

$$H \;=\; \sum_{r=1}^{S}\langle r|\hat{t}|s\rangle c^{\dagger}_{r}c_{s} \;+\; \frac{1}{2}\sum_{r,s,t,u}^{S}\langle r,s|\hat{v}|u,v\rangle c^{\dagger}_{r}c^{\dagger}_{s}c_{u}c_{t}\;. \tag{9.98}$$

In many cases the Hamiltonian is spin-independent and the equivalent notation

$$H \;=\; \sum_{\substack{r,s=1\\ \sigma}}^{S}\langle r|\hat{t}|s\rangle c^{\dagger}_{r\sigma}c_{s\sigma} \;+\; \frac{1}{2}\sum_{\substack{r,s,t,u=1\\ \sigma,\sigma'}}^{S}\langle r,s|\hat{v}|t,u\rangle c^{\dagger}_{r\sigma}c^{\dagger}_{s\sigma'}c_{u\sigma'}c_{t\sigma} \tag{9.99}$$

will be used. In the latter case the indices r, s, t, u refer only to the orbital part of the single–particle basis.

If it were not for the two–particle contribution to the Hamiltonian, which represents the interactions between particles, the description of many–particle systems, e.g., evaluation of their stationary states and excitation energies, would be a simple exercise in linear algebra. Unfortunately, the two–particle operator makes the description of many–particle systems a very hard problem. The fortunate side of this is, however, that the two–particle operator representing interactions between particles induces a variety of interesting phenomena.

Actually, the study of problems governed by Hamiltonians of the type (9.98, 9.99) has preoccupied an important part of all intellectual efforts in Theoretical Physics during the past fifty years. In fact, it is one of the main intellectual achievements of Physics among the Sciences to have addressed systematically the study of systems composed of many strongly interacting components. The outcome of these studies is that even when interactions between components (particles) are simple, the concerted behaviour of interacting systems can deviate qualitatively from that of systems made up of independent components. Examples is the laser action, superconductivity, but also ordinary phenomena like freezing and evaporation. Often, the systems investigated involve a macroscopic number of components such that statistical mechanical approaches are envoked. The great generality of the concepts developed in the context of many–particle systems can be judged from the fact

that today these concepts are providing insight into the functioning of biological brains, another prototypical systems of many strongly interacting components, namely of neurons[3].
Before continuing one may finally point out that the material world as we know it and as it establishes the varieties of natural substances, ranging from nuclei to the molecules of living systems , ultimately depend in a crucial way on the fermion character of its constituent building blocks, electrons and nucleons. If it were'nt for the fermion nature, all material systems would condensate into states which would depend little on particle number. The *Aufbau principle*, according to which nuclei and atoms change their qualitative properties when they grow larger, would not exist. The electronic properties of atoms with different numbers of electrons would differ little, Chemistry essentially would know only one element and Life would not exist.

Exercise 9.4.1: Imagine that in a closed, water-filled jar all electrons of water turn their fermion nature into a boson nature. What might happen?

Independent-Particle Hamiltonian

A many–fermion system governed by an independent-particle Hamiltonian, i.e., a Hamiltonian without a two–particle operator contribution accounting for interactions among the particles, can be described in a rather straightforward way. *We will restrict our description in the following to systems composed of an even number (2N) of particles and to spin-independent interactions.* The Hamiltonian of such system is

$$H_o \;=\; \sum_{\substack{r,s=1\\ \sigma}}^{S} \langle r|\hat{t}|s\rangle c^{\dagger}_{r\sigma} c_{s\sigma} \tag{9.100}$$

We will denote the matrix elements of $\hat{t}$ as $\langle r|\hat{t}|s\rangle \;=\; t_{rs}$.

Transformation to a New Set of Creation and Annihilation Operators

Our aim is to represent the Hamiltonian (9.100) in a form in which the factors $c^{\dagger}_{r\sigma} c_{s\sigma}$ become occupation number operators. In such a representation H_o is diagonal and the stationary states can be stated readily. To alter the representation of H_o we apply a unitary transformation $\mathbf{U}$ to the single–particle states $|r\rangle$ to obtain a new basis of states $|m)$, i.e., $\{|m), m \;=\; 1, 2, \ldots S\}$, where

$$|m) \;=\; \sum_{r=1}^{S} U_{rm} |r\rangle \; . \tag{9.101}$$

The unitary property of U_{rn}

$$\mathbf{U}^{\dagger}\mathbf{U} \;=\; \mathbf{U}\,\mathbf{U}^{\dagger} \;=\; \mathbb{1} \tag{9.102}$$

or

$$\sum_{r=1}^{S} U *_{rm}\, U_{rn} \;=\; \delta_{mn} \; , \quad \sum_{m=1}^{S} U_{rm} U *_{sm} \;=\; \delta_{rs} \tag{9.103}$$

[3] An account of some of these efforts can be found in *Modelling Brain Function – The World of Attractor Neural Networks* by D.J. Amit (Cambridge University Press, New York, 1989)

allows one to express conversely $|r\rangle$ in terms of $|m)$

$$|r\rangle \;=\; \sum_{m=1}^{S} U^*_{rm}|m) \;. \tag{9.104}$$

One can, hence, expand

$$t_{rs} \;=\; \sum_{mn}^{S} \tilde{t}_{mn} U_{rm} U^*_{sn} \tag{9.105}$$

where

$$\tilde{t}_{mn} \;=\; (m|\hat{t}|n) \;=\; \sum_{r,s=1}^{S} t_{rs} U^*_{rm} U_{sn} \;=\; \left(U^\dagger \hat{t} U\right)_{mn} \tag{9.106}$$

which together with (9.100) yields

$$H_o \;=\; \tilde{t}_{mn} d^\dagger_{m\sigma} d_{n\sigma} \tag{9.107}$$

where

$$d^\dagger_{n\sigma} \;=\; \sum_{r=1}^{S} U_{rn} c^\dagger_{r\sigma} \;, \quad d_{n\sigma} \;=\; \sum_{r=1}^{S} U^*_{rn} c_{r\sigma} \tag{9.108}$$

These operators describe the creation and annihilation operators of fermions in states $|n)$ which are linear combinations (9.101) of states $|r\rangle$. The unitary property (9.103) allows one to express [c.f. (9.104)]

$$c^\dagger_{r\sigma} \;=\; \sum_{m=1}^{S} U^*_{rm} d^\dagger_{m\sigma} \;, \quad c_{s\sigma} \;=\; \sum_{n=1}^{S} U_{sn} d_{n\sigma} \;. \tag{9.109}$$

The operators (9.108) obey the same anti-commutation properties (9.45, 9.46) as $c^\dagger_{r\sigma}$ and $c_{r\sigma}$, namely,

$$[d_{m\sigma}, d_{n\sigma'}]_+ \;=\; 0 \;; \quad [d^\dagger_{m\sigma}, d^\dagger_{n\sigma'}]_+ \;=\; 0 \tag{9.110}$$

$$[d_{m\sigma}, d^\dagger_{n\sigma'}]_+ \;=\; \delta_{mn}\, \delta_{\sigma\sigma'} \tag{9.111}$$

and, accordingly, they are Fermion creation and annihilation operators. In a basis of states

$$\prod_{j=1}^{N} d^\dagger_{n_j\sigma_j} \; |0\rangle \tag{9.112}$$

, i.e., of N-Fermion states in which single particle states $|n_j)$ as defined in (9.101) are occupied, the operators $d^\dagger_{n\sigma}$ and $d_{n\sigma}$, behave exactly like the operators $c^\dagger_{r\sigma}$ and $c_{r\sigma}$ behave for states $|\Psi^F(\mathcal{N})\rangle$; for example, the expressions drived above for the matrix elements of one- and two-particle operators hold in an analogous way for $d^\dagger_{n\sigma}$ and $d_{n\sigma}$.

We demonstrate here the anti-commutation property (9.111), the anti-commutation properties (9.110) can be demonstrated similarly. The l.h.s. of (9.111) can be written, using (9.108) and (9.46),

$$[d_{m\sigma}, d^\dagger_{n\sigma'}]_+ \;=\; \sum_{r,s} U^*_{rm} U_{sn} \, [c_{r\sigma}, c^\dagger_{s\sigma'}]_+ \;=\; \delta_{\sigma\sigma'} \sum_{r} U^*_{rm} U_{rn} \;. \tag{9.113}$$

The unitarity property $\sum_r U^*_{rm} U_{rn} \;=\; \delta_{mn}$ yields immediately identity (**??**).

Diagonal Representation

The transformation (9.101) gives us the freedom to choose the matrix (9.106) diagonal, i.e.,

$$\tilde{t}_{mn} \;=\; \epsilon_n \, \delta_{mn} \; . \tag{9.114}$$

In this case H_o has the desired form

$$H_o \;=\; \sum_{n=1}^{S} \epsilon_n d^{\dagger}_{n\sigma} d_{n\sigma} \tag{9.115}$$

and involves solely occupation number operators $\hat{\tilde{N}}_{n\sigma} \;=\; d^{\dagger}_{n\sigma} d_{n\sigma}$. It is, hence, a simple matter to state many–particle states in the new representation.
Before proceeding we like to address the issue how the new representation, i.e., transformation matrices U_{rn} and energy values ϵ_n, is obtained. The condition (9.114) together with (9.106) is equivalent to

$$\sum_{s=1}^{S} t_{rs} U_{sn} \;=\; \epsilon_n U_{rn} \quad \forall r, r = 1, 2, \ldots S \tag{9.116}$$

which follows from (9.106) and the unitary property of U_{rn}. This equation poses the eigenvalue problem for the hermitian matrix (t_{rs}). The corresponding eigenvalues $\epsilon_n, n \;=\; 1, 2, \ldots S$ are real, the associated (properly normalized) eigenvectors V_n are the columns of (U_{rn}), i.e., $V_n^T \;=\; (U_{1n}, U_{2n}, \ldots U_{Sn})$.
Eigenstates of (9.115) can be stated immediately since any many–particle wave function in the occupation number representation is suitable. We apply for this purpose (9.57) to the case of $2N$ particles. The $2N$ fermion state

$$\prod_{j=1}^{2N} d^{\dagger}_{n_j \, \sigma_j} |0\rangle \quad \text{where } (n_j, \sigma_j) \;\neq\; (n_k, \sigma_k) \text{ for } j \neq k \tag{9.117}$$

are eigenstates of (9.115) with eigenvalues

$$E(n_1, \sigma_1;\, n_2, \sigma_2;\, \ldots n_{2N}, \sigma_{2N};\,) \;=\; \sum_{j=1}^{2N} \epsilon_{n_j} \; . \tag{9.118}$$

Ground State

In case of an ordering $\epsilon_m \;<\; \epsilon_n$ for $m < n$ the state of lowest energy, the so-called ground state, is

$$|\Phi_o\rangle \;=\; \prod_{j=1}^{N} d^{\dagger}_{j\,\alpha} d^{\dagger}_{j\,\beta} |0\rangle \; . \tag{9.119}$$

In this state the N lowest orbital eigenstates of t_{rs} are occupied each by an electron with spin $|\alpha\rangle \;=\; |\frac{1}{2}, \frac{1}{2}\rangle$ and $|\beta\rangle \;=\; |\frac{1}{2}, -\frac{1}{2}\rangle$. A *non-degenerate* orbital state which is occupied by two fermions, i.e., a fermion in a spin state $|\frac{1}{2},\, \frac{1}{2}\rangle$ as well as a fermion in a spin state $|\frac{1}{2},\, -\frac{1}{2}\rangle$ is called a *closed*

shell. The ground state has only closed shells. We will demonstrate now that this property endows the ground state with total spin zero.
In order to investigate the total spin of $|\Phi_o\rangle$ we apply to this state the total spin operator $\hat{S}^2$ as given by (9.97). The spin operator in the present representation of single-particle states is

$$\hat{S}^2 \;=\; \frac{1}{2}\hat{N} + \frac{1}{4}\sum_{m,n=1}^{S}(\hat{\bar{N}}_{m\alpha} - \hat{\bar{N}}_{m\beta})(\hat{\bar{N}}_{n\alpha} - \hat{\bar{N}}_{n\beta}) - \sum_{m,n=1}^{S} d^\dagger_{m\alpha}d^\dagger_{n\beta}d_{m\beta}d_{n\alpha} \tag{9.120}$$

where the occupation number operators refer to the single-particle states $|m)$. The action of the operator (9.120) is particularly simple for closed shells. One can conclude immediately that the second term in (9.97), namely, $\frac{1}{4}\sum_{m,n=1}^{S}(\hat{\bar{N}}_{m\alpha} - \hat{\bar{N}}_{m\beta})(\hat{\bar{N}}_{n\alpha} - \hat{\bar{N}}_{n\beta})$ does not give any contribution if either $|m)$ or $|n)$ are closed shells. Similarly, the third term $-\sum_{m,n=1}^{S} c^\dagger_{m\alpha}c^\dagger_{n\beta}c_{m\beta}c_{n\alpha}$ does not give a contribution if $m \neq n$ and either $|m)$ or $|n)$ are closed shells. In case of $m = n$ it gives a contribution '1' for each closed shell which cancels the contribution of the first term. Alltogether, one can conclude that $|\Phi_o\rangle$ is an eigenstate of $\hat{S}^2$ with eigenvalue zero, i.e., is a *singlet state*.

Excited States

We want to construct now excited states for the system governed by the independent-particle Hamiltonian (9.100). Obviously, the states with energy closest to the ground state are those in which a particle is promoted from the highest occupied state $|N)$ to the lowest unoccupied state $|N+1)$. There are four such states, namely,

$$\begin{aligned}
|\alpha,\alpha\rangle\rangle &= d^\dagger_{N+1\alpha}d_{N\alpha}|\Phi_o\rangle \\
|\alpha,\beta\rangle\rangle &= d^\dagger_{N+1\alpha}d_{N\beta}|\Phi_o\rangle \\
|\beta,\alpha\rangle\rangle &= d^\dagger_{N+1\beta}d_{N\alpha}|\Phi_o\rangle \\
|\beta,\beta\rangle\rangle &= d^\dagger_{N+1\beta}d_{N\beta}|\Phi_o\rangle
\end{aligned} \tag{9.121}$$

All four states have the same excitation energy, i.e., energy above the ground state, of $\Delta E = \epsilon_{N+1} - \epsilon_N$. However, the states differ in their spin character. The two states $|\alpha,\beta\rangle\rangle$ and $|\beta,\alpha\rangle\rangle$ are eigenstates of $\hat{S}^2$ given in (9.120), both with eigenvalues 2

$$\hat{S}^2|\alpha,\beta\rangle\rangle \;=\; 2\,|\alpha,\beta\rangle\rangle\,; \quad \hat{S}^2||\beta,\alpha\rangle\rangle \;=\; 2\,|\beta,\alpha\rangle\rangle\,. \tag{9.122}$$

This property can be derived as follows: The two states are obviously diagonal with respect to the following contribution to $\hat{S}^2$

$$\hat{\Sigma}_1 \;=\; \frac{1}{2}\hat{N} + \frac{1}{4}\sum_{m,n=1}^{N-1}(\hat{N}_{m\alpha} - \hat{N}_{m\beta})(\hat{N}_{n\alpha} - \hat{N}_{n\beta}) - \sum_{m,n=1}^{N-1} d^\dagger_{m\alpha}d^\dagger_{n\beta}d_{m\beta}d_{n\alpha} \tag{9.123}$$

which acts only on the $N-1$ closed shells (except for $\hat{N}$) of the two states and has an eigenvalue $N + 0 - (N-1) = 1$ in both cases. The remaining contributions to $\hat{S}^2$ which act on partially occupied orbitals $|N\rangle$ and $|N+1\rangle$ are

$$\hat{\Sigma}_2 \;=\; \frac{1}{4}\sum_{m,n=N}^{N+1}(\hat{N}_{m\alpha} - \hat{N}_{m\beta})(\hat{N}_{n\alpha} - \hat{N}_{n\beta}) \tag{9.124}$$

and

$$\hat{\Sigma}_3 \;=\; -\sum_{m,n=N}^{N+1} d^\dagger_{m\alpha} d^\dagger_{n\beta} d_{m\beta} d_{n\alpha} \; . \tag{9.125}$$

Contributions to $\hat{S}^2$ acting on states $|N+2\rangle, |N+3\rangle, \ldots$ do not need to be considered since they give vanishing contributions. The two states $|\alpha,\beta\rangle\rangle$, $|\beta,\alpha\rangle\rangle$ are, of course, also eigenstates of $\hat{\Sigma}_2$, both with eigenvalues 1. The action of $\hat{\Sigma}_3$ on the two states produces , for example, for $|\alpha,\beta\rangle\rangle$

$$\hat{\Sigma}_3|\alpha,\beta\rangle\rangle \;=\; -\sum_{m,n=N}^{N+1} d^\dagger_{m\alpha} d^\dagger_{n\beta} d_{m\beta} d_{n\alpha} d^\dagger_{N+1\alpha} d_{N\beta}|\Phi_o\rangle \;=\; 0 \tag{9.126}$$

which follows from the occurence of squares of fermion operators which, of course, vanish. The same result holds for $|\beta,\alpha\rangle\rangle$. One can, hence, conclude that (9.122) is correct.
An eigenvalue '2' of the spin operator $\hat{S}^2$ identifies the states $|\alpha,\beta\rangle\rangle$ and $|\beta,\alpha\rangle\rangle$ as triplet states. The remaining states $|\alpha,\alpha\rangle\rangle$ and $|\beta,\beta\rangle\rangle$ are not eigenstates of $\hat{S}^2$, however, the linear combinations $\sqrt{1/2}(|\alpha,\alpha\rangle\rangle \pm |\beta,\beta\rangle\rangle$ qualify as eigenstates, one with eigenvalue zero (singlet) and one with eigenvalue '2' (triplet).

Exercise 9.4.2: Construct four operators $\hat{O}_{\ell m}$

$$\hat{O}_{\ell m} \;=\; \sum_{\sigma,\sigma'} \gamma^{\ell m}_{\sigma,\sigma'} d^\dagger_{N+1,\sigma} d_{N\sigma'} \tag{9.127}$$

such that $\hat{O}_{\ell m}|\Phi_o\rangle$ are triplet and singlet states, i.e., apropriate eigenstates of the operators $\hat{S}^2$ and $\hat{S}_3$.

Example: $2N$ **Independent Electrons on a Ring**

In order to illustrate the procedure to obtain eigenstates of one-particle Hamiltonians (9.100) outlined above we consider a system of $2N$ electrons which move in a set of atomic orbitals $|r\rangle$, $r = 1, 2, \ldots 2N$ which are located on a ring. The system is assumed to posses a $2N$–fold symmetry axis and interactions connect only orbital states $|r\rangle \rightarrow |r \pm 1\rangle$. We identify the states $|2N+1\rangle = |1\rangle$ to avoid cumbersome summation limits, etc. The system is described by the Hamiltonian

$$\hat{H}_o \;=\; -t \sum_{\substack{n=1 \\ \sigma}}^{2N} \left(c^\dagger_{n+1\,\sigma} c_{n\,\sigma} \;+\; c^\dagger_{n\,\sigma} c_{n+1\,\sigma} \right) \; . \tag{9.128}$$

The cyclic property of the system is expressed through

$$c_{2N+1\,\sigma} \;=\; c_{1\,\sigma} \; ; \quad c^\dagger_{2N+1\,\sigma} \;=\; c^\dagger_{1\,\sigma} \tag{9.129}$$

The symmetry of the Hamiltonian suggests to choose a new representation defined through the operators ($r = 1, 2, \ldots 2N$)

$$d_{r\sigma} \;=\; \frac{1}{\sqrt{2N}} \sum_{n=1}^{2N} e^{-irn\pi/N} \, c_{n\sigma} \tag{9.130}$$

$$d^\dagger_{r\sigma} \;=\; \frac{1}{\sqrt{2N}} \sum_{n=1}^{2N} e^{irn\pi/N}\, c^\dagger_{n\sigma} \tag{9.131}$$

(9.130, 9.131) constitute a unitary transformation $\mathbf{U}$ defined through $U_{rn} \;=\; \frac{1}{\sqrt{2N}} e^{irn\pi/N}$. The unitarity property follows from

$$\sum_{r=1}^{2N} e^{irs\pi/N} \;=\; 0 \quad \text{for } 0 < s < 2N \;., \tag{9.132}$$

an identity which can be derived employing the well-known expression for a finite geometric series

$$\sum_{s=1}^{m} a^s \;=\; a\,\frac{1-a^m}{1-a} \;. \tag{9.133}$$

Application to the l.h.s. of (9.132) gives for $r \neq 0,\, 2N,\, 4N, \ldots$

$$e^{is\pi/N}\,\frac{1 \,-\, e^{2N\,is\pi/N}}{1 \,-\, e^{is\pi/N}} \tag{9.134}$$

which, indeed, vanishes for integer s. One can then express[cf. (9.109)]

$$c_{n\sigma} \;=\; \frac{1}{\sqrt{2N}} \sum_{r=1}^{2N} e^{irn\pi/N}\, d_{r\sigma} \tag{9.135}$$

$$c^\dagger_{n\sigma} \;=\; \frac{1}{\sqrt{2N}} \sum_{r=1}^{2N} e^{-irn\pi/N}\, d^\dagger_{r\sigma} \tag{9.136}$$

and, thereby, one obtains the new representation of $\hat{H}_o$

$$\hat{H}_o \;=\; -t \sum_{\substack{r,s=1\\ \sigma}}^{2N} \tilde{t}_{rs}\, d^\dagger_{r\sigma} d_{s\sigma} \tag{9.137}$$

where

$$\tilde{t}_{rs} \;=\; e^{-ir\pi/N}\,\frac{1}{2N}\sum_{n=1}^{2N} e^{i(s-r)n\pi/N} \;+\; e^{is\pi/N}\,\frac{1}{2N}\sum_{n=1}^{2N} e^{i(r-s)n\pi/N} \quad . \tag{9.138}$$

Using (9.132) one can conclude

$$\tilde{t}_{rs} \;=\; \left(e^{ir\pi/N} \;+\; e^{-ir\pi/N} \right) \delta_{rs} \tag{9.139}$$

from which follows

$$\hat{H}_o \;=\; \sum_{\substack{r=1\\ \sigma}}^{2N} \left(-2t\,\cos\frac{r\pi}{N} \right)\; d^\dagger_{r\sigma} d_{r\sigma} \;. \tag{9.140}$$

The Hamiltonian is now diagonal and the construction outlined above can be applied.

Exercise 9.4.3: Construct the ground state and the lowest energy excited state(s) for a system of $2N$ electrons moving in a linear chain of single-electron orbitals $|n\rangle$, $n = 1, 2, \ldots 2N$ with interactions between neighbouring $(n, n \pm 1)$ orbitals and Hamiltonian

$$\hat{H}_o \;=\; -\,t \sum_{\substack{n=1 \\ \sigma}}^{2N-1} \left(c^\dagger_{n+1\,\sigma} c_{n\,\sigma} \;+\; c^\dagger_{n\,\sigma} c_{n+1\,\sigma} \right) . \tag{9.141}$$

State the excitation energy ΔE.

9.5 Self-Consistent Field Theory

Observations of many-fermion systems show that properties of such systems often can be explained to a surprisingly good degree on the basis of the assumption that the fermions move like independent particles. The most famous example is the periodic table of the elements. The regularities of the elements can be rationalized in terms of electrons moving in hydrogen atom-type orbitals, i.e., in states which are constructed according to the 'Aufbauprinzip' in a manner which neglects the mutual repulsion between electrons. A similar principle accounts approximately for properties of nuclei as described by the nuclear shell model. The properties of molecules can be understood largely in terms of models which place electrons into so-called molecular orbitals in which the electrons move as if they were not interacting with other electrons. Many electronic properties of solids can be understood in a similar way, i.e., assuming that electrons move independently from each other in so-called bands, e.g., valence bands or conduction bands. Of course, properties of many-fermion properties deviant from such simple description is then of as much interest as independent fermion descriptions are useful.

Since independent-particle behaviour is so universal one may wonder why the presence of particle-particle interactions, i.e., the everpresent Coulomb repulsion between electrons, does not spoil it. The reason is mainly connected with the fact that most many-fermion systems are found in their ground state or removed from it through low energy excitations, and that independent-particle behaviour surfaces mainly because it applies well to the ground state. There are two reasons why this is so: first, if one places fermions into an independent-particle ground state of the type (9.119) then perturbations due to pair interactions according to the Pauli exclusion principle can only involve independent particle states not occupied in the ground state, i.e., those with energy *above* that of the (energetically) highest occupied single-particle state. Hence, the fermion nature restricts the possibility for perturbations on the system, in particular, if one can choose the single-particle states such that the residual perturbations are small. We will present in this and the following section a method which constructs such optimal single-fermion states. These states do not altogether neglect the pair interactions, rather they assume that each particle experiences the average interaction due to the fermions frozen into the ground state.

A second reason why independent-particle models can be successful is that the pair interaction for electrons is the slowly decaying Coulomb interaction. The slow decay of the interaction makes the motion of any one electron rather independent of the exact position of most other electrons, i.e., one expects that mean-field descriptions should be rather sufficient.

In this section we will consider systems of $2N$ fermions described by the spin-independent Hamiltonian

$$H \;=\; \sum_{\substack{r,s=1\\ \sigma}}^{S} \langle r|\hat{t}|s\rangle c^{\dagger}_{r\sigma}c_{s\sigma} \;+\; \frac{1}{2}\sum_{\substack{r,s,t,u=1\\ \sigma,\sigma'}}^{S} \langle r,s|\hat{v}|t,u\rangle c^{\dagger}_{r\sigma}c^{\dagger}_{s\sigma'}c_{u\sigma'}c_{t\sigma} \tag{9.142}$$

and derive a single-particle operator which approximates this Hamiltonian.
In our formulas below we will adopt strictly the convention that indices r, s, t, u refer to the initial basis of single-particle states $|r\rangle, r = 1, 2, \ldots, S$ on which (9.142) is based. We will adopt a second set of single-particle states $\{|\tilde{m}\rangle, m = 1, 2, \ldots S\}$ the elements of which will be labelled by indices m, n, p, q. The states $|\tilde{m}\rangle$ are connected with the states $|r\rangle$ through $(m = 1, 2, \ldots S)$

$$|\tilde{m}\rangle \;=\; \sum_{r=1}^{S} U_{rm}\,|r\rangle\;; \quad |r\rangle \;=\; \sum_{m=1}^{S} U^{*}_{rm}\,|\tilde{m}\rangle\;. \tag{9.143}$$

These S states are associated with the creation and annihilation operators

$$\begin{aligned} d^{\dagger}_{m\sigma} \;&=\; \sum_{r=1}^{S} U_{rm}c^{\dagger}_{r\sigma} \\ d_{m\sigma} \;&=\; \sum_{r=1}^{S} U^{*}_{rm}c_{r\sigma} \end{aligned} \tag{9.144}$$

defined as in (9.108). The states $|\tilde{m}\rangle$ serve to define a reference state of the system

$$|\Phi_o(\mathbf{U})\rangle \;=\; \prod_{j=1}^{N} d^{\dagger}_{j\,\alpha}d^{\dagger}_{j\,\beta}|0\rangle\;. \tag{9.145}$$

which will play a pivotal role: it is this the state in which the fermions are assumed to be moving and relative to which the mean interactions acting on individual fermions is determined.
$\mathbf{U} = (U_{rm})$ as defined in (9.143) with $r, m = 1, 2, \ldots S$ is a unitary matrix. If one restricts $m = 1, 2, \ldots N$, as in in (9.145), the corresponding $\mathbf{U} = (U_{rm})$ forms an $S \times N$ matrix and, naturally, is not unitary.

Mean-Field Potential

The mean field for the reference state $|\Phi_o(\mathbf{U})\rangle$ is defined in a straightforward way by averaging the two-particle contribution to (9.142) over this reference state to turn the contribution into an effective one-particle operator. This is done as follows:

$$\begin{aligned} &\hat{V}_{mf}\left(|\Phi_o(\mathbf{U})\rangle\right) \;= \\ &\frac{1}{2}\sum_{\substack{r,s,t,u=1\\ \sigma,\sigma'}}^{S} \langle r,s|\hat{v}|t,u\rangle\Big(\langle\langle c^{\dagger}_{r\sigma}c^{\dagger}_{s\sigma'}\rangle\rangle c_{u\sigma'}c_{t\sigma} \;+\; c^{\dagger}_{r\sigma}c^{\dagger}_{s\sigma'}\langle\langle c_{u\sigma'}c_{t\sigma}\rangle\rangle \\ &\qquad + c^{\dagger}_{r\sigma}\langle\langle c^{\dagger}_{s\sigma'}c_{u\sigma'}\rangle\rangle c_{t\sigma} \;+\; c^{\dagger}_{s\sigma'}\langle\langle c^{\dagger}_{r\sigma}c_{t\sigma}\rangle\rangle c_{u\sigma'} \\ &\qquad - c^{\dagger}_{r\sigma}\langle\langle c^{\dagger}_{s\sigma'}c_{t\sigma}\rangle\rangle c_{u\sigma'} \;-\; c^{\dagger}_{s\sigma'}\langle\langle c^{\dagger}_{r\sigma}c_{u\sigma'}\rangle\rangle c_{t\sigma} \quad \Big) \end{aligned} \tag{9.146}$$

Here $\langle\langle \quad \cdots \quad \rangle\rangle$ denotes the average

$$\langle\langle \mathcal{O} \rangle\rangle \;=\; \langle \Phi_o(\mathbf{U}) |\, \mathcal{O}\, | \Phi_o(\mathbf{U}) \rangle \;. \tag{9.147}$$

Since the reference state $|\Phi_o(\mathbf{U})\rangle$ is defined in terms of the single-particle states $|\tilde{m}\rangle$ it is preferable to switch the representation of (9.146) accordingly. Since the averages affect only two creation-annihilation operators actually a mixed representation is most suitable

$$\begin{aligned}
\hat{V}_{mf}\left(|\Phi_o(\mathbf{U})\rangle\right) \;&=\; \frac{1}{2} \sum_{\substack{m,n,t,u=1 \\ \sigma,\sigma'}}^{S} \langle \tilde{m}, \tilde{n} | \hat{v} | t, u \rangle \langle\langle d^\dagger_{m\sigma} d^\dagger_{n\sigma'} \rangle\rangle c_{u\sigma'} c_{t\sigma} \\
&+ \frac{1}{2} \sum_{\substack{r,s,m,n=1 \\ \sigma,\sigma'}}^{S} \langle r, s | \hat{v} | \tilde{m}, \tilde{n} \rangle c^\dagger_{r\sigma} c^\dagger_{s\sigma'} \langle\langle d_{m\sigma'} d_{n\sigma} \rangle\rangle \\
&+ \frac{1}{2} \sum_{\substack{r,m,n,t=1 \\ \sigma,\sigma'}}^{S} \langle r, \tilde{m} | \hat{v} | t, \tilde{n} \rangle c^\dagger_{r\sigma} \langle\langle d^\dagger_{m\sigma'} d_{n\sigma'} \rangle\rangle c_{t\sigma} \\
&+ \frac{1}{2} \sum_{\substack{m,s,n,u=1 \\ \sigma,\sigma'}}^{S} \langle \tilde{m}, s | \hat{v} | \tilde{n}, u \rangle c^\dagger_{s\sigma'} \langle\langle d^\dagger_{m\sigma} d_{n\sigma} \rangle\rangle c_{u\sigma'} \\
&- \frac{1}{2} \sum_{\substack{r,m,n,u=1 \\ \sigma,\sigma'}}^{S} \langle r, \tilde{m} | \hat{v} | \tilde{n}, u \rangle c^\dagger_{r\sigma} \langle\langle d^\dagger_{m\sigma'} d_{n\sigma} \rangle\rangle c_{u\sigma'} \\
&- \frac{1}{2} \sum_{\substack{m,s,t,n=1 \\ \sigma,\sigma'}}^{S} \langle \tilde{m}, s | \hat{v} | t, \tilde{n} \rangle c^\dagger_{s\sigma'} \langle\langle d^\dagger_{m\sigma} d_{n\sigma'} \rangle\rangle c_{t\sigma}
\end{aligned} \tag{9.148}$$

where, for example,

$$\langle r, \tilde{m} |\, \hat{v}\, | t, \tilde{n} \rangle \;=\; \sum_{s,u}^{S} \langle r, s |\, \hat{v}\, t, u \rangle\, U^*_{sm}\, U_{un} \;. \tag{9.149}$$

The remaining matrix elements appearing in (9.148) are obtained in a similar way by transforming only two of the four single-particle states into the new representation.
For the averages $\langle\langle \quad \cdots \quad \rangle\rangle$ in (9.148) one obtains, by means of the rules (9.84),

$$\begin{aligned}
\langle\langle d^\dagger_{m\sigma} d^\dagger_{n\sigma'} \rangle\rangle \;&=\; \langle \Phi_o(\mathbf{U}) | d^\dagger_{m\sigma} d^\dagger_{n\sigma'} | \Phi_o(\mathbf{U}) \rangle \;=\; 0 \\
\langle\langle d_{m\sigma} d_{n\sigma'} \rangle\rangle \;&=\; \langle \Phi_o(\mathbf{U}) | d_{m\sigma} d_{n\sigma'} | \Phi_o(\mathbf{U}) \rangle \;=\; 0 \\
\langle\langle d^\dagger_{m\sigma} d_{n\sigma'} \rangle\rangle \;&=\; \langle \Phi_o(\mathbf{U}) | d^\dagger_{m\sigma} d_{n\sigma'} | \Phi_o(\mathbf{U}) \rangle \\
&=\; \begin{cases} \delta_{mn}\delta_{\sigma\sigma'} & m \le N \\ 0 & m > N \end{cases}
\end{aligned} \tag{9.150}$$

and, hence,

$$\hat{V}_{mf}\left(|\Phi_o(\mathbf{U})\rangle\right) \;=\; \frac{1}{2} \sum_{m \le N} \sum_{\substack{r,t=1 \\ \sigma,\sigma'}}^{S} \langle r, \tilde{m} | \hat{v} | t, \tilde{n} \rangle c^\dagger_{r\sigma} c_{t\sigma}\; \delta_{\sigma'\sigma'}$$

$$+\frac{1}{2}\sum_{m\leq N}\sum_{\substack{s,u=1\\ \sigma,\sigma'}}^{S}\langle\tilde{m},s|\hat{v}|\tilde{n},u\rangle c^{\dagger}_{s\sigma'}c_{u\sigma'}\;\delta_{\sigma\sigma}$$

$$-\frac{1}{2}\sum_{m\leq N}\sum_{\substack{r,u=1\\ \sigma}}^{S}\langle r,\tilde{m}|\hat{v}|\tilde{n},u\rangle c^{\dagger}_{r\sigma}c_{u\sigma}$$

$$-\frac{1}{2}\sum_{m\leq N}\sum_{\substack{s,t=1\\ \sigma}}^{S}\langle\tilde{m},s|\hat{v}|t,\tilde{n}\rangle c^{\dagger}_{s\sigma}c_{t\sigma}\;. \tag{9.151}$$

Carrying out the sum $\sum_\sigma \delta_{\sigma\sigma} = 2$ leads to a factor 2 for the first two terms. Exploiting the symmetry $\langle r,s|\,\hat{v}\,|t,u\rangle = \langle s,r|\,\hat{v}\,|u,t\rangle$ and renaming dummy summation indices one can demonstrate that term one and term two as well as term three and four are identical and one obtains

$$\begin{aligned}\hat{V}_{mf}\left(|\Phi_o(\mathbf{U})\rangle\right) &= 2\sum_{\substack{r,m,t=1\\ \sigma,\sigma'}}^{S}\langle r,\tilde{m}|\hat{v}|t,\tilde{n}\rangle c^{\dagger}_{r\sigma}c_{t\sigma}\;\delta_{\sigma'\sigma'}\\ &\quad-\sum_{\substack{r,m,u=1\\ \sigma,\sigma'}}^{S}\langle r,\tilde{m}|\hat{v}|\tilde{n},u\rangle c^{\dagger}_{r\sigma}c_{u\sigma'}\end{aligned} \tag{9.152}$$

By means of expression (9.149) for the matrix elements in the mixed representation one can state the right hand side explicitly in terms of U_{rm}. The one-particle operator (9.152) can then be written in the form

$$\hat{V}_{mf}\left(|\Phi_o(\mathbf{U})\rangle\right) = \sum_{\substack{r,s\\ \sigma}}\langle r|\,\hat{v}_{mf}\left(|\Phi_o(\mathbf{U})\rangle\right)\,|s\rangle\,c^{\dagger}_{r\sigma}c_{s\sigma} \tag{9.153}$$

where

$$\langle r|\,\hat{v}_{mf}\left(|\Phi_o(\mathbf{U})\rangle\right)\,|s\rangle = \sum_{t,u}\left(\,2\,\langle r,t|\,\hat{v}\,|s,u\rangle - \langle r,t|\,\hat{v}\,|u,s\rangle\,\right)\left(\sum_{m\leq N}U^{*}_{tm}U_{um}\right) \tag{9.154}$$

The mean field approximation replaces then the Hamiltonian (9.142) by $\hat{H}_{mf}(\mathbf{U})$ defined through

$$\hat{H}_{mf}(\mathbf{U}) = \sum_{\substack{r,s=1\\ \sigma}}^{S}\left(\,\langle r|\hat{t}|s\rangle + \langle r|\,\hat{v}_{mf}\left(|\Phi_o(\mathbf{U})\rangle\right)\,|s\rangle\,\right)c^{\dagger}_{r\sigma}c_{s\sigma} \tag{9.155}$$

which is a function of the $S\times N$–matrix

$$\mathbf{U} = (U_{rm})_{r=1,2,\ldots S;\,m=1,2,\ldots N} \tag{9.156}$$

which defines the reference state $|\Phi_o(\mathbf{U})\rangle$. The mean field approximation, as introduced here, leaves open the question how the reference state should be chosen. At this point this state is completely arbitrary. We will address now a proper choice of the reference state.

9.6 Self-Consistent Field Algorithm

The Self-Consistent Field (SCF) approximation, often also referred to as the Hartree-Fock approximation, is based on the mean field approach and provides an algorithm to construct a reference state $|\Phi_o(\mathbf{U})\rangle$ for a $2N$ fermion system described by a spin-independent Hamiltonian (9.142). The procedure determines the reference state as the ground state of the independent-particle Hamiltonian (9.155) following the method outlined in Section 9.4. This procedure, however, can achieve this goal only iteratively, assuming in an intial step (1) a properly chosen reference state, determining in a step (2) the corresponding mean field Hamiltonian (9.155), and obtaining in a step (3) the ground state of this one-particle Hamiltonian according to the construction in Section 9.4 and defining this as the new reference state; steps (2) and (3) are being repeated M times until the procedure converges, i.e., the reference state resulting from step $2M+1$ (within numerical error) is equal to the reference state resulting from step $2M-1$. The state thus determined is referred to as the self-consistent independent-particle ground state, the independent-particle nature stemming from the fact that the functional form of the ground state, i.e., (9.119, 9.145), is exact only for an independent-particle Hamiltonian. We will argue below that the self-consistent field ground state, under conditions which often are realized, is the lowest energy independent-particle ground state one can construct.
Let us state now the construction of the self-consistent field ground state in more detail.

SCF-Algorithm, Step 1: Choosing an Initial Reference State

One defines the Hamiltonian

$$\hat{H}^{(1)}_{mf} \;=\; \sum_{\substack{r,s=1\\ \sigma}}^{S} \langle r|\hat{t}|s\rangle c^{\dagger}_{r\sigma} c_{s\sigma} \tag{9.157}$$

and determines the associated diagonal representation defined through

$$\sum_{s=1}^{S} \langle r|\hat{t}|s\rangle U^{(1)}_{sm} \;=\; \epsilon^{(1)}_m \, U^{(1)}_{rm} \;, \quad r = 1,2,\ldots S \;, \quad m = 1,2,\ldots S \;. \tag{9.158}$$

where the labels m are ordered to obey the condition

$$\epsilon^{(1)}_m \;< \epsilon^{(1)}_n \quad \text{for } m \;<\; n \;. \tag{9.159}$$

One defines the reference state $|\Phi_o(\mathbf{U}^{(1)})\rangle$ using the definition (9.145), i.e. $\mathbf{U}^{(1)}$ is the $S\times N$–matrix of the first N column vectors of $U^{(1)}_{rm},\ r = 1,2,\ldots S \;, \quad m = 1,2,\ldots S$.

SCF-Algorithm, Step $2M$, $M = 1,2,\ldots$: Determine Mean Field Hamiltonian

In this step the mean field Hamiltonian

$$\begin{aligned} \hat{H}^{(M)}_{mf} \;&=\; \sum_{\substack{r,s=1\\ \sigma}}^{S} \Big(\langle r|\hat{t}|s\rangle \;+\; \langle r|\, \hat{v}_{mf} \left(|\Phi_o(\mathbf{U}^{(M)})\rangle \right) |s\rangle \Big) \, c^{\dagger}_{r\sigma} c_{s\sigma} \\ &=\; \sum_{\substack{r,s=1\\ \sigma}}^{S} \langle r|\hat{h}^{(M)}_{mf}|s\rangle \, c^{\dagger}_{r\sigma} c_{s\sigma} \end{aligned} \tag{9.160}$$

is evaluated, i.e., the $S \times S$–matrix

$$\langle r|h_{mf}^{(M)}|s\rangle \;=\; \langle r|\hat{t}|s\rangle \;+\; \sum_{t,u=1}^{S} \left(2\langle r,t|\,\hat{v}\,|s,u\rangle \;-\; \langle r,t|\,\hat{v}\,|u,s\rangle \right) \left(\sum_{m=1}^{N} U_{tm}^{*(M)} U_{um}^{(M)} \right) \tag{9.161}$$

is calculated.

SCF-Algorithm, Step $2M+1$, $M = 1, 2, \ldots$: Diagonalize Mean Field Hamiltonian

In this step the eigenvalue problem

$$\sum_{s=1}^{S} \langle r|h_{mf}^{(M)}|s\rangle U_{sm}^{(M+1)} \;=\; \epsilon_m^{(M+1)}\, U_{rm}^{(M+1)}\,, \quad r = 1, 2, \ldots S\,,\; m = 1, 2, \ldots S \tag{9.162}$$

is solved adopting an ordering of the labels m which obeys the condition

$$\epsilon_m^{(M+1)} < \epsilon_n^{(M+1)} \quad \text{for } m \,<\, n\,. \tag{9.163}$$

The result yields the reference state $|\Phi_o(\mathbf{U}^{(M+1)})\rangle$ using the definition (9.145), i.e. $\mathbf{U}^{(M+1)}$ is the $S \times N$–matrix of the first N column vectors of $U_{rm}^{(M+1)}$, $r = 1, 2, \ldots S$, $m = 1, 2, \ldots S$.

SCF-Algorithm: Continuation and Convergence Condition

When step $2M+1$ is completed, step $2M+2$ is carried out, etc. The procedure is continued until it is detected that the one-particle density differences $|\sum_{m=1}^{N} U_{rm}^{*(M+1)} U_{um}^{(M+1)} \;-\; \sum_{m=1}^{N} U_{rm}^{*(M)} U_{um}^{(M)}|$ for $r, s \,=\, 1, 2 \ldots S$ do not exceed a preset threshold, indicating that the state converged.

Exercise 9.6.1: Let $\hat{P}_{rs}$ be the one-particle operator with the generic operator $\hat{p}_{rs} \,=\, |r\rangle\langle s|$, i.e.,

$$\langle t, \sigma|\hat{p}_{rs}|u, \sigma'\rangle \;=\; \delta_{tr}\delta_{su}\delta_{\sigma\sigma'}\,. \tag{9.164}$$

(a) Determine the expectation value of $\hat{P}_{rs}$ for the state as defined in (9.145).
(b) How can the expectation values of the operator $\hat{P}_{rr}$ be interpreted.
(c) Show that any spin-independent one-particle operator

$$\hat{F} \;=\; \sum_{\substack{r,s=1 \\ \sigma}}^{S} \langle r|\hat{f}|s\rangle\, c_{r\sigma}^{\dagger} c_{s\sigma} \tag{9.165}$$

can be written

$$\hat{F} \;=\; \sum_{r,s=1}^{S} \langle r|\hat{f}|s\rangle\, \hat{P}_{rs} \tag{9.166}$$

(d) Define a similar two-particle operator $\hat{P}_{rstu}$.
(e) Consider the creation operators

$$g_{q\sigma}^{\dagger} \;=\; \sum_{m=1}^{N} V_{mq}\, d_{m\sigma}^{\dagger} \tag{9.167}$$

which are connected with $d^\dagger_{m\sigma}$ through a unitary $N \times N$–matrix (V_{qm}). Note that this is **not** an $S \times S$–matrix! Show that the reference state defined through

$$\prod_{q=1}^{N} g^\dagger_{q\alpha} g^\dagger_{q\beta} |0\rangle \tag{9.168}$$

has the same expectation values for $\hat{P}_{rs}$ and $\hat{P}_{rstu}$ as the reference state (9.145).
(f) Can one distinguish the states (9.145) and (9.168) through a physical observation?
Exercise 9.6.2: Determine the SCF ground state and its energy expectation value for a system of two particles described through the Hamiltonian ($S = 2$)

$$\begin{aligned} H \;&=\; \sum_\sigma \Big(\epsilon \,(\, c^\dagger_{1\sigma} c_{1\sigma} \,+\, c^\dagger_{2\sigma} c_{2\sigma} \,) \;-\; t \,(\, c^\dagger_{1\sigma} c_{2\sigma} \,+\, c^\dagger_{2\sigma} c_{1\sigma}) \Big) \\ &+ 2v \,(\, c^\dagger_{1\alpha} c_{1\alpha} c^\dagger_{1\beta} c_{1\beta} \,+\, c^\dagger_{2\alpha} c_{2\alpha} c^\dagger_{2\beta} c_{2\beta} \,) \,+ v \sum_{\sigma,\sigma'} (\, c^\dagger_{1\sigma} c_{1\sigma} c^\dagger_{2\sigma'} c_{2\sigma'} \\ &+ c^\dagger_{2\sigma} c_{2\sigma} c^\dagger_{1\sigma'} c_{1\sigma'} \,) \,. \end{aligned} \tag{9.169}$$

9.7 Properties of the SCF Ground State

We want to investigate now the properties of the SCF ground state. We begin by summarizing the result of the SCF algorithm.
We denote the representation which results from the SCF algorithm after its convergence as follows:

$$|\tilde{m}\rangle \;=\; \sum_{r=1}^{S} U^{(SCF)}_{rm} \,|r\rangle \,. \tag{9.170}$$

Here $|r\rangle$, $r = 1, 2, \ldots S$ denotes the initial single-particle states and $\left(U^{(SCF)}_{rm}\right)$ is the unitary $S \times S$–transformation matrix obtained in (9.162,9.163). For this representation holds

$$\langle \tilde{m}| \,\hat{t}\, |\tilde{n}\rangle \;+\; \sum_{m'}^{N} \big(\,2\langle \tilde{m}\tilde{m}'| \,\hat{v}\, |\tilde{n}\tilde{m}'\rangle \;-\; \langle \tilde{m}\tilde{m}'| \,\hat{v}\, |\tilde{m}'\tilde{n}\rangle \,\big) \;=\; \epsilon^{(SCF)}_m \,\delta_{mn} \tag{9.171}$$

where the convention (9.163), i.e.,

$$\epsilon^{(SCF)}_m \,< \epsilon^{(SCF)}_n \quad \text{for } m \,<\, n \tag{9.172}$$

is obeyed. Equation (9.171) implies that for the mean field Hamiltonian holds

$$\hat{H}_{mf}(\mathbf{U}^{(SCF)}) \;=\; \sum_{\substack{m=1 \\ \sigma}}^{S} \epsilon^{(SCF)}_m \, d^\dagger_{m\sigma} d_{m\sigma} \,, \tag{9.173}$$

i.e., the mean-field Hamiltonian is diagonal in the SCF representation. Finally, the SCF ground state is

$$\|SCF\rangle \;=\; \prod_{m=1}^{N} d^{\dagger}_{m\alpha} d^{\dagger}_{m\beta} |0\rangle \; . \tag{9.174}$$

The first property we consider is the total spin character of $\|SCF\rangle$. Since this state is composed only of closed shells one can conclude following Section 9.4 that $\|SCF\rangle$ is a total singlet state.
We like to determine next the energy expectation value of $\|SCF\rangle$. Within the mean field approximation as described by (9.173) holds

$$\langle SCF\|\hat{H}_{mf}(\mathbf{U}^{(SCF)})\|SCF\rangle \;=\; 2\sum_{r=1}^{N} \epsilon_m^{(SCF)} \; . \tag{9.175}$$

However, one can also determine the expectation value of $\|SCF\rangle$ for the Hamiltonian (9.142), i.e., $\langle SCF\|\hat{H}\|SCF\rangle$. Employing expressions (9.84) and (9.93) for the expectation values (diagonal elements) of the one-particle and two-particle part of the Hamiltonian (9.142), exploiting the spin-independence of (9.142), one obtains

$$\begin{aligned} &\langle SCF\|\hat{H}\|SCF\rangle \;= \\ &2\sum_{m=1}^{N} \langle \tilde{m}|\hat{t}|\tilde{m}\rangle \;+\; \sum_{m,m'=1}^{N} \left(2\langle \tilde{m}\tilde{m}'|\,\hat{v}\,|\tilde{m}\tilde{m}'\rangle \;-\; \langle \tilde{m}\tilde{m}'|\,\hat{v}\,|\tilde{m}'\tilde{m}\rangle \right) \; . \end{aligned} \tag{9.176}$$

Comparision with (9.171) yields

$$\begin{aligned} &\langle SCF\|\hat{H}\|SCF\rangle \;= \\ &2\sum_{m=1}^{N} \epsilon_m^{(SCF)} \;-\; \sum_{m,m'=1}^{N} \left(2\langle \tilde{m}\tilde{m}'|\,\hat{v}\,|\tilde{m}\tilde{m}'\rangle \;-\; \langle \tilde{m}\tilde{m}'|\,\hat{v}\,|\tilde{m}'\tilde{m}\rangle \right) \; . \end{aligned} \tag{9.177}$$

The second term originates from the fact that in the mean field approximation one assumes that each of the fermions is subject to an average pair interaction involving a $2N$-particle reference state. Since the system under consideration has only $2N$ particles altogether, the mean field potential $\hat{V}_{mf}\left(|\Phi_o(\mathbf{U})\rangle\right)$ defined in (9.146) counts a particle twice, once as a member of the ground state, and once as a probe particle being subject to the mean pair interaction. This over-counting leads to the correction term in (9.177).

Exercise 9.7.1: Reformulate (9.171) in terms of matrix elements $\langle r|\hat{t}|s\rangle$, $\langle r,s|\hat{v}|t,u\rangle$ and $U_{rm}^{(SCF)}$. Show that the resulting eigenvalue problem of the type (9.162) is non-linear in $U_{rm}^{(SCF)}$.
Exercise 9.7.2: Derive (9.177).

9.8 Mean Field Theory for Macroscopic Systems

The SCF algorithm has been developed in Sections 9.4–9.7 for finite systems. In the present Section we want to adapt the algorithm to systems containing a macroscopically large number of fermions. We consider as an example the Hubbard model of an infinite linear lattice and apply the model to describe magnetic instabilities in metals.

The Hubbard Model

The Hubbard model serves today the important role as the simplest manifestation of strongly correlated electron systems which arise in many instances in molecular and solid state physics, for example, in the two-dimensional copper oxide lattices of high temperature superconductors. The one-dimensional Hubbard model is described by the Hamiltonian

$$\hat{H} = -t \sum_{r\sigma} \left(c^\dagger_{r+1,\sigma} c_{r\sigma} + c^\dagger_{r\sigma} c_{r+1,\sigma} \right) + \frac{v}{2} \sum_{\substack{r \\ \sigma\sigma'}} c^\dagger_{r\sigma} c^\dagger_{r\sigma'} c_{r\sigma'} c_{r\sigma} \ . \tag{9.178}$$

Here the index r, $r \in \mathbb{Z}$, describes the sites of a linear lattice. We assume that there are altogether $S = 2N_0$ lattice sites, labeled $r = -N_0+1, \ldots, N_0$ which are populated by $2N$ electrons (we choose an even number of electrons for convenience). Both N_0 and N are macroscopically large numbers. The operator $c^\dagger_{r\sigma}$ ($c_{r\sigma}$) creates (destroys) an electron with spin σ ($\sigma = \alpha, \beta$ for 'up' and 'down' spins, respectively) in state $|r\rangle$ at lattice site r. t describes the coupling of state $|r\rangle$ to states $|r \pm 1\rangle$ at the two neighboring lattice sites; t is assumed to be a positive, real number. According to (9.178) v contributes only in case that two electrons occupy the same lattice site, i.e., v represents the 'on-site' Coulomb repulsion.
The first term on the r.h.s. of (9.178), is identical to that of the independent–particle Hamiltonian H_0 (9.128), i.e.,

$$\hat{H}_o = -t \sum_{r\sigma} \left(c^\dagger_{r+1,\sigma} c_{r\sigma} + c^\dagger_{r\sigma} c_{r+1,\sigma} \right) \ . \tag{9.179}$$

The *potential energy* term, i.e., the second term on ther.h.s. of (9.178), in the usual two–particle operator form, reads

$$\hat{V} \ = \ \frac{1}{2} \sum_{\substack{r,s,t,u \\ \sigma\sigma'}} \langle r, s|\hat{v}|t, u\rangle \, c^\dagger_{r\sigma} c^\dagger_{s\sigma'} c_{u\sigma'} c_{t\sigma} \ . \tag{9.180}$$

where

$$\langle r, s|\hat{v}|u, t\rangle = v \ \delta_{ru} \delta_{st} \delta_{rs} \ . \tag{9.181}$$

The Hubbard model, as stated through Hamiltonian (9.178), is characterized through the parameters t, v of the Hubbard Hamiltonian (9.178) and through the so-called *filling factor* n

$$n = \frac{2N}{S} = \frac{N}{N_0} \ . \tag{9.182}$$

n can assume values $0 \leq n \leq 2$. The case $n = 1$ is termed the *half filled band* case, referring to the fact that in this case the *band* of single particle energies (9.192) derived below is filled half.
In spite of the simplicity of its Hamiltonian the Hubbard model, except in case of one-dimensional systems, cannot be solved exactly. Due to the lack of an exact solution in dimensions higher than one, approximation schemes like the self-consistent field approximation play an important role.

Since we are dealing presently with a macroscopic system, boundary effects are assumed to be negligible, a freedom which we employ to adopt so-called *periodic boundary conditions* like those for the example "$2N$ independent electrons on a ring" on page 264. Accordingly, we identify $|r + N_0\rangle = |r\rangle$ and later let N_0 go to infinity.

SCF Ground State for the Hubbard Model

We seek to determine the ground state of the Hubbard model stated by (9.178) within the framework of the self-consistent field theory. For this purpose we apply the SCF theory presented in Section 9.6. Accordingly, we assume that the SCF ground state is given by (9.174), i.e., by

$$||SCF\rangle = \prod_{m=0}^{N-1} d^\dagger_{m\alpha} d^\dagger_{m\beta} |0\rangle \ , \tag{9.183}$$

where the operators $d^\dagger_{m\sigma}$ are related to the original creation operators $c^\dagger_{r\sigma}$ through the unitary transformation $\mathbf{U}$ defined in (9.144). The self-consistent field Hamiltonian $\hat{H}_{mf}$ which corresponds to the Hubbard Hamiltonian (9.178) can be determined by applying (9.155, 9.154). Using (9.181, 9.179), one obtains for the mean field Hamiltonian

$$\hat{H}_{mf}(\mathbf{U}) = \hat{H}_0 + v \sum_{r,\sigma} \left(\sum_{m=0}^{N-1} U^*_{rm} U_{rm} \right) c^\dagger_{r\sigma} c_{r\sigma} \ . \tag{9.184}$$

We are now ready to apply *step 1* of the SCF algorithm and diagonalize term $\hat{H}_0$. This task has been solved already on page 264. The unitary transformation which diagonalizes $\hat{H}_0$, in fact, is

$$U_{rm} = \frac{1}{\sqrt{2N_0}} \exp\left(irm\pi/N_0\right) \ . \tag{9.185}$$

According to (9.140), the operator $\hat{H}_0$ can be re-written in the diagonal form

$$\hat{H}_0 = \sum_{\substack{m=-N_0+1 \\ \sigma}}^{N_0} \epsilon_m \, d^\dagger_{m\sigma} d_{m\sigma} \tag{9.186}$$

where

$$\epsilon_m = -2t \cos \frac{m\pi}{N_0} \ . \tag{9.187}$$

The energy levels are labeled such that $\epsilon_0 < \epsilon_{\pm 1} < \ldots < \epsilon_{\pm(N_0-1)} < \epsilon_{N_0}$ holds as can be readily verified.

We can now embark on *step 2* of the SCF algorithm. Inserting (9.185) into (9.184) and using (9.186) one obtains for the mean field Hamiltonian

$$\hat{H}^{(2)}_{mf} = \sum_{\substack{m=-N_0+1 \\ \sigma}}^{N_0} \epsilon_m \, d^\dagger_{m\sigma} d_{m\sigma} + v \frac{N}{2N_0} \sum_{r\sigma} c^\dagger_{r\sigma} c_{r\sigma} \ . \tag{9.188}$$

Expressing $c^\dagger_{r\sigma}$, $c_{r\sigma}$ through $d^\dagger_{m\sigma}$, $d_{n\sigma}$ according to (9.109) and using (9.185) one can prove

$$\sum_{r\sigma} c^\dagger_{r\sigma} c_{r\sigma} = \sum_{\substack{m=-N_0+1 \\ \sigma}}^{N_0} d^\dagger_{m\sigma} d_{m\sigma} \; . \tag{9.189}$$

and, hence,

$$\hat{H}_{mf} = \hat{H}^{(2)}_{mf} = \sum_{\substack{m=-N_0+1 \\ \sigma}}^{N_0} \left(\epsilon_m + \frac{vn}{2}\right) d^\dagger_{m\sigma} d_{m\sigma} \tag{9.190}$$

We have used in the latter expression the definition (9.182) of the filling factor n [c.f. (9.182)]. The Hamiltonian $\hat{H}_{mf}$, as given in (9.190), is already diagonal, i.e., the self–consistency condition is exactly met and the SCF algorithm converged after two steps. In other words, the ground state of the Hubbard model in the self-consistent field approximation can be determined exactly. The energy E_{mf} of this state can be calculated readily by using (9.177) and

$$\langle \tilde{m}\tilde{m}'|\hat{v}|\tilde{m}\tilde{m}'\rangle = \langle \tilde{m}\tilde{m}'|\hat{v}|\tilde{m}'\tilde{m}\rangle = \frac{v}{2N_0}$$

which holds in the present case. E_{mf} is then

$$E_{mf} = 2\sum_{m=0}^{N-1}\left(\epsilon_m + \frac{vn}{2}\right) - N\frac{vn}{2} \;=\; 2\sum_{m=0}^{N-1}\left(\epsilon_m + \frac{vn}{4}\right) \tag{9.191}$$

where ϵ_m is given in (9.187). Apparently, the electrons in the present description behave like independent particles with energies $\bar{\epsilon}_m = \epsilon_m + \frac{vn}{4}$.
So far we have not exploited the fact that N_0 and N are macroscopically large quantities. When N_0 becomes macroscopically large the single particle discrete energy levels (9.187) form a quasi-continuous energy band. Indeed, for $k_m = m\pi/N_0$ holds $k_m \in \left\{-\pi + \frac{1}{N_0}, -\pi + \frac{2}{N_0} \ldots, \pi\right\}$ and, in the limit $N_0 \to \infty$, holds $k \equiv k_m \in]-\pi, \pi]$. The energy ϵ_m can be expressed as a function of a continuous variable $k \in]-\pi, \pi]$, namely, through the so-called *dispersion law*

$$\epsilon(k) = -2t\cos k \; , \qquad -\pi \le k \le \pi \; . \tag{9.192}$$

This dispersion law is presented in Fig. 9.1. One can see that $-2t \le \epsilon(k) \le 2t$ holds. The bottom of the energy band corresponds to $\epsilon(0) = -2t$ and the width of the energy band is $4t$. The ground state of the system, i.e., the state with the lowest possible energy, can be obtained, according to the Pauli principle, by filling up this energy band with electrons from the bottom of the band (which corresponds to $k = 0$) to a maximum energy, called the *Fermi energy*, denoted by ϵ_F (see Fig. 9.1).

Alternative Description of the Mean Field Approximation

The state (9.183) is not the only candidate for the mean field ground state of the Hubbard model. To demonstrate this we consider an alternative formulation of the mean field approximation for Hamiltonian (9.178). Indeed, there exist several ways of formulating mean field approximations, even for one and the same Hamiltonian. Usually, the results of different formulations agree qualitatively, but may differ quantitatively.

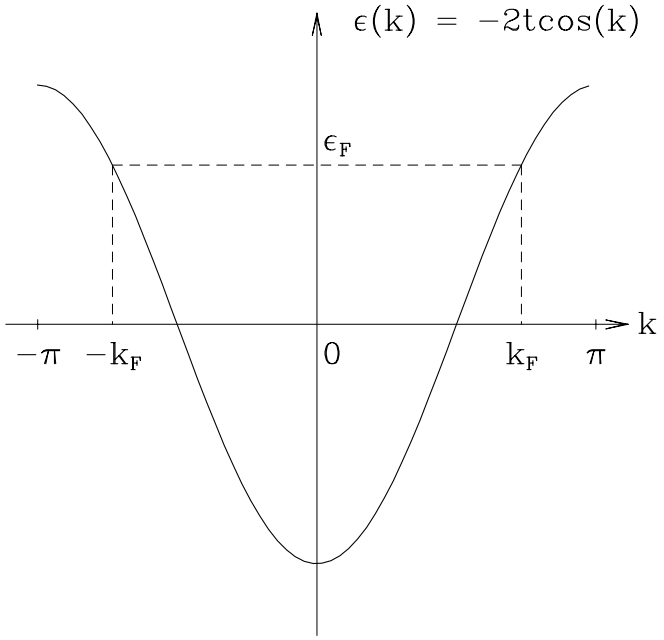

Figure 9.1: The dispersion law $\epsilon(k)$ for independent electrons on an infinite one dimensional lattice. $\epsilon_F = \epsilon(\pm k_F)$ denotes the Fermi energy.

First, let us express the interaction term in (9.178) in terms of the occupation number operators $\hat{N}_{r\sigma} = c^\dagger_{r\sigma} c_{r\sigma}$. The anti-commutation properties (9.45, 9.46) of the fermionic creation and annihilation operators yield

$$c^\dagger_{r\sigma} c^\dagger_{r\sigma'} c_{r\sigma'} c_{r\sigma} = -c^\dagger_{r\sigma} c^\dagger_{r\sigma'} c_{r\sigma} c_{r\sigma'} =$$

$$c^\dagger_{r\sigma} c_{r\sigma} c^\dagger_{r\sigma'} c_{r\sigma'} - c^\dagger_{r\sigma} c_{r\sigma} \delta_{\sigma\sigma'} = \hat{N}_{r\sigma} \hat{N}_{r\sigma'} - \hat{N}^2_{r\sigma} \delta_{\sigma\sigma'} \ , \tag{9.193}$$

where, in the last term on the right hand side, we have employed (9.56). Inserting (9.193) into (9.178) and performing the summation over the spin indices results in

$$\hat{H} = \hat{H}_0 + v \sum_r \hat{N}_{r\alpha} \hat{N}_{r\beta} \ . \tag{9.194}$$

For a given reference state, say the one given in (9.183), the operator $\hat{N}_{r\sigma}$ can be written

$$\hat{N}_{r\sigma} = \langle N_{r\sigma} \rangle + \delta \left(N_{r\sigma} \right) \ , \tag{9.195}$$

where $\langle N_{r\sigma} \rangle$ is the mean occupation number of the one particle state $|r\sigma\rangle$, i.e.,

$$\langle N_{r\sigma} \rangle \ = \ \langle SCF || N_{r\sigma} || SCF \rangle \ , \tag{9.196}$$

and where $\delta \left(N_{r\sigma} \right) = \hat{N}_{r\sigma} - \langle N_{r\sigma} \rangle$ describes the *fluctuations* of $\hat{N}_{r\sigma}$, i.e., the deviation of $\hat{N}_{r\sigma}$ from its mean value $\langle N_{r\sigma} \rangle$ for the corresponding reference state. The mean field approximation neglects the

fluctuations to second order and the mean field Hamiltonian is obtained from (9.194) by dropping all the terms which contain the fluctuations to second order. In this approximation one can express

$$\begin{aligned}\hat{N}_{r\alpha}\hat{N}_{r\beta} &= \left(\langle N_{r\alpha}\rangle + \delta\left(N_{r\alpha}\right)\right)\left(\langle N_{r\beta}\rangle + \delta\left(N_{r\beta}\right)\right) \\ &\approx \langle N_{r\alpha}\rangle\langle N_{r\beta}\rangle + \langle N_{r\alpha}\rangle\delta\left(N_{r\beta}\right) + \langle N_{r\beta}\rangle\delta\left(N_{r\alpha}\right) \\ &= \langle N_{r\alpha}\rangle\hat{N}_{r\beta} + \langle N_{r\beta}\rangle\hat{N}_{r\alpha} - \langle N_{r\alpha}\rangle\langle N_{r\beta}\rangle \end{aligned} \tag{9.197}$$

and the corresponding mean field Hamiltonian becomes

$$\hat{H}_{mf} = \hat{H}_0 + v\sum_r\left(\langle N_{r\alpha}\rangle\hat{N}_{r\beta} + \langle N_{r\beta}\rangle\hat{N}_{r\alpha}\right) - v\sum_r\langle N_{r\alpha}\rangle\langle N_{r\beta}\rangle\ . \tag{9.198}$$

Let us assume that the ground state of the Hubbard model, in the mean field approximation, is given by (9.183). Because of

$$\begin{aligned}\langle N_{r\sigma}\rangle &= \langle c^\dagger_{r\sigma}c_{r\sigma}\rangle \;=\; \sum_{m,m'}U_{rm}U^*_{rm'}\langle d^\dagger_{m\sigma}d_{m'\sigma}\rangle \\ &= \sum_{m=0}^{N-1}U_{rm}U^*_{rm} \;=\; \frac{N}{2N_0} \;=\; \frac{n}{2}\,,\end{aligned}$$

holds

$$\begin{aligned}\hat{H}_{mf} &= \hat{H}_0 + \frac{mv}{2}\sum_{r\sigma}c^\dagger_{r\sigma}c_{r\sigma} - 2N_0\frac{vn^2}{2} \\ &= \sum_{m\sigma}\left(\epsilon_m + \frac{nv}{2}\right)d^\dagger_{m\sigma}d_{m\sigma} - N\frac{vn}{2}\ ,\end{aligned} \tag{9.199}$$

which is identical to expression (9.191) for the ground state energy. Note that the procedure employed in (9.195), i.e., separating the occupation number operator into a mean value plus fluctuation and neglecting the fluctuations in 2nd order, yields essentially the same mean field Hamiltonian (9.198) as the one obtained by using the mean field potential (9.146).

Spin-Polarized Mean Field Ground State

We want to consider now a ground state for $\hat{H}_{mf}$ defined through

$$\langle N_{r\sigma}\rangle = n_\sigma = \text{const} \tag{9.200}$$

allowing, however, that n_α and n_β assume different values. For such state the mean occupation number $n_{r\sigma}$ is uniform at all lattice sites, but the mean number of particles with spin α can be different from the mean number of particles with spin β. Therefore, the ground state of the system can have a non-zero local spin and, consequently, non-vanishing magnetization. In case $n_\alpha = n_\beta$ the following construction will lead to a ground state which coincides with the non-magnetic ground state (9.183) .
To determine a magnetic ground state we note

$$\sum_r\hat{N}_{r\sigma} = \sum_{mm'}\left(\sum_r U_{rm}U^*_{rm'}\right)d^\dagger_{m\sigma}d_{m'\sigma} = \sum_{mm'}\delta_{mm'}\hat{N}_{m\sigma} = \sum_m\hat{N}_{m\sigma}\ ,$$

from which we obtain

$$n_\sigma = \frac{1}{2N_0}\sum_m \langle N_{m\sigma}\rangle \ . \tag{9.201}$$

The mean field Hamiltonian is then

$$\hat{H}_{mf} = \sum_m \left[(\epsilon_m + vn_\beta)\,\hat{N}_{m\alpha} + (\epsilon_m + vn_\alpha)\,\hat{N}_{m\beta}\right] - 2N_0 v n_\alpha n_\beta \ . \tag{9.202}$$

This Hamiltonian describes a system of non-interacting electrons with a spin-dependent dispersion law

$$\epsilon_{m\sigma} = \epsilon_m + vn_{-\sigma} \ . \tag{9.203}$$

The actual values of n_σ ($\sigma = \alpha, \beta$) are determined by minimizing the energy density of the ground state

$$\mathcal{E}_{mf} \equiv \frac{\langle H_{mf}\rangle}{2N_0} = \frac{1}{2N_0}\sum_{m,\sigma}\left[\epsilon_{m\sigma}\langle N_{m\sigma}\rangle\right] - vn_\alpha n_\beta \tag{9.204}$$

with respect to n_α and n_β, subject to the constraint

$$n = n_\alpha + n_\beta \ . \tag{9.205}$$

Such minimization is realized through the method of *Lagrangian multipliers*. According to this method one minimizes

$$\tilde{\mathcal{E}}_{mf} = \mathcal{E}_{mf} + \mu\,(n - n_\alpha - n_\beta) \ , \tag{9.206}$$

where μ is the Lagrangian multiplier considered an independent variable, i.e., $\tilde{\mathcal{E}}_{mf}$ is minimized with respect to n_α, n_β and μ. The additional term in (9.206) ascertains that condition (9.205) is met.

At this point we exploit the fact that our system is macroscopically large, i.e., $N_0 \sim 10^{23}$. In this limit the discrete energy spectrum (9.203) is provided by the continuous function

$$\epsilon_\sigma(k) = \epsilon(k) + vn_{-\sigma} \ , \tag{9.207}$$

where $\epsilon(k)$ is given by (9.192). This last equation tells us that the electrons with spin α (β) are accommodated by an energy sub–band $\epsilon_\alpha(k)$ ($\epsilon_\beta(k)$) which is obtained from the dispersion law of the non-interactive electrons $\epsilon(k)$ by an overall shift of vn_β (vn_α). The ground state (corresponding to the lowest possible energy) of the many electron system is obtained by filling these two energy sub–bands with electrons up to the same maximum energy value, the so-called Fermi energy $\epsilon_F = \mu$ (see below), as is shown schematically in Figure 9.2a. Since $\epsilon_\beta(k) - \epsilon_\alpha(k) = v(n_\alpha - n_\beta)$, one can see that an uneven occupation by electrons of the two energy bands yields a relative shift of the energy bands with respect to each other, e.g., if $n_\alpha > n_\beta$ then $\epsilon_\beta(k) > \epsilon_\alpha(k)$, such that the larger n_σ, the smaller is $\epsilon_\sigma(k)$ for a given k. Therefore, one can expect the system to lower its energy by assuming $n_\alpha \neq n_\beta$ and, hence, a spin–polarized ground state.

The values of n_α and n_β are determined by minimizing the energy density (9.206). For this purpose the sum in (9.206) needs to be evaluated. In the limit $N_0 \to \infty$ this sum can be expressed as an integral. In fact, for any function $f\left(\frac{m\pi}{N_0}\right)$ holds (compare with the definition of a definite integral as the limit of the corresponding Riemann sum)

$$\lim_{N_0\to\infty}\frac{1}{2N_0}\sum_{m=-N_0+1}^{N_0} f\left(\frac{m\pi}{N_0}\right) = \int_{-\pi}^{\pi}\frac{dk}{2\pi}f(k) \ . \tag{9.208}$$

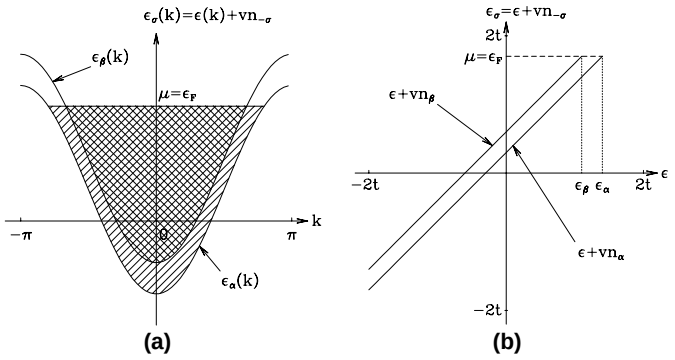

Figure 9.2: (a) Relative position of the two energy sub–bands $\epsilon_\alpha(k)$ and $\epsilon_\beta(k)$ for $\Delta = n_\alpha - n_\beta > 0$. The shaded areas represent the filled portions of these bands by electrons. (b) Graphical definition of the limiting energies ϵ_α and ϵ_β.

If the function f depends explicitly only on $\epsilon(k)$ one can state

$$\int_{-\pi}^{\pi} \frac{dk}{2\pi} f\left(\epsilon(k)\right) = \int_{-\infty}^{\infty} \rho(\epsilon) d\epsilon f(\epsilon) \tag{9.209}$$

where

$$\rho(\epsilon) = \int_{-\pi}^{\pi} \frac{dk}{2\pi} \delta\left(\epsilon - \epsilon(k)\right) \ . \tag{9.210}$$

Here $\delta(x)$ is the *Dirac–delta* function and $\rho(\epsilon)$, which is usually called the *density of states*, gives the the number of available one particle states per site, unit energy and a given spin orientation of the particle.
For a given dispersion law $\epsilon(k)$ the density of states $\rho(\epsilon)$ can be calculated by employing equation (9.210). In our case $\epsilon(k)$ is given by (9.192) and, therefore, holds

$$\rho(\epsilon) = \int_{-\pi}^{\pi} \frac{dk}{2\pi} \delta(\epsilon + 2t\cos k) \ . \tag{9.211}$$

In order to calculate the integral we recall the following property of the Dirac–delta function

$$\delta\left[f(x)\right] = \sum_i \frac{\delta(x - x_i)}{|f'(x_i)|} \ , \tag{9.212}$$

where x_i are the simple roots of the function $f(x)$. Since the equation $f(k) \equiv 2t\cos k + \epsilon = 0$ has two simple roots, namely $k_{1,2} = \pm(\pi - \arccos(\epsilon/2t))$, and noting

$$|f'(k)| = |2t\sin k| = 2t\sqrt{1-\cos^2 k} = \sqrt{(2t)^2 - \epsilon^2} \ ,$$

one obtains

$$\delta(\epsilon - \epsilon(k)) = \frac{\delta(k + \pi - \arccos(\epsilon/2t)) + \delta(k - \pi + \arccos(\epsilon/2t))}{\sqrt{(2t)^2 - \epsilon^2}} \ .$$

Inserting this last result into (9.211) and using

$$\int_{-\pi}^{\pi} dk \delta(k \pm (\pi - \arccos(\epsilon/2t))) = \theta(2t - |\epsilon|) \ ,$$

where $\theta(x)$ is the *step function*, i.e., $\theta(x) = 1$ if $x > 0$ and $\theta(x) = 0$ if $x < 0$, one arrives at the following expression of the density of states

$$\rho(\epsilon) = \frac{\theta(2t - |\epsilon|)}{\pi\sqrt{(2t)^2 - \epsilon^2}} \; . \tag{9.213}$$

The presence of the θ function in the above formula guaranties that the density of states vanishes for $|\epsilon| > 2t$, i.e., outside the energy band $\epsilon(k)$; if we assume that ϵ is restricted to the interval $]-2t, 2t[$ then the θ function in (9.213) can simply be replaced by 1.
We can employ the results obtained to express the ground state energy density (9.204) through an integral expression. One obtains

$$\tilde{\mathcal{E}}_{mf} = \int_{-2t}^{\epsilon_\alpha} \epsilon\rho(\epsilon)d\epsilon + \int_{-2t}^{\epsilon_\beta} \epsilon\rho(\epsilon)d\epsilon + vn_\alpha n_\beta + \mu(n - n_\alpha - n_\beta) \; , \tag{9.214}$$

where ϵ_σ denotes the value of $\epsilon(k)$ which corresponds to the top of the filled portion of the energy sub–band $\epsilon_\sigma(k)$ [c.f. Fig. 9.2], i.e.,

$$\epsilon_F = \epsilon_\alpha + vn_\beta = \epsilon_\beta + vn_\alpha \; . \tag{9.215}$$

n_α and n_β in (9.214) are given by the sum (9.201). Replacing again the sum by an integral over energy one can write

$$n_\sigma \; = \; \int_{-2t}^{\epsilon_\sigma} \rho(\epsilon)d\epsilon \tag{9.216}$$

Using (9.213) and carrying out the resulting integral yields

$$n_\sigma = \frac{1}{\pi} \arcsin(\epsilon_\sigma/2t) \; . \tag{9.217}$$

Since $\tilde{\mathcal{E}}_{mf}$ [c.f. (9.206)] depends only on continuous quantities, namely, on $\epsilon_\alpha, \epsilon_\beta$ and μ, the necessary conditions for a ground state of minimum energy are

$$\frac{\partial\tilde{\mathcal{E}}_{mf}}{\partial\epsilon_\alpha} = 0 \; , \qquad \frac{\partial\tilde{\mathcal{E}}_{mf}}{\partial\epsilon_\beta} = 0 \; , \qquad \frac{\partial\tilde{\mathcal{E}}_{mf}}{\partial\mu} = 0 \; . \tag{9.218}$$

The derivatives can be readily determined and the conditions (9.218) read

$$\frac{\partial\tilde{\mathcal{E}}_{mf}}{\partial\epsilon_\alpha} = \epsilon_\alpha + vn_\beta - \mu = 0 \; , \tag{9.219}$$

$$\frac{\partial\tilde{\mathcal{E}}_{mf}}{\partial\epsilon_\beta} = \epsilon_\beta + vn_\alpha - \mu = 0 \; , \tag{9.220}$$

and

$$\frac{\partial\tilde{\mathcal{E}}_{mf}}{\partial\mu} = n - n_\alpha - n_\beta = 0 \; . \tag{9.221}$$

Equations (9.219–9.221) and (9.216) allow one, in principle, to determine the unknown quantities ϵ_α, ϵ_β, μ, n_α and n_β as a function of the parameters of the Hubbard model, namely, of t, v and n. From (9.219, 9.220) μ can be readily obtained

$$\mu = \frac{1}{2}\,(\epsilon_\alpha + \epsilon_\beta) + \frac{vn}{2} \; , \tag{9.222}$$

Comparision of (9.222) and (9.215) reveals that μ is indeed equal to the Fermi energy ϵ_F (see also Figure 9.2b).
One still needs to determine ϵ_α and ϵ_β. For this purpose we consider the *magnetization* of the mean field ground state

$$\Delta \equiv n_\alpha - n_\beta \; . \tag{9.223}$$

$\Delta = 0$ corresponds to the ground state (9.183) without magnetization. One can express Δ as a function of ϵ_α and ϵ_β in two different ways. First, from (9.219–9.220) and (9.223 one obtains

$$\Delta = \frac{\epsilon_\alpha - \epsilon_\beta}{v} \; , \tag{9.224}$$

and second, from (9.217) and (9.223) follows

$$\Delta = \int_{\epsilon_\beta}^{\epsilon_\alpha} \rho(\epsilon) d\epsilon = \int_0^{v\Delta} \rho\left(\epsilon_\beta + \epsilon\right) d\epsilon \; . \tag{9.225}$$

Defining the function

$$f(\Delta) = \int_0^{v\Delta} \rho\left(\epsilon_\beta + \epsilon\right) d\epsilon \; , \tag{9.226}$$

one can obtain Δ by solving (cf. (9.226)

$$\Delta = f(\Delta) \; . \tag{9.227}$$

Since $f(0) = 0$ one can infer that $\Delta = 0$ is always a solution (the so called *paramagnetic* solution) of condition (9.227).
Equation (9.227) can be solved graphically. For this purpose one plots $f(\Delta)$ versus Δ as is shown schematically in Figure 9.3. We assume in the following discussion that the implicit Δ dependence of ϵ_β in $f(\Delta)$ can be neglected.
From the definition (9.226) follows that $f(\Delta)$ is a monotonically increasing function of Δ. Indeed, the slope of $f(\Delta)$ is positive for all $\Delta \geq 0$, as reflected by the expression

$$\frac{d[f(\Delta)]}{d\Delta} = v\rho(\epsilon_\beta + \Delta) = \frac{v}{\pi\sqrt{(2t)^2 - (v\Delta + \epsilon_\beta)^2}} > 0 \; . \tag{9.228}$$

Since the total number of states per site is finite, $f(\Delta)$ converges to a maximum value as $\Delta \to \Delta_{max} = n$. Accordingly, condition (9.227) will have a second, non trivial, so called *ferromagnetic* solution, if, and only if, the slope of $f(\Delta)$ at the origin is larger than 1 [c.f. Figure 9.3]. If the slope of $f(\Delta)$ at the origin is less than 1, condition (9.227) has only the trivial solution $\Delta = 0$.
The slope of $f(\Delta)$ at the origin depends on the Hubbard model parameter v. For v above a critical value v_c, the Hubbard model has a ground state with $\Delta \neq 0$, i.e., a magnetic ground state. One can determine v_c by equating the slope of $f(\Delta)$ at the origin to 1, i.e., through the condition [c.f. (9.228)]

$$v_c \rho\left(\epsilon_\beta\right) = 1 \; , \tag{9.229}$$

This cindition is known as the *Stoner criterion* and gives the critical value of v which determines the onset of the ferromagnetic long range order. The Stoner criterion (9.229) has a wider range of validity than one can infer from the present analysis of the Hubbard model.

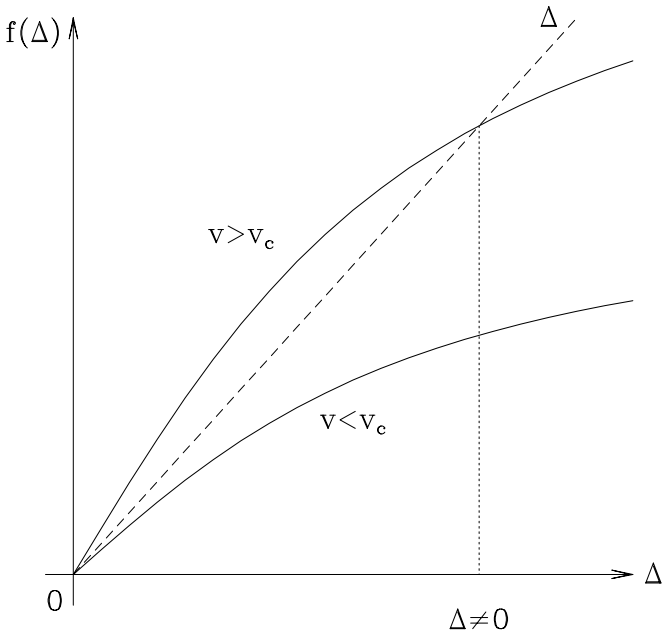

Figure 9.3: Graphical solution of the mean field equation $\Delta = f(\Delta)$.

By parameterizing ϵ_α and ϵ_β

$$\epsilon_\alpha = 2t \sin x \ , \qquad \epsilon_\beta = 2t \sin y \ , \tag{9.230}$$

one obtains from (9.219, 9.220, 9.205) the following set of equations determining x, y and, hence, ϵ_α, ϵ_β

$$x + y = \pi(n-1) \tag{9.231}$$

$$x - y = \pi \frac{2t}{v} (\sin x - \sin y) = \pi \Delta \ . \tag{9.232}$$

For a given $\frac{2t}{v}$ the values of x and y can be obtained numerically and other relevant quantities mentioned above can be calculated.
We like to determine finally the dependence of $\frac{v_c}{2t}$ on the filling factor n. The corresponding analytical expression provides the phase diagram of the ground state: when v approaches v_c from above, the magnetization Δ of the ground state vanishes and remains zero for values $v < v_c$. Equation (9.232) states that $x - y$ is proportional to Δ. Since Δ vanishes near v_c we set $x = y + \delta$ where δ is a small quantity. From (9.231) follows

$$y = \frac{\pi}{2}(n-1) - \frac{\delta}{2} \approx \frac{\pi}{2}(n-1) \ . \tag{9.233}$$

Employing the approximation $\sin(y+\delta) - \sin y \approx \delta \cos y$ for small δ, (9.232) together with (9.233) yield the desired expression

$$\frac{v_c}{2t} = \pi \cos\left[\frac{\pi}{2}(n-1)\right] \ . \tag{9.234}$$

The resulting phase diagram of the ground state, i.e., the plot of $\frac{v_c}{2t}$ vs. n, is presented in Figure 9.4. As already mentioned, the ground state is characterized by the quantities (v, t, n). Accordingly, any

mean field ground state is represented by a point in the phase diagram. The magnetic nature of the ground state of the system depends on whether the representative point lies inside the ferromagnetic or inside the paramagnetic domain of the phase diagram.

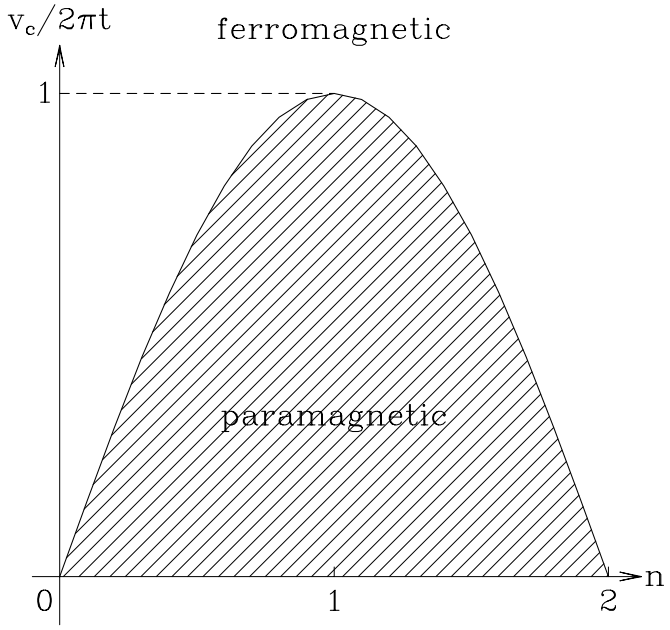

Figure 9.4: Ground state phase diagram of the mean field Hamiltonian (9.202).

Concluding Remarks

At the end of our analysis of the mean field ground state of the one-dimensional Hubbard model, it is natural to ask oneself if the results obtained reflect, at least qualitatively, the properties of the real ground state of the Hubbard model. Well, the answer is no. The real ground state of the one-dimensional Hubbard model is quite different in nature from the mean field ground state discussed here. The reason is that the effect of quantum fluctuations, which are neglected in the mean field theory, in one spatial dimension is very strong.
Nevertheless, the analysis presented above is not quite useless. First, once we specify a class of possible states to which the real ground state might belong to, the method described above gives a systematic way of singling out the state with the lowest possible energy which might be a good candidate for the real ground state of the system. Second, since in one spatial dimension there are many exact results available, the application of the mean field theory for these systems provides an excellent testing opportunity of these theories by comparing their predicted results with the exact ones. Third, the mean field theory of the one-dimensional Hubbard model can be extended in a straightforward way to higher spatial dimensions. In general, the effect of quantum fluctuations is getting less important as the dimensionality of the system is increased. For example, in three spatial dimensions the theory presented above works fine in the case of the transitional–metal oxides such as NiO and CoO. However, strong electron correlation effects , even in these materials, can lead to serious modifications of the mean field ground state.

In case of two spatial dimensions things are more complicated. On the one hand, the lack of exact solutions, and on the other hand, the strong effect of quantum fluctuations of the strongly correlated electron system described by the Hubbard Hamiltonian makes all the presently existing solutions questionable. In fact, in the case of the copper oxide high temperature superconductors, which involve strongly correlated quasi two-dimensional electron systems, a reliable microscopic theory is still lacking. The available mean field theories cannot account for all the striking, unusual physical properties of these materials.