Вторичное квантование

C.1 Creation and Annihilation Operators

The name "second quantization" is misleading. This formalism has nothing to do with the further quantizing of quantum mechanics. It is just an alternative formulation of the usual quantum mechanics, which has turned out to be very useful for handling the many-body problem. It can be used for bosons and fermions, and we will give a short introduction and some important formulae.

We start with a complete orthogonal set of single-particle states $|\nu\rangle$, where ν stands for a set of quantum numbers, for example,

(i) space coordinate $\mathbf{r}$, spin $s \equiv s_z$ $|\mathbf{r}, s\rangle$;
(ii) the quantum numbers of an oscillator basis $|nljm\rangle$.

Orthogonality and completeness are expressed as

$$\langle\nu|\nu'\rangle = \delta_{\nu\nu'}, \qquad \sum_{\nu} |\nu\rangle\langle\nu| = 1. \tag{C.1}$$

(For continuous quantum numbers such as $\mathbf{r}$, the $\delta_{\nu\nu'}$ will mean $\delta(\mathbf{r}-\mathbf{r}')$ and the sum $\sum_\nu$ is to be replaced by $\int d^3r$.)

The coordinate representation of the state $|\nu\rangle$ is given by

$$\varphi_\nu(1) = \varphi_\nu(\mathbf{r}_1, s_1) = \langle\mathbf{r}_1, s_1|\nu\rangle. \tag{C.2}$$

Starting with this set of single-particle states, we can construct a complete orthogonal set of totally *symmetric* N-body wave functions

$$\Phi_{\nu_1\ldots\nu_N}(1,\ldots,N) = \mathfrak{N}\sum_{P} P\{\varphi_{\nu_1}(1)\cdots\varphi_{\nu_N}(N)\}, \tag{C.3}$$

where the sum runs over all permutations $(\nu_1 \ldots \nu_N)$ of the numbers $(1 \ldots N)$ and $\mathfrak{N}$ is a normalization constant.

Any arbitrary, totally *symmetric* N-body wave function can be represented in this basis:

$$\Psi(1,\ldots,N) = \sum_{\nu_1 \ldots \nu_N} c_{\nu_1 \ldots \nu_N} \Phi_{\nu_1 \ldots \nu_N}(1,\ldots,N). \tag{C.4}$$

We can also give to each of the single-particle states a number $(\nu = 1, 2, \ldots)$ (in the case of continuous quantum numbers, we must first introduce a finite box) and characterize the wave function $\Phi_{\nu_1 \ldots \nu_N}$ by the "occupation numbers" $\{n_\nu\}$, which tell how often a particular number ν is contained in the N numbers $(\nu_1, \ldots, \nu_N)$. Obviously, we have

$$\sum_\nu n_\nu = N \tag{C.5}$$

and

$$\begin{aligned}\Phi_{\{n_\nu\}}(1,\ldots,N) &= \Phi_{\nu_1 \ldots \nu_N}(1,\ldots,N)\\ &= \frac{1}{\sqrt{N!}} \frac{1}{\sqrt{n_1! n_2! \ldots}} \sum_P P\{\varphi_{\nu_1}(1) \ldots \varphi_{\nu_N}(N)\}.\end{aligned} \tag{C.6}$$

Such a state describes a boson system. In complete analogy, we can construct totally antisymmetric-basis wave functions

$$\Phi_{\{n_\nu\}}(1,\ldots,N) = \frac{1}{\sqrt{N!}} \sum_P \operatorname{sign}(P) P\{\varphi_{\nu_1}(1) \ldots \varphi_{\nu_N}(N)\}. \tag{C.7}$$

They are called *Slater determinants* and describe fermion systems. In this case the numbers n_ν only take the values 0 or 1, otherwise (C.7) would vanish identically.

We can now construct a Hilbert space which contains a vacuum (no particle) $|-\rangle$, all the one-particle states, all the symmetrized (or antisymmetrized) two-particle states, and so on...

$$\mathcal{H} = \{\mathcal{H}_0, \mathcal{H}_1, \mathcal{H}_2, \dots\}. \tag{C.8}$$

The wave functions $\Phi_{\{n_\nu\}}$ correspond to basis states $|n_1, n_2, \dots\rangle$ in this Hilbert space, which are characterized by the occupation numbers (occupation number representation), such that

$$\Phi_{\{n_\nu\}}(1, \dots, N) = \langle 1, \dots, N | n_1, n_2 \dots \rangle. \tag{C.9}$$

These states are orthonormalized

$$\langle n_1', n_2', \dots n_\nu' \dots | n_1, n_2 \dots n_\nu \dots \rangle = \delta_{n_1 n_1'} \cdot \delta_{n_2 n_2'} \cdots \delta_{n_\nu n_\nu'} \cdots. \tag{C.10}$$

First we shall study boson systems and define an "*annihilation operator*" B_ν by

$$B_\nu | n_1, n_2, \dots, n_\nu, \dots \rangle = \sqrt{n_\nu}\, | n_1, n_2, \dots, n_\nu - 1, \dots \rangle. \tag{C.11}$$

The operator B_ν lowers the occupation number in the state with the number ν by one. An N-body state goes over into an $(N-1)$-body state.

The matrix elements of B_ν are

$$\langle n_1', n_2', \ldots, n_\nu', \ldots | B_\nu | n_1, n_2, \ldots, n_\nu, \ldots \rangle = \sqrt{n_\nu}\, \delta_{n_1 n_1'} \ldots \delta_{n_\nu' n_\nu - 1} \cdots \tag{C.12}$$

or

$$\langle n_1, n_2, \ldots, n_\nu, \ldots | B_\nu^+ | n_1', n_2', \ldots, n_\nu', \ldots \rangle = \sqrt{n_{\nu'} + 1}\, \delta_{n_1 n_1'} \ldots \delta_{n_\nu n_\nu' + 1} \cdots \tag{C.13}$$

This is valid for all basis states $\langle n_1, n_2 \ldots |$. We therefore find

$$B_\nu^+ | n_1, n_2, \ldots, n_\nu, \ldots \rangle = \sqrt{n_\nu + 1}\, | n_1, n_2, \ldots, n_\nu + 1, \ldots \rangle . \tag{C.14}$$

B_ν^+ "creates" a particle in the state with the number ν. Therefore, it is called a "*creation operator* in the state ν." It is the Hermitian conjugate operator to B_ν.

From this definition we gain the fact that

$$(B_\mu B_\nu^+ - B_\nu^+ B_\mu) | n_1, n_2, \ldots, n_\nu, \ldots, n_\mu \ldots \rangle$$

$$= \begin{cases} \left(\sqrt{n_\nu + 1}\, \sqrt{n_\mu} - \sqrt{n_\mu}\, \sqrt{n_\nu + 1} \right) | n_1, \ldots, n_\nu + 1, \ldots, n_\mu - 1, \ldots \rangle = 0 & \text{for } \nu \neq \mu, \\ \left(\sqrt{n_\nu + 1}\, \sqrt{n_\nu + 1} - \sqrt{n_\nu}\, \sqrt{n_\nu} \right) | n_1, \ldots, n_\nu, \ldots \rangle & \text{for } \nu = \mu, \end{cases} \tag{C.15}$$

and hence get the commutation relations.

$$[B_\mu, B_\nu^+] = B_\mu B_\nu^+ - B_\nu^+ B_\mu = \delta_{\mu\nu}. \tag{C.16}$$

In the same way, we may show that

$$[B_\mu, B_\nu] = [B_\nu^+, B_\mu^+] = 0. \tag{C.17}$$

The state with the occupation numbers $|0,0,0\ldots\rangle = |-\rangle$ is the *vacuum*. We thus have

$$B_\nu|-\rangle = 0 \qquad \text{for all } \nu \tag{C.18}$$

and

$$|n_1, n_2, \ldots, n_\nu, \ldots\rangle = \frac{1}{\sqrt{n_1! n_2! \cdots n_\nu! \cdots}} \prod_\mu (B_\mu^+)^{n_\mu}|-\rangle. \tag{C.19}$$

The relation (C.11) follows from (C.16) to (C.19), which was our definition of the operators B_ν. We can therefore also go in the opposite direction and start with a set of operators B_ν, B_ν^+ which obey boson commutation relations and construct the many-body Hilbert space from (C.17) and (C.18).

The operator $B_\nu^+ B_\nu$ is called the particle-number operator for the state ν:

$$B_\nu^+ B_\nu |n_1, \ldots, n_\nu, \ldots\rangle = n_\nu |n_1, \ldots, n_\nu, \ldots\rangle. \tag{C.20}$$

We now address ourselves to a fermion system. We shall use small Latin letters a_ν^+, a_ν for the creation and annihilation operators of fermions. Since n_ν can only have the values 0 and 1, we may define the action of the operators as

$$a_\nu|n_1,\ldots,n_\nu=1,\ldots\rangle=|n_1,\ldots,n_\nu=0,\ldots\rangle,\qquad a_\nu|n_1,\ldots,n_\nu=0,\ldots\rangle=0, \tag{C.21}$$

from which we get

$$a_\nu^+|n_1,\ldots,n_\nu=0,\ldots\rangle=|n_1,\ldots,n_\nu=1,\ldots\rangle,\qquad a_\nu^+|n_1,\ldots,n_\nu=1,\ldots\rangle=0, \tag{C.22}$$

and

$$\begin{gathered}\left[a_\mu,a_\nu^+\right]_+ := \left\{a_\mu,a_\nu^+\right\} := a_\mu a_\nu^+ + a_\nu^+ a_\mu = \delta_{\mu\nu},\\ \left[a_\mu,a_\nu\right]_+ = \left[a_\mu^+,a_\nu^+\right]_+ = 0.\end{gathered} \tag{C.23}$$

The vacuum is again given by $|-\rangle=|0,0,\ldots\rangle$ and we have

$$a_\nu|-\rangle=0 \qquad \text{for all } \nu, \tag{C.24}$$

hence

$$|n_1,\ldots,n_\nu,\ldots\rangle=\prod_\mu (a_\mu^+)^{n_\mu}|-\rangle=a_{\nu_1}^+\ldots a_{\nu_N}^+|-\rangle. \tag{C.25}$$

C.2 Field Operators in the Coordinate Space*

Using the single-particle wave functions $\varphi_\nu(\mathbf{r}, s)$ in Eq. (C.2) we can define creation and annihilation operators $a^+(\mathbf{r}, s), a(\mathbf{r}, s)$, which depend on the coordinates $\mathbf{r}$ and $s^\dagger$:

$$a(\mathbf{r}, s) = \sum_\nu \varphi_\nu(\mathbf{r}, s) a_\nu ; \qquad a^+(\mathbf{r}, s) = \sum_\nu \varphi_\nu^*(\mathbf{r}, s) a_\nu^+ . \tag{C.26}$$

With Eq. (C.1) we can invert this relation,

$$a_\nu = \sum_s \int d^3r\, \varphi_\nu^*(\mathbf{r}, s) a(\mathbf{r}, s), \qquad a_\nu^+ = \sum_s \int d^3r\, \varphi_\nu(\mathbf{r}, s) a^+(\mathbf{r}, s), \tag{C.27}$$

and gain the commutators

$$\left[a(\mathbf{r}, s), a^+(\mathbf{r}', s')\right]_+ = \sum_{\nu\nu'} \varphi_\nu(\mathbf{r}, s) \varphi_{\nu'}^*(\mathbf{r}', s') \left[a_\nu, a_{\nu'}^+\right]_+ = \delta_{ss'} \delta(\mathbf{r} - \mathbf{r}') \tag{C.28}$$

and

$$\left[a(\mathbf{r}, s), a(\mathbf{r}', s')\right]_+ = \left[a^+(\mathbf{r}, s), a^+(\mathbf{r}', s')\right]_+ = 0. \tag{C.29}$$

We can express the many-body wave function (C.7) by

$$\Phi_{\{n_\nu\}}(1, \ldots, N) = \frac{1}{\sqrt{N!}} \langle - | a(N) \ldots a(1) | n_1, n_2, \ldots n_\nu \ldots \rangle \tag{C.30}$$

and

$$|n_1, n_2, \ldots n_\nu \ldots\rangle = \int d1 \ldots dN \frac{1}{\sqrt{N!}} \Phi_{\{n_\nu\}}(1, \ldots, N) a^+(1) \ldots a^+(N) |-\rangle. \tag{C.31}$$

C.3 Representation of Operators

Starting from a vacuum $|-\rangle$, we have expressed all states in the many-body Hilbert space $\mathcal{H}$ by creation and annihilation operators a_ν^+, a_ν. The same will be done for operators in the following. We have to distinguish between one- and two-body operators.

A *one-body operator* as, for example, the kinetic energy or the total momentum of an N-particle system, is given as the sum of N operators $\hat{f}_i$ which always act on the coordinate of the particle i:

$$\hat{F} = \sum_{i=1}^{N} \hat{f}_i. \tag{C.32}$$

Its matrix elements in the $|\nu\rangle$ representation are

$$f_{\nu\nu'} = \langle\nu|\hat{f}|\nu'\rangle, \tag{C.33}$$

that is,

$$\hat{f}_i \varphi_\nu(i) = \sum_{\nu'} f_{\nu'\nu} \varphi_{\nu'}(i). \tag{C.34}$$

The representation of $\hat{F}$ in the operators a_ν^+, a_ν is given by

$$\hat{F} = \sum_{\nu\nu'} f_{\nu\nu'} a_\nu^+ a_{\nu'} . \tag{C.35}$$

To show this, we have to prove

$$\sum_i \hat{f}_i \Phi(1,\dots,N) = \langle 1,\dots,N | \sum_{\nu\nu'} f_{\nu\nu'} a_\nu^+ a_{\nu'} | \Phi \rangle . \tag{C.36}$$

On the l.h.s, from Eqs. (C.30), (C.26) and (C.34) up to a factor $1/\sqrt{N!}$ we gain

$$\begin{aligned}
&\sum_i \hat{f}_i \langle - | a(N) \dots a(i) \dots a(1) | \Phi \rangle \\
&\quad = \sum_i \sum_{\nu_1 \dots \nu_N} \hat{f}_i \varphi_{\nu_N}(N) \dots \varphi_{\nu_i}(i) \dots \varphi_{\nu_1}(1) \langle - | a_{\nu_N} \dots a_{\nu_1} | \Phi \rangle \\
&\quad = \sum_i \sum_\nu \sum_{\nu_1 \dots \nu_N} f_{\nu\nu_i} \varphi_{\nu_N}(N) \dots \varphi_\nu(i) \dots \varphi_{\nu_1}(1) \langle - | a_{\nu_N} \dots a_{\nu_1} | \Phi \rangle .
\end{aligned}$$

This is identical to the r.h.s.:

$$\begin{aligned}
&\sum_{\nu\nu'} \sum_{\nu_1 \dots \nu_N} f_{\nu\nu'} \varphi_{\nu_N}(N) \dots \varphi_{\nu_1}(1) \langle - | a_{\nu_N} \dots a_{\nu_1} a_\nu^+ a_{\nu'} | \Phi \rangle \\
&\quad = \sum_i \sum_\nu \sum_{\nu_1 \dots \nu_N} f_{\nu_i\nu} \varphi_{\nu_N}(N) \dots \varphi_{\nu_1}(1) \langle - | a_{\nu_N} \dots a_\nu \dots a_{\nu_1} | \Phi \rangle .
\end{aligned}$$

We give next a few examples:

The kinetic energy

$$\hat{T} = \sum_i \hat{t}_i = \sum_i \frac{-\hbar^2}{2m} \Delta_i, \tag{C.37}$$

$$\begin{aligned} \hat{T} &= \sum_{\nu\nu'} \sum_s \int d^3r\, \varphi^*_\nu(\mathbf{r}, s) \frac{-\hbar^2}{2m} \Delta \varphi_{\nu'}(\mathbf{r}, s) a^+_\nu a_{\nu'} \\ &= \sum_s \int d^3r\, a^+(\mathbf{r}, s) \frac{-\hbar^2}{2m} \Delta a(\mathbf{r}, s). \end{aligned} \tag{C.38}$$

The single-particle density (see Appendix D)

$$\hat{\rho}(\mathbf{r}) = \sum_{i=1}^{N} \delta(\mathbf{r} - \hat{\mathbf{r}}_i). \tag{C.39}$$

$\hat{\mathbf{r}}_i$ is the coordinate operator of the *i*th particle; $\mathbf{r}$ is a number.

$$\hat{\rho}(\mathbf{r}) = \sum_{\nu\nu'} \sum_s \int d^3r'\, \varphi^*_\nu(\mathbf{r}', s) \delta(\mathbf{r} - \mathbf{r}') \varphi_{\nu'}(\mathbf{r}', s) a^+_\nu a_{\nu'} = \sum_s a^+(\mathbf{r}, s) a(\mathbf{r}, s). \tag{C.40}$$

The particle number

$$\begin{aligned} \hat{N} &= \sum_\nu a^+_\nu a_\nu = \sum_\nu \sum_{ss'} \int d^3r\, d^3r'\, \varphi_\nu(\mathbf{r}, s) \varphi^*_\nu(\mathbf{r}', s') a^+(\mathbf{r}, s) a(\mathbf{r}', s') \\ &= \int \hat{\rho}(\mathbf{r})\, d^3r. \end{aligned} \tag{C.41}$$

In the most general case, $\hat f$ will be an integral operator (a "nonlocal" one-particle operator):

$$\hat f\,\varphi(\mathbf{r},s)=\sum_{s'}\int d^3r'\; f_{ss'}(\mathbf{r},\mathbf{r}')\,\varphi(\mathbf{r}',s'). \tag{C.42}$$

A *two-particle operator* as, for example, a two-body interaction, is given by a sum of operators v_{ij} which act on the coordinates of the particles i and j.

$$V=\sum_{i<j=1}^{N} v_{ij}. \tag{C.43}$$

In the most general case, v_{ij} will be an integral operator in two variables, with matrix elements

$$v_{\mu\nu\mu'\nu'}=\langle\mu\nu|v|\mu'\nu'\rangle=\int d1\,d2\,d3\,d4\,\varphi_\mu^*(1)\varphi_\nu^*(2)\,v(1,2,3,4)\,\varphi_{\mu'}(3)\varphi_{\nu'}(4). \tag{C.44}$$

In complete analogy to Eq. (C.35), we can show that V can be written as

$$V=\tfrac{1}{2}\sum_{\mu\nu\mu'\nu'} v_{\mu\nu\mu'\nu'}\,a_\mu^+ a_\nu^+ a_{\nu'} a_{\mu'}=\tfrac{1}{4}\sum_{\mu\nu\mu'\nu'} \bar v_{\mu\nu\mu'\nu'}\,a_\mu^+ a_\nu^+ a_{\nu'} a_{\mu'}, \tag{C.45}$$

with the antisymmetrized matrix element

$$\bar v_{\mu\nu\mu'\nu'}=\langle\mu\nu|v|\mu'\nu'\rangle-\langle\mu\nu|v|\nu'\mu'\rangle. \tag{C.46}$$

Very often we use local two-body interactions of the form (we neglect spin)

$$v_{ij} = v(\mathbf{r}_i, \mathbf{r}_j). \tag{C.47}$$

In this case, we can verify Eq. (C.45) immediately with Eq. (C.40):

$$\begin{aligned}\tfrac{1}{2}\sum_{\mu\nu\mu'\nu'} v_{\mu\nu\mu'\nu'} a_\mu^+ a_\nu^+ a_{\nu'} a_{\mu'} &= -\tfrac{1}{2}\int d^3r\, d^3r'\, a^+(\mathbf{r}) a^+(\mathbf{r}') v(\mathbf{r}, \mathbf{r}') a(\mathbf{r}) a(\mathbf{r}') \\ &= \tfrac{1}{2}\left(\int d^3r\, d^3r'\, v(\mathbf{r}, \mathbf{r}') \hat{\rho}(\mathbf{r}) \hat{\rho}(\mathbf{r}') - \int d^3r\, v(\mathbf{r}, \mathbf{r}) \hat{\rho}(\mathbf{r})\right) \\ &= \tfrac{1}{2}\left(\sum_{i \neq j} v(\mathbf{r}_i, \mathbf{r}_j) - \sum_i v(\mathbf{r}_i, \mathbf{r}_i)\right) = \sum_{i<j=1}^{N} v(\mathbf{r}_i, \mathbf{r}_j).\end{aligned} \tag{C.48}$$

C.4 Wick's Theorem

In practical applications of the second quantization, Wick's theorem has turned out to be very useful. It is a rule which allows a very simple reordering of a set of N-operators a or a^+, which have the property that the commutator (in the case of bosons) or the anticommutator (in the case of fermions) of two arbitrarily chosen operators of this set is a number.

We first define the T-product (time ordered product) of a product of operators $a(t_2), a(t_3), a^+(t_1) \ldots$ to be the one where the field operators have been reordered in such a way that the time arguments are increasing from right to left (an odd permutation gives a minus sign):

$$T\{a(t_1) a^+(t_3) a(t_2) a^+(t_4)\} = -a(t_1) a(t_2) a^+(t_3) a^+(t_4) \qquad t_1 > t_2 > t_3 > t_4. \tag{C.49}$$

In a *normal ordered* product, the field operators are ordered in such a way that all creation operators are to the left of all annihilation operators* (again, an odd permutation gives a minus sign):

$$N\{a_\nu a_\mu a_\rho a_\sigma^+\} =: a_\nu a_\mu a_\rho a_\sigma^+ := -a_\sigma^+ a_\nu a_\mu a_\rho. \tag{C.50}$$

The *contraction* $\widehat{UV}$ of two field operators U and V is defined as

$$\widehat{UV} = T\{UV\} - N\{UV\}. \tag{C.51}$$

With these definitions, *Wick's Theorem* [Wi 50] can be stated as:

$$\begin{aligned} T\{UVW\ldots XYZ\} &= N\{UVW\ldots XYZ\} + N\{\widehat{UV}W\ldots XYZ\} \\ &\quad + \cdots + N\{UVW\ldots X\widehat{YZ}\} + N\{\widehat{UV}W\ldots \widehat{XY}Z\} \\ &\quad + \cdots + N\{\widehat{UV}\widehat{W\ldots X}\widehat{YZ}\} + \cdots . \end{aligned} \tag{C.52}$$

The time ordered product of field operators is therefore equal to their normal ordered product plus the normal ordered products with one contraction (in all possible ways), plus the normal ordered product with two contractions, and so on. Care has to be taken in the removal of a contraction out of a normal ordered product, as this can give a minus sign:

$$N\{\overparen{UV}XY\} = \overparen{UV}N\{XY\}; N\{\overparen{UVX}Y\} = -\overparen{UX}N\{VY\}. \quad \text{(C.53)}$$

(For the proof of Wick's theorem see, e.g., Thouless [Th 61b].)

Wick's theorem is especially useful for the calculation of ground state expectation values of time ordered products of field operators (e.g., the expectation value of particle operators with respect to the quasi-particle vacuum in Chap. 6). The result is equal to the r.h.s. of (C.52), where all operators have been contracted in all possible ways.

If there are time-independent field operators, as in (C.45), then the given order is to be defined as time ordered. The contraction of time-independent operators is especially simple; for example, we get:

$$\overparen{a_\mu a_\nu^+} = a_\mu a_\nu^+ - N\{a_\mu a_\nu^+\} = \delta_{\mu\nu}. \quad \text{(C.54)}$$

Применение оболочечной модели к проблеме многих тел

2.5 The Shell Model Approach to the Many-Body Problem

The single-particle model takes into account the individual nucleons. It therefore provides a microscopic description of the nucleus. This is certainly only an approximation of the exact many-body problem. We will see, however, in the following, that the shell model can be used as a basis for more elaborate many-body theories, so before we talk about further details of the model, we want to discuss some general properites of the single particle model.

The microscopic theory of the nucleus is usually based on the following three properties.

(i) The nucleus is a quantum mechanical many-body system.
(ii) The velocities in the nucleus are small enough so that one can neglect relativistic effects $[(v/c)^2 \sim 1/10]$.
(iii) The interaction between the nucleons has a two-body character.

A full microscopic theory of the nucleus would then be given by the solution of the many-body Schrödinger equation

$$H\Psi = \left\{ \sum_{i=1}^{A} -\frac{\hbar^2}{2m}\Delta_i + \sum_{i<j}^{A} v(i,j) \right\} \Psi(1,\ldots,A) = E\Psi(1,\ldots,A), \tag{2.19}$$

where i represents all coordinates of the ith nucleon, for instance,

$$(i) = (\mathbf{r}_i, s_i, t_i), \tag{2.20}$$

where t_i will be $\frac{1}{2}$ for neutrons and $-\frac{1}{2}$ for protons. With the assumption of the nuclear shell model, the above equation reduces to the much simpler equation

$$H_0\Psi = \left\{ \sum_{i=1}^{A} h_i \right\} \Psi = \sum_{i=1}^{A} \left\{ -\frac{\hbar^2}{2m}\Delta_i + V(i) \right\} \Psi = E\Psi. \tag{2.21}$$

The solutions Ψ of Eq. (2.21) are anti-symmetrized products of single-particle functions, which are eigenfunctions to the single-particle Hamiltonian h_i:

$$h_i\phi_k(i)=\epsilon_k\phi_k(i). \tag{2.22}$$

The functions ϕ_k provide an orthogonal basis for an occupation number representation within the framework of second quantization (see Appendix C). To each level k corresponds a pair of creation and annihilation operators a_k^+, a_k which create or annihilate particles with wave function ϕ_k. Since nucleons are Fermions, each level can be occupied only once, and the operators a_k, a_k^+ obey Fermi commutation relations (C. 23).

The shell model Hamiltonian H_0 has the form

$$H_0=\sum\epsilon_k a_k^+ a_k.$$

Using the bare vacuum $|-\rangle$ its eigenfunctions can be represented as

$$|\Phi_{k_1\ldots k_A}\rangle=a_{k_1}^+\ldots a_{k_A}^+|-\rangle.$$

They are Slater determinants

$$\Phi_{k_1\ldots k_A}(1,\ldots,A)=\begin{vmatrix}\phi_{k_1}(1) & \cdots & \phi_{k_1}(A)\\ \vdots & & \vdots\\ \phi_{k_A}(1) & & \phi_{k_A}(A)\end{vmatrix} \tag{2.23}$$

with eigenvalues

$$E_{k_1\ldots k_A}=\epsilon_{k_1}+\cdots+\epsilon_{k_A}. \tag{2.24}$$

In the ground state the levels are filled successively according to their energy (see Fig. 2.6)

$$|\Phi_0\rangle=a_1^+\ldots a_A^+|-\rangle. \tag{2.25}$$

Thus we have for closed shells the following unique prescription for the construction of the A particle ground state as well as for the A particle excitation spectrum: Starting with the $(1s_{1/2})$ level, one has to occupy each level $|nsljm\rangle$ with just one particle until all A particles are used up. We thus obtain an A nucleon ground state where all different quantum states are occupied with just one particle up to the Fermi level (the highest occupied level); above the Fermi level all levels are unoccupied.

The independent particle picture of the nucleus is different from that in an atom in the sense that in a nucleus there are *two* different kinds of particles, the proton and the neutron, whereas in an atom there is only the

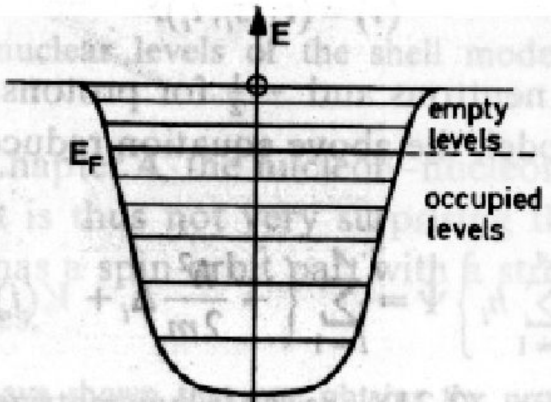
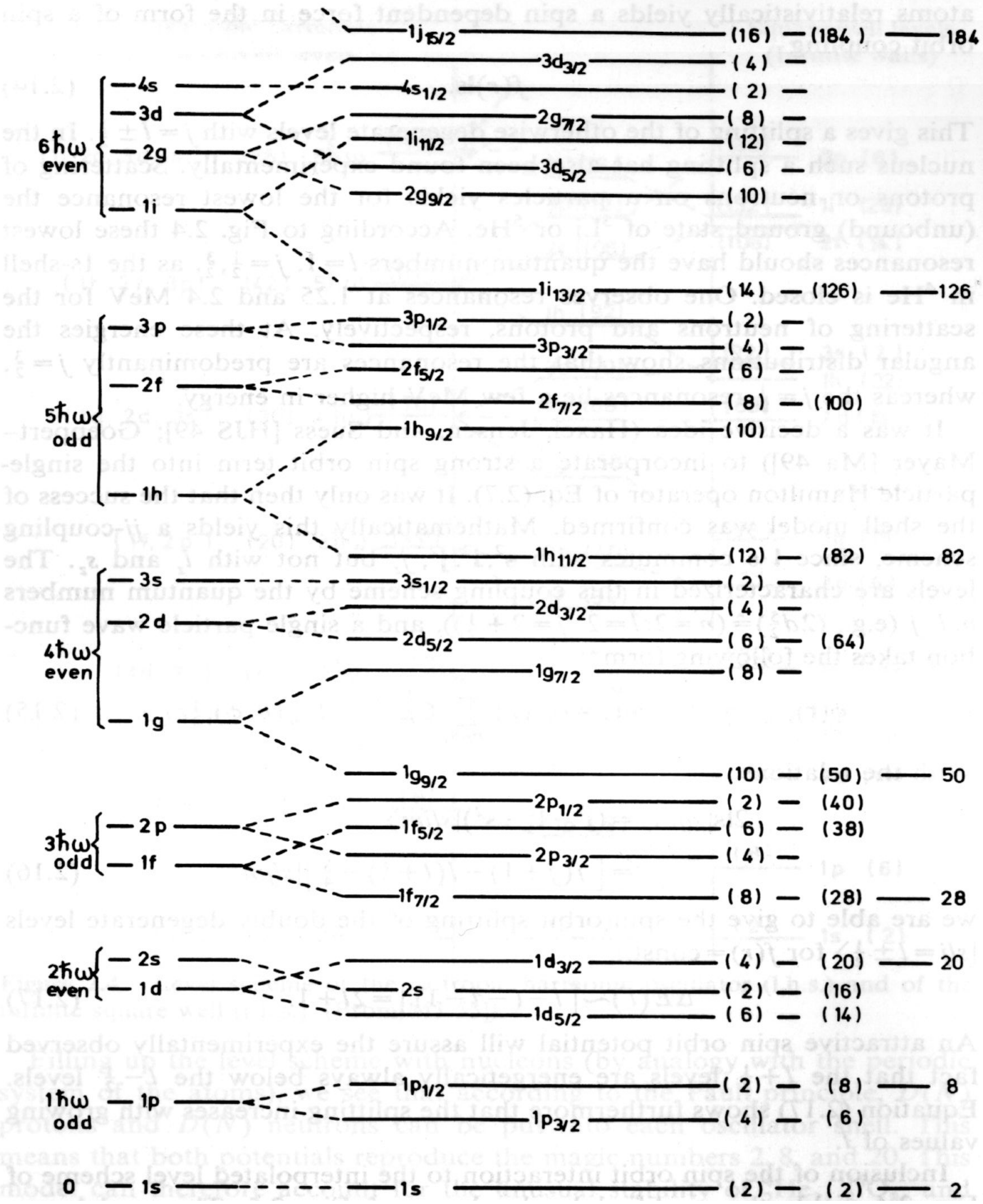


Figure 2.6. Shell model potential and Fermi level.


6ħω even
4s
3d
2g
1i
1j15/2 (16) (184) 184
3d3/2 (4)
4s1/2 (2)
2g7/2 (8)
1i11/2 (12)
3d5/2 (6)
2g9/2 (10)
1i13/2 (14) (126) 126
5ħω odd
3p
2f
1h
3p1/2 (2)
3p3/2 (4)
2f5/2 (6)
2f7/2 (8) (100)
1h9/2 (10)
1h11/2 (12) (82) 82
4ħω even
3s
2d
1g
3s1/2 (2)
2d3/2 (4)
2d5/2 (6) (64)
1g7/2 (8)
1g9/2 (10) (50) 50
3ħω odd
2p
1f
2p1/2 (2) (40)
1f5/2 (6) (38)
2p3/2 (4)
1f7/2 (8) (28) 28
2ħω even
2s
1d
1d3/2 (4) (20) 20
2s (2) (16)
1d5/2 (6) (14)
1ħω odd
1p
1p1/2 (2) (8) 8
1p3/2 (4) (6)
0
1s
1s (2) (2) 2

electron. Protons and neutrons feel different average potentials for two reasons:

(i) Protons also interact via the *Coulomb force*. One therefore usually adds the potential of a homogeneously charged sphere

$$V_C(\mathbf{r}) = \begin{cases} \dfrac{Ze^2}{R}\,\dfrac{1}{2}\left(3-\left(\dfrac{r}{R}\right)^2\right) & r \leqslant R, \\[2ex] \dfrac{Ze^2}{r} & r > R. \end{cases} \tag{2.26}$$

Sometimes (see Sec. 2.8), this feature is approximated by using different potential parameters for protons and neutrons.

(ii) The *symmetry energy* [see Eq. (1.4)] favors a configuration with an equal number of protons and neutrons. Because of the Coulomb repulsion for heavier nuclei, one has a neutron excess: If, in the nucleus, we replace a neutron by a proton, we gain symmetry energy and lose Coulomb energy. Since the Coulomb energy is already taken into account by Eq. (2.26), there must be an additional difference between the single-particle potential for protons and neutrons, which is caused by the symmetry energy. The *nuclear* part of the proton potential is therefore deeper (see Fig. 2.7, dashed line).

These two effects go in opposite directions, but they do not cancel. In the end, the Fermi surfaces for protons and neutrons must be equal, otherwise protons would turn into neutrons by β-decay or vice versa, whichever is energetically favored.

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In $N \neq Z$ nuclei, energy levels with the same quantum numbers for protons and neutrons are therefore shifted with respect to one another by an amount Δ_ϵ resulting from a positive contribution Δ_C from the Coulomb force and a negative contribution $-\Delta_S$ from the symmetry energy

$$\epsilon_{nlj}^{(p)} - \epsilon_{nlj}^{(n)} = \Delta_\epsilon = \Delta_C - \Delta_S . \tag{2.27}$$

In heavy nuclei, this difference is such that the protons and neutrons at the Fermi surface belong to different major shells.

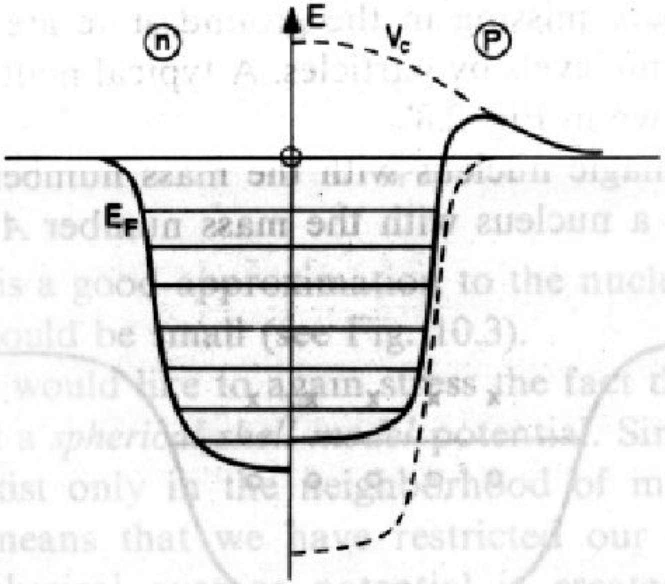

Figure 2.7. Comparison of the shell model potential for neutrons and protons in a nucleus with neutron excess.

The Fermi level coincides in this case with the $1d_{3/2}$ level (see Fig. 2.5).

If we use the indices i, j for the levels below the Fermi surface ($\epsilon_i \leqslant \epsilon_F$), and the indices m, n for the levels above the Fermi surface ($\epsilon_n > \epsilon_F$), the lowest excitations in the shell model are then *ph* excitations of the form

$$|\Phi_{mi}\rangle := a_m^+ a_i |\Phi_0\rangle = \pm a_m^+ a_1^+ \ldots a_{i-1}^+ a_{i+1}^+ \ldots a_A^+ |-\rangle \tag{2.28}$$

with excitation energy $\epsilon_{mi} = \epsilon_m - \epsilon_i$.

In fact one has observed such states in magic nulcei. They are, however, not the lowest states. As we have already seen in Chapter 1, there are low-lying collective states which cannot be explained in the independent particle model.

The Slater determinants (2.23) form a *complete set* of states for the A nulceon system [Lö 55]. Each state of the system is characterized by the distribution of the nucleons among the levels of the single particle potential, that is, by the "occupation numbers" of the levels. It is usual to classify all excited states by taking the ground state as a reference state. The nucleons that are missing in the ground state are denoted by holes, those above the Fermi levels by particles. A typical multiparticle–multihole configuration is shown in Fig. 2.8

Starting from a magic nucleus with the mass number A, we can add a particle and obtain a nucleus with the mass number $A+1$. If we put the

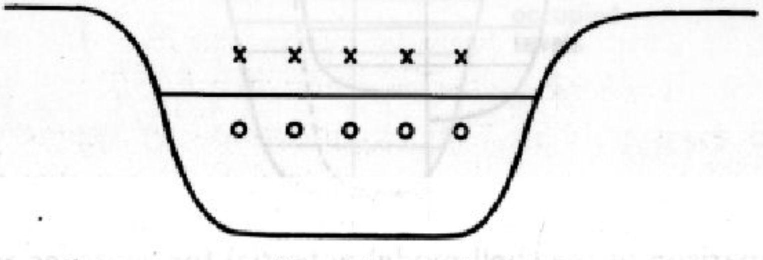

Figure 2.8. Schematic representation of a typical five-particle (crosses), five-hole (open circles) state.

particle into the level m, the wavefunction is

$$|\Phi_m\rangle = a_m^+|\Phi_0\rangle \tag{2.29}$$

and we get the energy difference

$$\epsilon_m = E_m(A+1) - E_0(A). \tag{2.30}$$

In this way one is able to measure the single-particle energies (see Sec. 2.7). These are the simplest states in $A+1$ nuclei. More complicated states have a $2p-1h$ structure, and so on. In complete analogy, there are $1h$, $1p-2h$, etc., states in $A-1$ nuclei.

It often turns out to be very convenient to define quasiparticles by the operators

$$\begin{aligned} &\alpha_m^+ = a_m^+, \qquad &&\alpha_m = a_m, \qquad &&\text{for } \epsilon_m > \epsilon_F; \\ &\alpha_i^+ = a_i, \qquad &&\alpha_i = a_i^+, \qquad &&\text{for } \epsilon_i \leqslant \epsilon_F. \end{aligned} \tag{2.31}$$

These quasiparticles are again fermions. They are particles for states above, and holes for states below, the Fermi surface, so that we have

$$\alpha_k|\Phi_0\rangle = 0, \tag{2.32}$$

that is, the ground state of the magic nucleus is a "vacuum" with respect to these quasi-particles; ph states are two-quasi-particle states, and so on. The multi-quasi-particle states

$$|\Phi_{k_1\ldots k_N}\rangle = \alpha_{k_1}^+ \ldots \alpha_{k_N}^+|\Phi_0\rangle \tag{2.33}$$

form a complete orthogonal set in the many-body Hilbert space.

Метод Хартри-Фока

5.2 The General Variational Principle

We first want to show that the exact Schrödinger equation

$$H|\Psi\rangle = E|\Psi\rangle \tag{5.2}$$

is equivalent to the variational equation

$$\delta E[\Psi] = 0, \tag{5.3}$$

with

$$E[\Psi] = \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle}\,. \tag{5.4}$$

The variation (5.3) can be obtained from (5.4):

$$\langle\delta\Psi|H-E|\Psi\rangle + \langle\Psi|H-E|\delta\Psi\rangle = 0. \tag{5.5}$$

Since $|\Psi\rangle$ is, in general, a complex function, we can carry out the variation over the real and imaginary part independently, which is equivalent to carrying out the variation over $|\delta\Psi\rangle$ and $\langle\delta\Psi|$ independently. To see this we use the fact that Eq. (5.5) is valid for arbitrary infinitesimal $|\delta\Psi\rangle$. We can replace $|\delta\Psi\rangle$ by $i|\delta\Psi\rangle$ and get

$$-i\langle\delta\Psi|H-E|\Psi\rangle + i\langle\Psi|H-E|\delta\Psi\rangle. \tag{5.6}$$

Together with Eq. (5.5), we find

$$\langle \delta\Psi | H - E | \Psi \rangle = 0 \tag{5.7}$$

and the complex conjugate equation. Since $|\delta\Psi\rangle$ is arbitrary, Eq. (5.7) is equivalent to the eigenvalue problem (5.2).

The approximation of such variational methods consists of the fact that $|\Psi\rangle$ is usually restricted to a set of mathematically simple trial wave functions. As soon as the true function is not in this set, the minimal solution is no longer the exact eigenfunction, but only an approximation. The variational method is especially well suited for determining the ground state, since for any trial wave function $|\Psi\rangle$ we can show that

$$E[\Psi] \geqslant E_0, \tag{5.8}$$

and thus E_0 will always be the lower bound of a variational calculation. To prove this, we develop the trial wave function in terms of the exact eigenfunctions of the Hamiltonian:

$$|\Psi\rangle = \sum_{n=0}^{\infty} a_n |\Psi_n\rangle \tag{5.9}$$

with

$$H|\Psi_n\rangle = E_n |\Psi_n\rangle. \tag{5.10}$$

This yields

$$E[\Psi] = \frac{\sum_{nn'} a_n^* a_n E_n \delta_{nn'}}{\sum_n |a_n|^2} \geqslant \frac{\sum_n |a_n|^2 E_0}{\sum_n |a_n|^2} = E_0, \tag{5.11}$$

which is precisely Eq. (5.8). In cases where the ground state energy is not degenerate, the equality sign in (5.11) is valid, if and only if all the coefficients a_n with $n \neq 0$ vanish, that is, $|\Psi\rangle$ is proportional to $|\Psi_0\rangle$. If we are interested in the first excited state, we then have to carry out the variation within the subspace entirely orthogonal to $|\Psi_0\rangle$, that is, over all the wave functions $|\Psi\rangle$ with $a_0 = 0$. Within this subspace $|\Psi_1\rangle$ has the minimal expectation value of H. To find $|\Psi_1\rangle$, we must carry out the variation with the subsidiary condition $\langle \Psi_1 | \Psi_0 \rangle = 0$. In principle we can continue and calculate the whole spectrum using this method.

In practice, however, we do not know $|\Psi_0\rangle$ exactly. From a variation in a restricted subset of the Hilbert space, we find only an approximation $|\Phi_0\rangle$. For the calculation of an approximation $|\Phi_1\rangle$ to the first excited state $|\Psi_1\rangle$, we have to solve the variational equation (5.3) with the supplementary condition that $|\Phi_1\rangle$ is orthogonal to $|\Phi_0\rangle$:

$$\langle \Phi_1 | \Phi_0 \rangle = 0. \tag{5.12}$$

For the second excited state, we must have two supplementary conditions, namely:

$$\langle \Phi_2 | \Phi_1 \rangle = 0; \quad \text{and} \quad \langle \Phi_2 | \Phi_0 \rangle = 0. \tag{5.13}$$

These supplementary conditions are coupled to the problem via Lagrange parameters. We thus see that for higher excited states this method quickly gets rather complicated, therefore it has been applied mainly for the calculation of the ground state. Sometimes, however, these conditions are simply fulfilled because of symmetry properties, as, for example, is the case for states with different angular momentum quantum numbers. We will see in Chapter 7 how to calculate a whole rotational band where the determination of each level is no more complicated than that of the ground state.

So far we have shown that for a certain trial wave function, the ground state energy is always larger than or equal to the exact ground state energy and corresponds to an extremum. In actual calculations, we have to make sure that this extremum actually corresponds to a *minimum*, that is, we must calculate the second derivative of the energy functional, for example, with respect to certain parameters. In the case of the Hartree–Fock or Hartree–Fock–Bogoliubov theory, we will come back to this point (in Chapter 7).

In order to decide which of two variational approaches (i.e., two sets of trial wave functions) is the better one, we have two criteria:

(i) If one set of the trial wave functions is a subset of the other, the larger set is usually the better one, because it contains the first's set minimum.

(ii) Since the exact E_0 is a lower bound, we may hope that out of two trial wave functions, the one for which the corresponding energy is closest to E_0 is better.

Both criteria are, however, not exact statements. Pathological examples can be found which contradict them.

We finish this section with the remark that the variation principle is only valid in this form for a linear eigenvalue problem of the type (5.2). In cases where the Hamiltonian itself depends on the wave function we want to determine, we have to be very careful in applying this principle.

5.3 The Derivation of the Hartree–Fock Equation

5.3.1 The Choice of the Set of Trial Wave Functions

Using the fact that the shell model has provided a suitable approximation for the qualitative explanation of many nuclear properties, we shall assume that there is an average single-particle potential (later to be called the *Hartree–Fock potential*)

$$H^{\mathrm{HF}} = \sum_{i=1}^{A} h(i) \tag{5.14}$$

whose eigenfunction having the lowest eigenvalue E_0^{HF} is an approximation to the exact ground state function. This eigenfunction $\Phi(1\ldots A)$ is, as we have seen in Chapter 2, a *Slater determinant*

$$|\mathrm{HF}\rangle = |\Phi(1\ldots A)\rangle = \prod_{i=1}^{A} a_i^+ |-\rangle \tag{5.15}$$

in which the Fermion operators a_k^+, a_k correspond to the single-particle wave functions φ_k, which are themselves eigenfunctions of the single-particle Hamiltonian h, viz:

$$h(i)\varphi_k(i) = \epsilon_k \varphi_k(i), \qquad i = \{\mathbf{r}_i, s_i, t_i\}. \tag{5.16}$$

As we have seen in Section 2.5, we obtain the lowest eigenvalue of H^{HF} if one occupies the A lowest levels in the state $|\mathrm{HF}\rangle$ (Eq. 5.15). In the following, we will characterize the occupied levels in $|\mathrm{HF}\rangle$ by the letters i, j (hole states) and the empty levels by m, n (particle states). If we do not distinguish, we use the letters k, l, p, q.

The wave functions $\varphi_k(\mathbf{r}, s, t)$ are a coordinate space representation of the eigenstates $|k\rangle$ of the single-particle Hamiltonian h. Very often, we work in a configuration space based on some arbitrary complete and orthogonal set of single-particle wave functions $\{\chi_l\}$ (an example is the set of spherical harmonic oscillator wave functions). The function φ_k can be expanded on this basis:

$$\varphi_k = \sum_l D_{lk} \chi_l. \tag{5.17}$$

If, for each wave function χ_l, we define corresponding fermion creation and annihilation operators c_l^+, c_l (see Section C.1), we can similarly express the operators a_k^+ by the operators c_l^+:

$$a_k^+ = \sum_l D_{lk} c_l^+ . \tag{5.18}$$

Since both sets $\{\varphi_k\}$ and $\{\chi_l\}$ are complete and orthogonal, the transformation D has to be unitary:

$$D^+D = DD^+ = 1. \tag{5.19}$$

This fact also guarantees that the operators (a_k^+, a_k) and (c_l^+, c_l) both obey separate Fermi commutation relations.

As discussed in Section D.2, there is no one-to-one correspondence between a Slater determinant Φ of the form (5.15) and the set of single-particle states φ_k. Any unitary transformation which does not mix particle and hole states leaves Φ unchanged (at least up to an unimportant phase).

It is therefore more convenient to represent a Slater determinant $|\Phi\rangle$ by its single-particle density matrix (D.9):

$$\rho_{ll'} = \langle\Phi|c_{l'}^{+}c_l|\Phi\rangle. \tag{5.20}$$

From Eqs. (5.18) and (5.19), we get

$$\rho_{ll'} = \sum_{kk'} D_{lk} D_{l'k'}^{*} \langle\Phi|a_{k'}^{+}a_k|\Phi\rangle = \sum_{i=1}^{A} D_{li} D_{l'i}^{*} \tag{5.21}$$

because ρ is diagonal in the basis a_k^{+}, a_k with the eigenvalues (occupation numbers) 1 for $i \leqslant A$ (holes) and 0 for $i > A$ (particles). The trace of ρ is equal to the particle number.

As we show in Appendix D.2, there is a one-to-one correspondence between the Slater determinant Φ and its single-particle density ρ. Single-particle densities ρ of Slater determinants are characterized by the fact that they have only eigenvalues 0 or 1, that is,

$$\rho^2 = \rho. \tag{5.22}$$

ρ is therefore a projector in the space of single-particle wave functions onto the subspace spanned by the hole states φ_i.

In the same way, we can define a projector σ

$$\sigma = 1 - \rho \tag{5.23}$$

onto the subspace spanned by the particle states φ_m.

The *Hartree–Fock method* [Ha 28, Fo 30] is now defined in the following way. We use the set of Slater determinants $\{\Phi\}$ of the form (5.15) consisting of A arbitrary but orthogonal single-particle wave functions φ_i as trial wave functions and minimize the energy within this set. An equivalent statement would be that we use the set of all wave functions

$\{\Phi\}$ whose single particle density (5.20) has the property $\rho^2=\rho$ and $\operatorname{Tr}\rho=A$.

As we will see in the following sections, this variation will give us the possibility of determining the single-particle operator H^{HF}.

5.3.2 The Hartree–Fock Energy

Before we are able to carry out the variation which allows us to determine the HF-wave function Φ, we have to calculate the HF-energy

$$E^{\mathrm{HF}}=\langle\Phi|H|\Phi\rangle. \tag{5.24}$$

We start with the many-body Hamiltonian H and represent it in second quantization by the basis operators c_l^+, c_l (see Section C.1):

$$H=\sum_{l_1l_2} t_{l_1l_2}c_{l_1}^+c_{l_2}+\frac{1}{4}\sum_{l_1l_2l_3l_4}\bar{v}_{l_1l_2,\,l_3l_4}c_{l_1}^+c_{l_2}^+c_{l_4}c_{l_3}, \tag{5.25}$$

where

$$\bar{v}_{l_1l_2,\,l_3l_4}=v_{l_1l_2l_3l_4}-v_{l_1l_2l_4l_3}. \tag{5.26}$$

Wick's theorem (Sec. C.4) allows us to calculate the energy (5.24) as a functional of the single-particle density

$$E^{\mathrm{HF}}[\rho] = \sum_{l_1 l_2} t_{l_1 l_2} \langle \Phi | c_{l_1}^{+} c_{l_2} | \Phi \rangle + \frac{1}{4} \sum_{l_1 l_2 l_3 l_4} \bar{v}_{l_1 l_2 l_3 l_4} \langle \Phi | c_{l_1}^{+} c_{l_2}^{+} c_{l_4} c_{l_3} | \Phi \rangle$$

$$= \sum_{l_1 l_2} t_{l_1 l_2} \rho_{l_2 l_1} + \frac{1}{2} \sum_{l_1 l_2 l_3 l_4} \rho_{l_3 l_1} \bar{v}_{l_1 l_2 l_3 l_4} \rho_{l_4 l_2} \tag{5.27}$$

$$= \mathrm{Tr}\,(t\rho) + \frac{1}{2} \mathrm{Tr}_1 \mathrm{Tr}_1 (\rho \bar{v} \rho), \tag{5.28}$$

where $\mathrm{Tr}_1 \mathrm{Tr}_1 \ldots$ is an obvious shorthand notation. Eq. (5.28) does not depend on the basis. We can therefore use it to give an expression for the HF-energy in the HF-basis $\{\varphi_k\}$ in which ρ is diagonal with the eigenvalues 0 and 1

$$E^{\mathrm{HF}} = \sum_{i=1}^{A} t_{ii} + \frac{1}{2} \sum_{i,\, j=1}^{A} \bar{v}_{ij,\, ij}. \tag{5.29}$$

5.3.3 Variation of the Energy

To determine the HF-basis, we have to minimize the energy (5.28) for all product wave functions $|\Phi\rangle$ or for all densities ρ with the property $\rho^2 = \rho$. Since a small variation $\rho + \delta\rho$ has to be a projector again, we get

$$(\rho + \delta\rho)^2 = \rho + \delta\rho$$

or, up to linear terms in $\delta\rho$,

$$\delta\rho = \rho\, \delta\rho + \delta\rho\, \rho.$$

In the HF-basis, where ρ is diagonal, this means that the particle–particle (pp) and hole–hole (hh) matrix elements of $\delta\rho$ have to vanish, that is,

$$\rho\,\delta\rho\,\rho = \sigma\,\delta\rho\,\sigma = 0. \tag{5.30}$$

To make sure that we stay within the set of Slater determinants, therefore, we can only allow for variations $\delta\rho_{mi}$ and $\delta\rho_{im}$ of the *ph* and *hp* matrix elements of ρ in the HF-basis.

The variation of the energy (5.27) is then given by

$$\delta E = E[\rho + \delta\rho] - E[\rho] = \sum_{kk'} h_{kk'}\delta\rho_{k'k} = \sum_{mi} h_{mi}\delta\rho_{im} + c.c., \tag{5.31}$$

where the Hermitian matrix h is defined as

$$h_{kk'} = \frac{\partial E^{\mathrm{HF}}[\rho]}{\partial\rho_{k'k}}. \tag{5.32}$$

From Eq. (5.27), we obtain

$$h = t + \Gamma \tag{5.33}$$

with the *self-consistent field*

$$\Gamma_{kk'} = \sum_{ll'} \bar{v}_{kl'k'l}\,\rho_{ll'}. \tag{5.34}$$

Since arbitrary values of $\delta\rho_{mi}$ are allowed, we see from Eq. (5.31), that the condition $\delta E = 0$ for the HF-solution means that the *ph* matrix elements of h have to vanish,

$$h_{mi} = t_{mi} + \sum_{j=1}^{A} \bar{v}_{mjij} = 0 \qquad (\text{for } i \leqslant A, m > A), \tag{5.35}$$

in the basis where ρ is diagonal, that is, h does not mix particle and hole states of ρ and Eq. (5.35) is equivalent to

$$[h, \rho] = [t + \Gamma[\rho], \rho] = 0. \tag{5.36}$$

This is a nonlinear equation, and not easy to solve. It also states that h and ρ can be diagonalized simultaneously. Since the basis in which ρ is diagonal is determined only up to unitary transformations among the occupied levels or among the empty levels, we use this freedom and require that h shall be diagonal. This defines the *Hartree–Fock basis* and converts (5.36) into an eigenvalue problem.

$$h_{kk'} = t_{kk'} + \sum_{i=1}^{A} \bar{v}_{kik'i} = \epsilon_k \delta_{kk'}. \tag{5.37}$$

Considering the fact that this basis is given by the transformation D (5.18), we obtain the set of *Hartree–Fock equations*

$$\sum_{l'} h_{ll'} D_{l'k} = \sum_{l'} \left(t_{ll'} + \sum_{i=1}^{A} \sum_{pp'} \bar{v}_{lp'l'p} D_{pi} D^*_{p'i} \right) D_{l'k} = \epsilon_k D_{lk}, \tag{5.38}$$

which represent a Hermitian eigenvalue problem. It is nonlinear because the matrix h depends on the density ρ, that is, on the solution of the problem. The coefficients D_{lk} found by the solution of these equations determine the single-particle wave functions φ_k [Eq. (5.17)].

We have thus derived a single-particle Hamiltonian

$$H^{\mathrm{HF}} = \sum_{kk'} h_{kk'} a_k^+ a_{k'} = \sum_{kk'} (t+\Gamma)_{kk'} a_k^+ a_{k'}$$

$$= \sum_{kk'} \left(t_{kk'} + \sum_{j=1}^{A} \bar{v}_{kjk'j} \right) a_k^+ a_{k'} = \sum_k \epsilon_k a_k^+ a_k \tag{5.39}$$

with the properties required in Section (5.3.1): The Slater determinant $|\mathrm{HF}\rangle$, where the lowest A levels are occupied, corresponds to an energy E which is stationary against small variations of the wave function.

The single-particle Hamiltonian h contains, besides the kinetic energy t, a self-consistent field Γ (Eq. (5.34)), which depends on the density of the nucleus. It is a one-body field and averages over all two-body interactions. This point will become even clearer in the coordinate representation (Sec. 5.3.4). The energy expectation value of the HF-wave function $|\mathrm{HF}\rangle$ is given by Eqs. (5.29) and (5.37):

$$E_0^{\mathrm{HF}} = \sum_{i=1}^{A} \epsilon_i - \frac{1}{2} \sum_{ij=1}^{A} \bar{v}_{ijij}. \tag{5.40}$$

It is therefore not equal to the sum of single-particle energies [compare the discussion of this point in Sec. (2.8.6)].

5.3.4 The Hartree–Fock Equations in Coordinate Space

To give a better interpretation of the structure of Eq. (5.38), we write it down in the coordinate space. Assuming a local two-body potential which does not depend on spin or isospin, that is, a pure Wigner force (see Sec. 4.2), we find instead of Eq. (5.38):

$$-\frac{\hbar^2}{2m}\Delta\varphi_k(\mathbf{r})+\sum_{j=1}^{A}\int d\mathbf{r}'\, v(\mathbf{r},\mathbf{r}')\cdot\varphi_j^*(\mathbf{r}')\{\varphi_j(\mathbf{r}')\varphi_k(\mathbf{r})-\varphi_j(\mathbf{r})\varphi_k(\mathbf{r}')\}$$
$$=\epsilon_k\varphi_k(\mathbf{r}). \tag{5.41}$$

Defining the local Hartree potential

$$\Gamma_H(\mathbf{r})=\int d\mathbf{r}'\, v(\mathbf{r},\mathbf{r}')\sum_{j=1}^{A}|\varphi_j(\mathbf{r}')|^2=\int d\mathbf{r}'\, v(\mathbf{r},\mathbf{r}')\rho(\mathbf{r}') \tag{5.42}$$

and the nonlocal or exchange potential

$$\Gamma_{Ex}(\mathbf{r},\mathbf{r}')=-v(\mathbf{r},\mathbf{r}')\sum_{j=1}^{A}\varphi_j^*(\mathbf{r}')\varphi_j(\mathbf{r})=-v(\mathbf{r},\mathbf{r}')\rho(\mathbf{r},\mathbf{r}'), \tag{5.43}$$

we find that $\varphi_k(\mathbf{r})$ is the solution of a nonlocal Schrödinger equation

$$\left\{-\frac{\hbar^2}{2m}\Delta+\Gamma_H(\mathbf{r})\right\}\varphi_k(\mathbf{r})+\int d\mathbf{r}'\,\Gamma_{Ex}(\mathbf{r},\mathbf{r}')\varphi_k(\mathbf{r}')=\epsilon_k\varphi_k(\mathbf{r}). \tag{5.44}$$

5.4 The Hartree–Fock Method in a Simple Solvable Model

As we will discuss in the last section of this chapter, all realistic HF calculations are very difficult numerical problems. In order to get some feeling about how this method works, we want to apply it to a very simple, exactly solvable model first proposed by Lipkin, Meshkov, and Glick [LMG 65], and which has been widely used to test all kinds of many-body theories (as we shall see later on). Let us

Furthermore, it is assumed that in the basis produced by the fixed potential of the core, the residual interaction of the nucleons in the two shells is of a very special form, being of the monopole–monopole type (see Chap. 4) and having essentially only one matrix element different from zero (a particle–hole matrix element of the RPA type (see Chap. 8)). The *model Hamiltonian* is then of the form

$$H = \epsilon K_0 - \tfrac{1}{2}V(K_+K_+ + K_-K_-), \tag{5.45}$$

with

$$K_0 = \frac{1}{2}\sum_{m=1}^{\Omega}(c^+_{+m}c_{+m} - c^+_{-m}c_{-m}); \quad K_+ = \sum_{m=1}^{\Omega} c^+_{+m}c_{-m}; \quad K_- = (K_+)^+, \tag{5.46}$$

where $\Omega = 2j+1$ and c^+_{+m}, c^+_{-m} create a particle in the upper and lower levels, respectively, and ϵ is the energy difference between the two levels (see Fig. 5.1). The operators $K_0, K_\pm$ fulfill the commutation relations of angular momenta.

$$[K_+, K_-] = 2K_0; \quad [K_0, K_\pm] = \pm K_\pm. \tag{5.47}$$

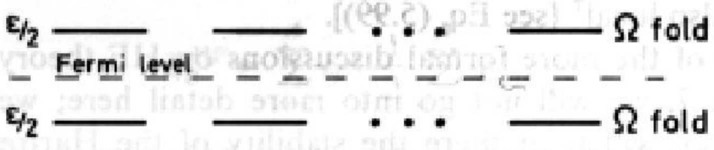

Figure 5.1. Level scheme in the schematic model.