INTRODUCTION TO THE MANY-BODY PROBLEM

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SPRING TERM 2010

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General literature

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1 Second quantization

1.1 Many-particle states

Single-particle states are represented by vectors $|\psi\rangle, |\phi\rangle$ of a Hilbert space $\mathcal{H}$. Two-particle states are constructed in terms of the tensor product $|\phi\rangle \otimes |\psi\rangle$, in short $|\phi\rangle|\psi\rangle$ with appropriate rules for addition, multiplication with a complex number and scalar product (see course on Quantum Mechanics). This construction is readily extended to an arbitrary number of particles. We will be mostly concerned with identical particles, for which the Hamiltonian is invariant under any permutation. In order to define permutation operators we number the particles according to the positions within the tensor product. Thus in the two-particle state

$$|\Psi\rangle = |\psi\rangle|\phi\rangle \tag{1.1}$$

the particle number 1 is in the state $|\psi\rangle$, particle number 2 in state $|\phi\rangle$. If the two single-particle states are different, the same holds for the states $|\Psi\rangle$ and

$$P_{12}|\Psi\rangle := |\phi\rangle|\psi\rangle \ . \tag{1.2}$$

The permutation operator is both Hermitean and unitary, and therefore its eigenvalues are ± 1, with eigenstates $\frac{1}{\sqrt{2}}(|\psi\rangle|\phi\rangle \pm |\phi\rangle|\psi\rangle)$. The Hamiltonian H must commute with P_{12} (see below), and therefore the eigenfunctions of H for two identical particles are either symmetric or antisymmetric.

Consider now three single-particle states $|\alpha\rangle, |\beta\rangle, |\gamma\rangle$, which we assume to be orthonormal, $\langle\alpha|\alpha\rangle = 1, \langle\alpha|\beta\rangle = 0$, and so on. The six permutation operators $P_{12}, P_{23}, P_{31}, P_{123}, (P_{123})^2$ and $P_{ij}^2 = E$ (unity), where the cyclic permutation P_{123} acts as $P_{123}|\alpha\rangle|\beta\rangle|\gamma\rangle = |\gamma\rangle|\alpha\rangle|\beta\rangle$, are not mutually commutative, but there exist four invariant subspaces, two one-dimensional and two two-dimensional spaces. One one-dimensional subspace consists of the state

$$\frac{1}{\sqrt{6}}\left(|\alpha\rangle|\beta\rangle|\gamma\rangle + |\beta\rangle|\alpha\rangle|\gamma\rangle + |\alpha\rangle|\gamma\rangle|\beta\rangle + |\gamma\rangle|\beta\rangle|\alpha\rangle + |\gamma\rangle|\alpha\rangle|\beta\rangle + |\beta\rangle|\gamma\rangle|\alpha\rangle\right),$$

which is symmetric under all permutation operators, the other one consists of the fully anti-symmetric state

$$\frac{1}{\sqrt{6}}\left(|\alpha\rangle|\beta\rangle|\gamma\rangle - |\beta\rangle|\alpha\rangle|\gamma\rangle - |\alpha\rangle|\gamma\rangle|\beta\rangle - |\gamma\rangle|\beta\rangle|\alpha\rangle + |\gamma\rangle|\alpha\rangle|\beta\rangle + |\beta\rangle|\gamma\rangle|\alpha\rangle\right),$$

which changes sign for the odd permutations P_{12}, P_{23}, P_{31} and is invariant under the even permutations $P_{123}, (P_{123})^2$. (A permutation is even if it is obtained by an even number of pair interchanges, otherwise it is odd.) The two states

$$\frac{1}{\sqrt{12}}\left(2|\alpha\rangle|\beta\rangle|\gamma\rangle + 2|\beta\rangle|\alpha\rangle|\gamma\rangle - |\alpha\rangle|\gamma\rangle|\beta\rangle - |\gamma\rangle|\beta\rangle|\alpha\rangle - |\gamma\rangle|\alpha\rangle|\beta\rangle - |\beta\rangle|\gamma\rangle|\alpha\rangle\right),$$

$$\frac{1}{2}\left(-|\alpha\rangle|\gamma\rangle|\beta\rangle + |\gamma\rangle|\beta\rangle|\alpha\rangle + |\gamma\rangle|\alpha\rangle|\beta\rangle - |\beta\rangle|\gamma\rangle|\alpha\rangle\right),$$

transform into a linear combination of each other under the action of the permutation operators, and the same holds for the remaining two states

$$\frac{1}{2}\left(-|\alpha\rangle|\gamma\rangle|\beta\rangle + |\gamma\rangle|\beta\rangle|\alpha\rangle - |\gamma\rangle|\alpha\rangle|\beta\rangle + |\beta\rangle|\gamma\rangle|\alpha\rangle\right),$$

$$\frac{1}{\sqrt{12}}\left(2|\alpha\rangle|\beta\rangle|\gamma\rangle - 2|\beta\rangle|\alpha\rangle|\gamma\rangle + |\alpha\rangle|\gamma\rangle|\beta\rangle + |\gamma\rangle|\beta\rangle|\alpha\rangle - |\gamma\rangle|\alpha\rangle|\beta\rangle - |\beta\rangle|\gamma\rangle|\alpha\rangle\right).$$

We apply the *principle of indistinguishability* (A. M. L. Messiah and O. W. Greenberg, Phys. Rev. **136**, B248 (1964)), according to which two states that differ only by a permutation of identical particles cannot be distinguished by any observation. This means that

$$\langle\Psi|A|\Psi\rangle = \langle\Psi|P_{ij}AP_{ij}|\Psi\rangle \tag{1.3}$$

for an arbitrary observable A and an arbitrary state $|\Psi\rangle$. Therefore

$$[A, P_{ij}] = 0\ , \tag{1.4}$$

i.e., any observable A commutes with any permutation operator.

The six permutation operators form a group, and their action on the states given above can be used for constructing irreducible representations of this group. There are two one-dimensional and one two-dimensional irreducible representations. Group theory is also useful for characterizing the eigenstates of any Hamiltonian which is invariant under permutations. It implies that matrix elements vanish between states belonging to different irreducible representations. These therefore can be used to label the energy eigenvalues, while their dimension is equal to the degeneracy of eigenvalues (if there are no accidental degeneracies).

It is an empirical fact that only fully symmetric or antisymmetric states are realized. Moreover, as proven in quantum field theory, particles with integer spin have only symmetric states (these particles are called *bosons*), whereas particles with half odd-integer spin have only antisymmetric states (these particles are called *fermions*). Antisymmetric states vanish if two single-particle states are identical. This is just the Pauli principle, according to which two fermions cannot occupy the same single-particle state.

1.2 Fock space

Often there exists a natural basis of single-particles states, for instance the states related to the energy levels of an atom or the Bloch states for a particle in a periodic potential. Let $\{|\phi_i\rangle\}$ be an orthonormal basis of the single-particle Hilbert space, $\langle\phi_i|\phi_j\rangle = \delta_{i,j}$. A basis for fully symmetric and anti-symmetric N-particle states is then given by

$$|\Psi\rangle_\pm = N_\pm \sum_p \begin{pmatrix} 1 \\ \text{sign } p \end{pmatrix} |\chi_{p_1}\rangle|\chi_{p_2}\rangle ... |\chi_{p_N}\rangle\ , \tag{1.5}$$

where $\chi_j \in \{|\phi_i\rangle\}$ are (not necessarily distinct) single-particle states, $N_\pm$ is a normalization factor, the sum runs over all $N!$ permutations $p = \begin{pmatrix} 1 & 2 & ... & N \\ p_1 & p_2 & ... & p_N \end{pmatrix}$

and sign $p = +1$ for permutations corresponding to an even number of transpositions and sign $p = -1$ otherwise. Instead of specifying the states (1.5) by all the single-particle states it is more convenient to indicate the number of times a single-particle state appears. Let us call n_i the number of times the state $|\phi_i\rangle$ appears in the product $|\chi_1\rangle|\chi_2\rangle...|\chi_N\rangle$. This number n_i is the *occupation number* of the state $|\phi_i\rangle$. Then the state (1.5) can be specified as

$$|\Psi\rangle_\pm = |n_1, n_2, \ldots\rangle_\pm \ , \tag{1.6}$$

where there are n_1 particles in $|\phi_1\rangle$, n_2 particles in $|\phi_2\rangle$ and so forth. For bosons $n_i = 0, 1, 2, 3, \ldots$, and for fermions $n_i = 0, 1$, according to the Pauli principle. For an N-particle state we have the restriction $\sum_i n_i = N$.

Two states $|n_1, n_2, ...\rangle, |n_1', n_2', ...\rangle$ are orthogonal if they differ in at least one occupation number, *i.e.* $n_i \neq n_i'$ for some number i. If all the occupation numbers coincide, we find

$$\langle\Psi_\pm|\Psi_\pm\rangle = N_\pm^2 \ N! \ n_1! \ n_2!... \tag{1.7}$$

Thus the normalization factor is $N_\pm = 1/\sqrt{N! \ n_1! \ n_2! \ ...}$, and we get

$$\langle n_1', n_2', ...|n_1, n_2, ...\rangle = \delta_{n_1,n_1'}\delta_{n_2,n_2'}... \tag{1.8}$$

It is important to realize that the *occupation number representation* (1.6) depends on the single-particle basis. In general one tries to make a judicious choice dictated by the physical problem at hand. To keep the notation simple we drop the subscript $\pm$ in (1.6). But one has to remember that the states in the occupation number representation are symmetric for bosons and antisymmetric for fermions.

The states $|n_1, n_2, ...\rangle$ form an orthonormal basis of the N-particle Hilbert space $\mathcal{H}_\pm^N$. Thus any state of $\mathcal{H}_\pm^N$ can be written as a linear combination

$$|\Psi\rangle = \sum_{\substack{n_1,n_2,\ldots \\ \sum n_i = N}} c(n_1, n_2, \ldots)|n_1, n_2, \ldots\rangle \ . \tag{1.9}$$

If we remove the restriction $\sum n_i = N$ we obtain a linear combination of states where the number of particles is not specified,

$$|\Psi\rangle = \sum_{n_1,n_2,\ldots} c(n_1, n_2, \ldots)|n_1, n_2, \ldots\rangle \ . \tag{1.10}$$

Two Hilbert spaces with different particle numbers have no state vector in common. Thus states of the form (1.9) belong to the Hilbert space formed by the direct sum

$$\bigoplus_{N=0}^{\infty} \mathcal{H}_\pm^N = \mathcal{F}_\pm \ .$$

In this expression $\mathcal{H}_\pm^0$ consists of the *vacuum state* $|0, 0, 0, \ldots\rangle$. The space $\mathcal{F}_\pm$ is called *Fock space*. It consists of symmetric (bosons) resp. antisymmetric (fermions) state vectors, the number of particles being unspecified. $\mathcal{F}_\pm$ is the appropriate Hilbert space for the formalism of second quantization.

1.3 Creation and annihilation operators

"Second quantization" does not mean that we quantize the theory once more, it merely provides an elegant formalism for dealing with many-fermion and many-boson systems. Formally, as will be shown later, the transition from the quantum theory for a single particle to a many-body theory can be made by replacing the wave functions by field operators. For electromagnetic fields this procedure would indeed correspond to a true quantization, but not in the present context.

a) Bosons

The creation operator $a_i^\dagger$ and annihilation operator a_i of a boson in the state $|\phi_i\rangle$ are defined by

$$\begin{aligned} a_i^\dagger|n_1, n_2, \ldots, n_i, \ldots\rangle &= \sqrt{n_i+1}\ |n_1, n_2, \ldots, n_i+1, \ldots\rangle\ , \\ a_i|n_1, n_2, \ldots, n_i, \ldots\rangle &= \sqrt{n_i}\ |n_1, n_2, \ldots, n_i-1, \ldots\rangle\ . \end{aligned} \tag{1.11}$$

In addition to these two relations we require these operators to be linear. In this way the creation and annihilation operators are completely specified. Relation (1.8) implies that the only non zero matrix elements of a_i are

$$\langle n_1, n_2, \ldots, n_i-1, \ldots |a_i|n_1, n_2, \ldots, n_i, \ldots\rangle = \sqrt{n_i}\ . \tag{1.12}$$

The only non zero matrix elements of $a_i^\dagger$ are

$$\langle n_1, n_2, \ldots, n_i, \ldots |a_i^\dagger|n_1, n_2, \ldots, n_i-1, \ldots\rangle = (n_i-1+1)^{\frac{1}{2}} = (n_i)^{\frac{1}{2}}\ . \tag{1.13}$$

Formulae (1.12) and (1.13) show that $a_i^\dagger$ is the adjoint of a_i. Eq. (1.11) allows to prove the algebraic relations

$$\begin{aligned} [a_i, a_j^\dagger] &= a_i a_j^\dagger - a_j^\dagger a_i = \delta_{ij}\ , \\ [a_i, a_j] &= [a_i^\dagger, a_j^\dagger] = 0\ . \end{aligned} \tag{1.14}$$

For $i = j$ the algebra is the same as that for the raising and lowering operators of the harmonic oscillator. Operators for different single-particle states $|\phi_i\rangle$ and $|\phi_j\rangle$ commute. To prove the first relation for $i = j$ we act with the operators $a_i a_i^\dagger$ and $a_i^\dagger a_i$ on a general state in Fock space,

$$\begin{aligned} a_i a_i^\dagger|..., n_i, ...\rangle &= \sqrt{n_i+1}\ a_i|..., n_i+1, ...\rangle &&= (n_i+1)|..., n_i, ...\rangle\ , \\ a_i^\dagger a_i|..., n_i, ...\rangle &= \sqrt{n_i}\ a_i^\dagger|..., n_i-1, ...\rangle &&= n_i|..., n_i, ...\rangle\ . \end{aligned}$$

Substracting the two relations we find $[a_i, a_i^\dagger]|..., n_i, ...\rangle = |..., n_i, ...\rangle$ for an arbitrary basis state, which proves the first relation in (1.14) for $i = j$. The other relations are demonstrated in the same way.

b) Fermions

The creation and annihilation operators, defined by

$$\begin{aligned} a_i^\dagger|n_1, n_2, \ldots, n_i, \ldots\rangle &= (1-n_i)(-1)^{\epsilon_i}|n_1, n_2, \ldots, n_i+1, \ldots\rangle\ , \\ a_i|n_1, n_2, \ldots, n_i, \ldots\rangle &= n_i(-1)^{\epsilon_i}|n_1, n_2, \ldots, n_i-1, \ldots\rangle\ , \end{aligned} \tag{1.15}$$

take into account the fermionic sign through the number of transpositions involved, $\epsilon_i = \sum_{s=1}^{i-1} n_s$. If state $|\phi_i\rangle$ is already occupied ($n_i = 1$), then we have $a_i^\dagger |n_1, n_2, ..., 1, ...\rangle = 0$, in agreement with the Pauli principle. As in the bosonic case one shows easily that $a_i^\dagger$ is the adjoint of a_i. These operators satisfy the algebra

$$\begin{aligned} \{a_i, a_j^\dagger\} &:= a_i a_j^\dagger + a_j^\dagger a_i = \delta_{ij} \ , \\ \{a_i, a_j\} &= \{a_i^\dagger, a_j^\dagger\} = 0 \ . \end{aligned} \tag{1.16}$$

In particular $a_i^2 = (a_i^\dagger)^2 = 0$, which is again an expression of the Pauli principle. The anticommutation relations for fermions (1.16) are proven in the same way as the commutation relations (1.14) for bosons.

c) Number operator

Eqs. (1.11) (1.15) imply for both Bose and Fermi statistics

$$a_i^\dagger a_i | \ldots, n_i, \ldots\rangle = n_i | \ldots, n_i, \ldots\rangle \ . \tag{1.17}$$

Thus the operator $a_i^\dagger a_i$ counts the number of particles in the state $|\phi_i\rangle$, and the total number of particles is measured by the operator

$$N = \sum_{i=1}^{\infty} a_i^\dagger a_i \ . \tag{1.18}$$

We have

$$N|n_1, n_2, n_3, \ldots\rangle = \sum_{i=1}^{\infty} n_i |n_1, n_2, n_3, \ldots\rangle \ . \tag{1.19}$$

d) Construction of states out of the vacuum

The vacuum state, corresponding to $n_1 = 0, n_2 = 0, \ldots$, is denoted by $|0\rangle$. Acting on $|0\rangle$ with products (or polynomials) of $a_i^\dagger$ and a_j yields states in Fock space. Using the definitions of $a_i^\dagger$ and a_j one shows that

$$|n_1, n_2, \ldots, n_i, \ldots\rangle = \frac{(a_1^\dagger)^{n_1}}{\sqrt{n_1!}} \frac{(a_2^\dagger)^{n_2}}{\sqrt{n_2!}} \cdots \frac{(a_i^\dagger)^{n_i}}{\sqrt{n_i!}} \cdots |0\rangle \ . \tag{1.20}$$

The Fock space is spanned by the states $|n_1, n_2, \ldots, n_i, \ldots\rangle$. Therefore an arbitrary state can be obtained by acting on $|0\rangle$ by some polynomial of creation operators $a_i^\dagger$.

To illustrate the formalism, we consider a few simple examples.

(1) As a first example we consider an atom where the single-particle states correspond to energy levels. With the operation (1.20), specified energy levels are occupied, for instance in

$$a_1^\dagger a_4^\dagger |0\rangle = |1, 0, 0, 1, 0, 0, \ldots\rangle$$

the operator $a_4^\dagger$ puts an electron into level 4, subsequently the operator $a_1^\dagger$ puts a second electron into level 1.

(2) The Fermi sea for free electrons can be written as

$$|\mathrm{F}\rangle = \prod_{\substack{\mathbf{k},\ |\mathbf{k}|<k_F \\ \sigma=\uparrow,\downarrow}} a^\dagger_{\mathbf{k}\sigma}|0\rangle \ ,$$

where $a^\dagger_{\mathbf{k}\sigma}$ creates an electron with momentum $\hbar\mathbf{k}$ and spin projection σ.

(3) The Bardeen-Cooper-Schrieffer state is given by

$$|\mathrm{BCS}\rangle = \prod_{\mathbf{k}}(u_{\mathbf{k}} + v_{\mathbf{k}} a^\dagger_{\mathbf{k}\uparrow} a^\dagger_{-\mathbf{k}\downarrow})|0\rangle, \quad |u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 = 1 \ ,$$

where $a^\dagger_{\mathbf{k}\uparrow}\ a^\dagger_{-\mathbf{k}\downarrow}$ creates a Cooper pair. Notice that this state is not an eigenstate of the particle number operator.

(4) Finally, a Bose condensate for N free bosons corresponds to

$$\frac{(a^\dagger_{\mathbf{k}=0})^N}{\sqrt{N!}}|0\rangle \ .$$

1.4 Quantum fields

For many applications the coordinate representation turns out to be useful. We introduce the family of operators $\Psi^\dagger(\mathbf{r})$ through the relation

$$\Psi^\dagger(\mathbf{r})|0\rangle := |\mathbf{r}\rangle. \tag{1.21}$$

Thus $\Psi^\dagger(\mathbf{r})$ creates a particle at $\mathbf{r}$. (Depending on the situation, one has also to specify some other quantum numbers, for instance the spin of an electron; in this case we will use the notation $\Psi^\dagger_\sigma(\mathbf{r})$.) Using the completeness of single-particle states $|\phi_i\rangle$, we arrive at

$$\Psi^\dagger(\mathbf{r})|0\rangle = \sum_i \langle\phi_i|\mathbf{r}\rangle|\phi_i\rangle = \sum_i \phi^*_i(\mathbf{r})\ a^\dagger_i|0\rangle. \tag{1.22}$$

Thus the operator $\Psi^\dagger(\mathbf{r})$ and the adjoint operator $\Psi(\mathbf{r})$ can also be defined with respect to a given basis,

$$\begin{aligned} \Psi^\dagger(\mathbf{r}) &= \sum_i \phi^*_i(\mathbf{r})\ a^\dagger_i \ , \\ \Psi(\mathbf{r}) &= \sum_i \phi_i(\mathbf{r})\ a_i \ . \end{aligned} \tag{1.23}$$

These operators are also called *quantum fields*. To obtain their properties, we will use extensively the closure and orthonormality relations for the single-particle wave functions

$$\begin{aligned} \sum_i \phi^*_i(\mathbf{r})\phi_i(\mathbf{r}') &= \delta(\mathbf{r}-\mathbf{r}') \ , \\ \int d^3r\ \phi^*_i(\mathbf{r})\phi_j(\mathbf{r}) &= \delta_{ij} \ . \end{aligned} \tag{1.24}$$

a) Spinless bosons

The commutation relations for the field operators of (spin zero) bosons are readily found using the definition (1.23) together with the closure relation of Eq. (1.24),

$$\begin{aligned}[\Psi(\mathbf{r}), \Psi^\dagger(\mathbf{r}')] &= \delta(\mathbf{r}-\mathbf{r}') \ , \\ [\Psi(\mathbf{r}), \Psi(\mathbf{r}')] &= [\Psi^\dagger(\mathbf{r}), \Psi^\dagger(\mathbf{r}')] = \ 0 \ . \end{aligned} \tag{1.25}$$

The particle number operator (1.18) can be expressed by the field operators (1.23), using the orthogonality relation of Eq. (1.24),

$$N = \int d^3r \, \Psi^\dagger(\mathbf{r})\Psi(\mathbf{r}) \ . \tag{1.26}$$

Thus $\Psi^\dagger(\mathbf{r})\Psi(\mathbf{r})$ can be interpreted as the density of particles at $\mathbf{r}$. This interpretation reminds us of the probability density for a particle in state $\psi(\mathbf{r})$ to be at $\mathbf{r}$, and it suggests that the transition from single-particle quantum mechanics to many-body theory is accomplished be replacing the wave function $\psi(\mathbf{r})$ by the operator $\Psi(\mathbf{r})$. The same rule will be found for other single-particle observables. From this point of view the expression "second quantization", although misleading, makes sense.

b) Fermions

For spin $\frac{1}{2}$ fermions we have to include the spin degrees of freedom labeled by $\sigma = \uparrow, \downarrow$,

$$a_i \to a_{i\sigma}, \qquad \Psi(\mathbf{r}) \to \Psi_\sigma(\mathbf{r}) \ . \tag{1.27}$$

Thus we treat the spin as an additional quantum number and do not write down explicitly the two-dimensional column vectors representing the spin states. The anticommutation relations (1.16) are replaced by

$$\begin{aligned}\{a_{i\sigma}, a^\dagger_{j\sigma'}\} &= \delta_{ij}\delta_{\sigma\sigma'} \ , \\ \{a_{i\sigma}, a_{j\sigma'}\} &= \{a^\dagger_{i\sigma}, a^\dagger_{j\sigma'}\} = 0 \ . \end{aligned} \tag{1.28}$$

Correspondingly, the field operators

$$\Psi_\sigma(\mathbf{r}) := \sum_i \phi_i(\mathbf{r}) \ a_{i\sigma} \tag{1.29}$$

satisfy the anticommutation relations

$$\begin{aligned}\{\Psi_\sigma(\mathbf{r}), \Psi^\dagger_{\sigma'}(\mathbf{r}')\} &= \delta(\mathbf{r}-\mathbf{r}')\delta_{\sigma\sigma'} \ , \\ \{\Psi_\sigma(\mathbf{r}), \Psi_{\sigma'}(\mathbf{r}')\} &= \{\Psi^\dagger_\sigma(\mathbf{r}), \Psi^\dagger_{\sigma'}(\mathbf{r}')\} = 0 \ . \end{aligned} \tag{1.30}$$

The number operator is given by

$$N = \sum_\sigma \int d^3r \, \Psi^\dagger_\sigma(\mathbf{r})\Psi_\sigma(\mathbf{r}) \ . \tag{1.31}$$

and therefore $\Psi^\dagger_\sigma(\mathbf{r})\Psi_\sigma(\mathbf{r})$ is the density of particles with spin σ at $\mathbf{r}$.

To be specific we consider electrons in a cubic box of size $V = L^3$ and apply periodic boundary conditions. A natural basis is given by the plane waves

$$\phi_{\mathbf{k}}(\mathbf{r}) = \langle \mathbf{r}|\mathbf{k}\rangle = \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{V^{\frac{1}{2}}} \ , \tag{1.32}$$

where $\mathbf{k} = \frac{2\pi}{L}\mathbf{n}$, $\mathbf{n} = (n_x, n_y, n_z) \in \mathbb{Z}^3$. The creation and annihilation operators of an electron with wave vector $\mathbf{k}$ and spin $\sigma \in \{\uparrow, \downarrow\}$ are $a^\dagger_{\mathbf{k}\sigma}$ and $a_{\mathbf{k}\sigma}$. The field operators of the electrons are therefore given by the Fourier transforms

$$\begin{aligned} \Psi^\dagger_\sigma(\mathbf{r}) &= \frac{1}{V^{\frac{1}{2}}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r}} a^\dagger_{\mathbf{k}\sigma} \ , \\ \Psi_\sigma(\mathbf{r}) &= \frac{1}{V^{\frac{1}{2}}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} a_{\mathbf{k}\sigma} \ . \end{aligned} \tag{1.33}$$

The density at point $\mathbf{r}$ is determined by the operator

$$n(\mathbf{r}) = \Psi^\dagger_\uparrow(\mathbf{r})\Psi_\uparrow(\mathbf{r}) + \Psi^\dagger_\downarrow(\mathbf{r})\Psi_\downarrow(\mathbf{r}) \tag{1.34}$$

and the total electron number operator is

$$N = \sum_{\sigma=\uparrow,\downarrow} \int_V d^3r \, \Psi^\dagger_\sigma(\mathbf{r})\Psi_\sigma(\mathbf{r}) = \sum_{\mathbf{k},\sigma} a^\dagger_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma} \ . \tag{1.35}$$

c) Many-particle wave functions

In the same way as many-particle states can be constructed by applying products of creation operators $a^\dagger_i$, defined with respect to a single-particle basis $\{|\phi_i\rangle\}$, to the vacuum state $|0\rangle$, we can generate states

$$|\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N\rangle := \Psi^\dagger(\mathbf{r}_1)\Psi^\dagger(\mathbf{r}_2)\ldots\Psi^\dagger(\mathbf{r}_N)|0\rangle \ , \tag{1.36}$$

or, for particles with non-zero spin,

$$|\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2, \ldots, \mathbf{r}_N\sigma_N\rangle := \Psi^\dagger_{\sigma_1}(\mathbf{r}_1)\Psi^\dagger_{\sigma_2}(\mathbf{r}_2)\ldots\Psi^\dagger_{\sigma_N}(\mathbf{r}_N)|0\rangle \ . \tag{1.37}$$

These are states where the N particles sit at the sites $\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N$ (possibly with spins $\sigma_1, \sigma_2, \ldots, \sigma_N$). They can be used for setting up a coordinate representation for any N-particle state.

Consider for example the particular state of N spin $\frac{1}{2}$ fermions

$$|1\tau_1, 2\tau_2, \ldots, N\tau_N\rangle := a^\dagger_{1\tau_1} a^\dagger_{2\tau_2} \ldots a^\dagger_{N\tau_N}|0\rangle \ , \tag{1.38}$$

where $a^\dagger_{i\tau_i}$ creates a particle in the state $|\phi_i\rangle$ with spin $\tau_i = \uparrow$ or $\downarrow$. The bra corresponding to the ket (1.37) is

$$\langle \mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2, \ldots, \mathbf{r}_N\sigma_N| = \langle 0|\Psi_{\sigma_N}(\mathbf{r}_N)\cdots\Psi_{\sigma_2}(\mathbf{r}_2)\Psi_{\sigma_1}(\mathbf{r}_1) \ . \tag{1.39}$$

Therefore, using Eq. (1.29), we find the coordinate representation

$$\begin{aligned} &\langle \mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2, \ldots, \mathbf{r}_N\sigma_N|1\tau_1, 2\tau_2, \ldots, N\tau_N\rangle \\ &= \sum_{i_1,\ldots,i_N} \phi_{i_1}(\mathbf{r}_1)\cdots\phi_{i_N}(\mathbf{r}_N) \ \langle 0|a_{i_N\sigma_N}\cdots a_{i_1\sigma_1} a^\dagger_{1\tau_1}\cdots a^\dagger_{N\tau_N}|0\rangle \ . \end{aligned} \tag{1.40}$$

The matrix element $\langle 0|a_{i_N\sigma_N}\cdots a_{i_1\sigma_1}a^\dagger_{1\tau_1}\cdots a^\dagger_{N\tau_N}|0\rangle$ is non-zero only if the sequence $(i_1, i_2, ..., i_N)$ is a permutation p of $(1, 2, ..., N)$. In this case one obtains (Wick's theorem, to be discussed later)

$$\langle 0|a_{i_N\sigma_N}\cdots a_{i_1\sigma_1}a^\dagger_{1\tau_1}\cdots a^\dagger_{N\tau_N}|0\rangle = \text{sign } p\ \delta_{\sigma_1,\tau_{p_1}}\cdots\delta_{\sigma_N,\tau_{p_N}}\ . \tag{1.41}$$

The many-body wave function representing the state $|1\tau_1, 2\tau_2, \ldots, N\tau_N\rangle$ is therefore given by

$$\langle \mathbf{r}_1\sigma_1, ..., \mathbf{r}_N\sigma_N|1\tau_1, ..., N\tau_N\rangle = \sum_p \text{sign } p\ \phi_{p_1}(\mathbf{r}_1)\delta_{\sigma_1,\tau_{p_1}}\cdots\phi_{p_N}(\mathbf{r}_N)\delta_{\sigma_N,\tau_{p_N}}\ , \tag{1.42}$$

where the summation runs over all the permutations $(p_1, p_2, \ldots, p_N)$. This expression can be recasted into the form of the so-called *Slater determinant*

$$\langle \mathbf{r}_1\sigma_1, ..., \mathbf{r}_N\sigma_N|1\tau_1, ..., N\tau_N\rangle = \begin{vmatrix} \langle \mathbf{r}_1\sigma_1|1\tau_1\rangle & \cdots & \langle \mathbf{r}_1\sigma_1|N\tau_N\rangle \\ \cdots & \cdots & \cdots \\ \langle \mathbf{r}_N\sigma_N|1\tau_1\rangle & \cdots & \langle \mathbf{r}_N\sigma_N|N\tau_N\rangle \end{vmatrix}\ , \tag{1.43}$$

where we have used the relation $\langle \mathbf{r}_i\sigma_i|j\tau_j\rangle = \phi_j(\mathbf{r}_i)\delta_{\sigma_i,\tau_j}$.

1.5 Representation of observables

We have already encountered the number operator which may be expressed in terms of creation and annihilation operators (in the basis $\{|\phi_i\rangle\}$), $N = \sum_i a^\dagger_i a_i$. Here we shall explain how to express general observables in terms of $a^\dagger_i$ and a_i. In order to keep the discussion concrete we concentrate on three special, but important observables, the kinetic energy of N particles

$$T = \sum_{i=1}^N \frac{\mathbf{p}_i^2}{2m}\ , \tag{1.44}$$

the external potential

$$V_{ext} = \sum_{i=1}^N U(\mathbf{r}_i) \tag{1.45}$$

and the two-body interaction

$$V_2 = \frac{1}{2}\sum_{i\neq j} V(\mathbf{r}_i, \mathbf{r}_j)\ . \tag{1.46}$$

The first and the second observables are one-body observables while the third one is a two-body observable. The following discussion is valid both for bosons and for fermions. For the sake of generality, the spin index (half-integer for fermions, zero or a positive integer for bosons) is explicitly displayed.

a) Kinetic energy

We start with the kinetic energy T which is diagonal in the basis of plane waves $|\mathbf{k},\sigma\rangle$. Thus we have

$$T|\mathbf{k}_1\sigma_1,\mathbf{k}_2\sigma_2,...,\mathbf{k}_N\sigma_N\rangle = \sum_{i=1}^{N}\left(\frac{\hbar^2\mathbf{k}_i^2}{2m}\right)|\mathbf{k}_1\sigma_1,\mathbf{k}_2\sigma_2,...,\mathbf{k}_N\sigma_N\rangle \ . \tag{1.47}$$

In second-quantized form the N-particle state is written as

$$|\mathbf{k}_1\sigma_1,\mathbf{k}_2\sigma_2,...,\mathbf{k}_N\sigma_N\rangle = a^\dagger_{\mathbf{k}_1\sigma_1}a^\dagger_{\mathbf{k}_2\sigma_2}...a^\dagger_{\mathbf{k}_N\sigma_N}|0\rangle \ . \tag{1.48}$$

The number of particles in the state $|\mathbf{k},\sigma\rangle$ is $a^\dagger_{\mathbf{k}\sigma}a_{\mathbf{k}\sigma}$, so we expect

$$T = \sum_{\mathbf{k},\sigma}\frac{|\hbar\mathbf{k}|^2}{2m}a^\dagger_{\mathbf{k}\sigma}a_{\mathbf{k}\sigma} \ . \tag{1.49}$$

In order to prove this statement we have to show that the application of this operator onto any N-particle state (1.48) reproduces Eq. (1.47). The following algebraic relation will be useful,

$$\left[a^\dagger_{\mathbf{k}\sigma}a_{\mathbf{k}\sigma},a^\dagger_{\mathbf{k}_i\sigma_i}\right] = a^\dagger_{\mathbf{k}_i\sigma_i}\delta_{\mathbf{k},\mathbf{k}_i}\delta_{\sigma,\sigma_i} \ . \tag{1.50}$$

It holds both for bosons and fermions. Applying this relation step by step, *i.e.*

$$\begin{aligned} &a^\dagger_{\mathbf{k}\sigma}a_{\mathbf{k}\sigma}a^\dagger_{\mathbf{k}_1\sigma_1}a^\dagger_{\mathbf{k}_2\sigma_2}...a^\dagger_{\mathbf{k}_N\sigma_N}|0\rangle = \\ &\quad\left[a^\dagger_{\mathbf{k}\sigma}a_{\mathbf{k}\sigma},a^\dagger_{\mathbf{k}_1\sigma_1}\right]a^\dagger_{\mathbf{k}_2\sigma_2}...a^\dagger_{\mathbf{k}_N\sigma_N}|0\rangle + a^\dagger_{\mathbf{k}_1\sigma_1}a^\dagger_{\mathbf{k}\sigma}a_{\mathbf{k}\sigma}a^\dagger_{\mathbf{k}_2\sigma_2}...a^\dagger_{\mathbf{k}_N\sigma_N}|0\rangle \ , \end{aligned} \tag{1.51}$$

we find

$$a^\dagger_{\mathbf{k}\sigma}a_{\mathbf{k}\sigma}a^\dagger_{\mathbf{k}_1\sigma_1}a^\dagger_{\mathbf{k}_2\sigma_2}...a^\dagger_{\mathbf{k}_N\sigma_N}|0\rangle = n_{\mathbf{k}\sigma}a^\dagger_{\mathbf{k}_1\sigma_1}a^\dagger_{\mathbf{k}_2\sigma_2}...a^\dagger_{\mathbf{k}_N\sigma_N}|0\rangle \ , \tag{1.52}$$

where $n_{\mathbf{k}\sigma}$ is the number of times the quantum number $\mathbf{k}\sigma$ appears in the state $|\mathbf{k}_1\sigma_1,\mathbf{k}_2\sigma_2,...,\mathbf{k}_N\sigma_N\rangle$. It is now obvious that Eq. (1.47) is fulfilled and therefore the kinetic energy is indeed given by Eq. (1.49).

Expression (1.49) is simple and intuitive because the underlying basis diagonalises the kinetic energy. It is useful to have T in coordinate basis. Inverting (1.33),

$$\begin{aligned} a^\dagger_{\mathbf{k}\sigma} &= \frac{1}{V^{\frac{1}{2}}}\int_V d^3r\, e^{i\mathbf{k}\cdot\mathbf{r}}\Psi^\dagger_\sigma(\mathbf{r}) \ , \\ a_{\mathbf{k}\sigma} &= \frac{1}{V^{\frac{1}{2}}}\int_V d^3r\, e^{-i\mathbf{k}\cdot\mathbf{r}}\Psi_\sigma(\mathbf{r}) \ , \end{aligned} \tag{1.53}$$

we obtain

$$\begin{aligned} \mathbf{k}^2a^\dagger_{\mathbf{k}\sigma}a_{\mathbf{k}\sigma} &= \frac{1}{V}\int_V d^3r\,\Psi^\dagger_\sigma(\mathbf{r})\nabla e^{i\mathbf{k}\cdot\mathbf{r}}\cdot\int_V d^3r'\,\Psi_\sigma(\mathbf{r}')\,\nabla' e^{-i\mathbf{k}'\cdot\mathbf{r}'} \\ &= \frac{1}{V}\int_V d^3r\, e^{i\mathbf{k}\cdot\mathbf{r}}\nabla\Psi^\dagger_\sigma(\mathbf{r})\cdot\int_V d^3r'\, e^{-i\mathbf{k}'\cdot\mathbf{r}'}\nabla'\Psi_\sigma(\mathbf{r}') \, , \end{aligned} \tag{1.54}$$

where we have used partial integration together with periodic boundary conditions ($V = L^3$, $k_\alpha = 2\pi\nu_\alpha/L$, $\alpha = x, y, z$). Using the relation [1]

$$\frac{1}{V}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} = \delta(\mathbf{r}-\mathbf{r}') \tag{1.55}$$

we get

$$T = \frac{\hbar^2}{2m}\sum_{\sigma}\int_V d^3r \nabla\Psi^\dagger_\sigma(\mathbf{r})\cdot\nabla\Psi_\sigma(\mathbf{r}) \ , \tag{1.56}$$

where the gradient operator acts only on the immediately following field operator.

b) External potential

The one-body potential V_{ext} is diagonal in coordinate space,

$$V_{ext}|\mathbf{r}_1\sigma_1, ..., \mathbf{r}_N, \sigma_N\rangle = \left(\sum_{i=1}^{N} U(\mathbf{r}_i)\right)|\mathbf{r}_1\sigma_1, ..., \mathbf{r}_N\sigma_N\rangle \ , \tag{1.57}$$

where in the state $|\mathbf{r}_1\sigma_1, ..., \mathbf{r}_N, \sigma_N\rangle$ one particle is at $\mathbf{r}_1$ with spin σ_1, one at $\mathbf{r}_2$ with spin σ_2, and so on, *i.e.*

$$|\mathbf{r}_1\sigma_1, ..., \mathbf{r}_N\sigma_N\rangle = \Psi^\dagger_{\sigma_1}(\mathbf{r}_1)...\Psi^\dagger_{\sigma_N}(\mathbf{r}_N)|0\rangle \ . \tag{1.58}$$

We claim now that the second-quantized representation of the external potential is given by

$$V_{ext} = \sum_\sigma \int d^3r U(\mathbf{r})\Psi^\dagger_\sigma(\mathbf{r})\Psi_\sigma(\mathbf{r}) = \int d^3r U(\mathbf{r})n(\mathbf{r}) \ . \tag{1.59}$$

The proof proceeds as above for the kinetic energy. We notice that the commutation relation

$$\left[\Psi^\dagger_\sigma(\mathbf{r})\Psi_\sigma(\mathbf{r}), \Psi^\dagger_{\sigma_i}(\mathbf{r}_i)\right] = \delta_{\sigma,\sigma_i}\delta(\mathbf{r}-\mathbf{r}_i)\Psi^\dagger_{\sigma_i}(\mathbf{r}_i) \tag{1.60}$$

holds both for bosons and fermions. Applying the operator (1.59) to the right-hand side of (1.58), we find indeed

$$\begin{aligned}\left(\sum_\sigma \int d^3r \ U(\mathbf{r})\Psi^\dagger_\sigma(\mathbf{r})\Psi_\sigma(\mathbf{r})\right)\Psi^\dagger_{\sigma_1}(\mathbf{r}_1)...\Psi^\dagger_{\sigma_N}(\mathbf{r}_N)|0\rangle \\ = \left(\sum_{i=1}^{N} U(\mathbf{r}_i)\right)\Psi^\dagger_{\sigma_1}(\mathbf{r}_1)...\Psi^\dagger_{\sigma_N}(\mathbf{r}_N)|0\rangle \ .\end{aligned} \tag{1.61}$$

The momentum representation of the external potential is easily obtained using Eq. (1.33),

$$\begin{aligned}V_{ext} &= \sum_\sigma \int d^3r \ U(\mathbf{r})\frac{1}{V}\sum_{\mathbf{k},\mathbf{k}'} e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}} a^\dagger_{\mathbf{k},\sigma}a_{\mathbf{k}',\sigma} \\ &= \frac{1}{V}\sum_{\mathbf{k},\mathbf{k}',\sigma}\tilde{U}(\mathbf{k}-\mathbf{k}')a^\dagger_{\mathbf{k},\sigma}a_{\mathbf{k}',\sigma} \ ,\end{aligned} \tag{1.62}$$

[1] In the theory of generalized functions one shows the relation $\sum_{n=-\infty}^{\infty}\delta(x-nL) = \frac{1}{L}\sum_{\nu=-\infty}^{\infty} e^{2\pi i\nu x/L}$. If x is limited to an interval of length L only one term of the l.h.s. survives.

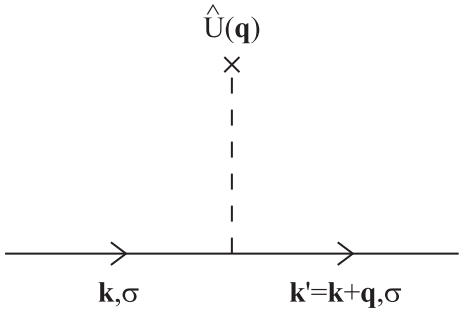

Figure 1: Diagram illustrating the scattering by an external potential.

where $\tilde{U}(\mathbf{q}) = \int d^3r\ e^{-i\mathbf{q}\cdot\mathbf{r}} U(\mathbf{r})$ is the Fourier transform of the potential. This result is illustrated by the diagram of Fig. 1. It can also be expressed in the plane-wave basis (1.32),

$$V_{ext} = \sum_{\mathbf{k},\mathbf{k}',\sigma} \int d^3r\ U(\mathbf{r}) \langle \mathbf{k}|\mathbf{r}\rangle\langle \mathbf{r}|\mathbf{k}'\rangle a^\dagger_{\mathbf{k},\sigma} a_{\mathbf{k}',\sigma}$$
$$= \sum_{\mathbf{k},\mathbf{k}',\sigma} \langle \mathbf{k}|U|\mathbf{k}'\rangle a^\dagger_{\mathbf{k},\sigma} a_{\mathbf{k}',\sigma}\ , \tag{1.63}$$

where we have used the completeness relation $\int d^3r\ |\mathbf{r}\rangle\langle\mathbf{r}| = 1$.

c) One-body operator with respect to an arbitrary single-particle basis

The general form of a one-body operator (in first-quantized form) is

$$O = \sum_{i=1}^{N} O_i\ , \tag{1.64}$$

where O_i acts only on the i-th particle. This labeling disappears for identical particles, and in second-quantized form the operator is written as

$$O = \sum_{m,n} \langle \phi_m|O_1|\phi_n\rangle\ a^\dagger_m a_n \tag{1.65}$$

with respect to a given single-particle basis $\{|\phi_n\rangle\}$, where O_1 is the one-body operator for a single particle. In order to prove the equivalence between the representations (1.64) and (1.65), we first show that the form (1.65) is the same for any single-particle basis. Let $b^\dagger_j, b_j$ describe creation and annihilation operators for a different single-particle basis $\{|\psi_j\rangle\}$, related to the original basis by the unitary transformation

$$|\phi_n\rangle = \sum_j \langle \psi_j|\phi_n\rangle\ |\psi_j\rangle\ . \tag{1.66}$$

This corresponds to the following relation between creation operators

$$a^\dagger_n = \sum_j \langle \psi_j|\phi_n\rangle\ b^\dagger_j\ . \tag{1.67}$$

The relation (1.33) between field operators $\Psi^\dagger_\sigma(\mathbf{r})$ and the creation operators $a^\dagger_{\mathbf{k},\sigma}$ is a special example of such a transformation. Inserting Eqs. (1.66) and (1.67) into the representation (1.65) and using the completeness relation $\sum_n |\phi_n\rangle\langle\phi_n| = 1$, we readily find

$$O = \sum_{j,j'} \langle\psi_j|O_1|\psi_{j'}\rangle \; b^\dagger_j b_{j'} \; , \tag{1.68}$$

i.e. indeed the same form as before. We can therefore choose any basis which is convenient for demonstrating the equivalence between the representations (1.64) and (1.65). The obvious choice is a basis consisting of eigenvectors $|\chi_l\rangle$ of O_1, $O_1|\chi_l\rangle = \omega_l|\chi_l\rangle$. This yields the diagonal representation $O = \sum_l \omega_l c^\dagger_l c_l$ in terms of the corresponding creation and annihilation operators. The proof for the equivalence between the representations (1.64) and (1.65) proceeds then in the same way as in the case of the kinetic energy.

d) Two-body operators

We will concentrate on a spin-independent two-body interaction as in Eq. (1.46) and proceed as in the case of V_{ext}. The operator V_2 is diagonal in coordinate space,

$$V_2|\mathbf{r}_1\sigma_1,\ldots,\mathbf{r}_N\sigma_N\rangle = \left(\frac{1}{2}\sum_{i\neq j} V_2(\mathbf{r}_i,\mathbf{r}_j)\right)|\mathbf{r}_1\sigma_1,\ldots,\mathbf{r}_N\sigma_N\rangle \; . \tag{1.69}$$

It will be shown below that the second-quantized expression is

$$V_2 = \frac{1}{2}\sum_{\sigma,\sigma'}\int d^3r \int d^3r' \; V_2(\mathbf{r},\mathbf{r}')\Psi^\dagger_\sigma(\mathbf{r})\Psi^\dagger_{\sigma'}(\mathbf{r}')\Psi_{\sigma'}(\mathbf{r}')\Psi_\sigma(\mathbf{r}) \; . \tag{1.70}$$

Often this expression is rewritten in terms of the density $n(\mathbf{r})$,

$$V_2 = \frac{1}{2}\int d^3r \int d^3r' \; V_2(\mathbf{r},\mathbf{r}') : n(\mathbf{r})n(\mathbf{r}') : \; . \tag{1.71}$$

This formula is quite familiar except that the operators are *normal ordered*. Normal order means that all the creation operators are put on the left of the annihilation operators and that for fermions one has to take into account the sign of the permutation involved in the rearrangement of the operators.

To show the equivalence of the first- and second-quantized representations, we verify that the application of Eq. (1.70) to a state $|\mathbf{r}_1\sigma_1,\ldots,\mathbf{r}_N\sigma_N\rangle$ reproduces Eq. (1.69). To this end we use the relation

$$\begin{aligned}&\left[\Psi^\dagger_\sigma(\mathbf{r})\Psi^\dagger_{\sigma'}(\mathbf{r}')\Psi_{\sigma'}(\mathbf{r}')\Psi_\sigma(\mathbf{r}), \Psi^\dagger_{\sigma_i}(\mathbf{r}_i)\right] \\ &= \Psi^\dagger_{\sigma_i}(\mathbf{r}_i)\left(\delta_{\sigma,\sigma_i}\delta_{\mathbf{r},\mathbf{r}_i}\Psi^\dagger_{\sigma'}(\mathbf{r}')\Psi_{\sigma'}(\mathbf{r}') + \delta_{\sigma',\sigma_i}\delta_{\mathbf{r}',\mathbf{r}_i}\Psi^\dagger_\sigma(\mathbf{r})\Psi_\sigma(\mathbf{r})\right) \; ,\end{aligned} \tag{1.72}$$

which is easily proven for both bosons and fermions. We use this relation to move the field operators in Eq. (1.70) through the operators in the state (1.58)

$$\begin{aligned}&\Psi^\dagger_\sigma(\mathbf{r})\Psi^\dagger_{\sigma'}(\mathbf{r}')\Psi_{\sigma'}(\mathbf{r}')\Psi_\sigma(\mathbf{r})\Psi^\dagger_{\sigma_1}(\mathbf{r}_1)\cdots\Psi^\dagger_{\sigma_N}(\mathbf{r}_N)|0\rangle \\ &= \sum_{i=1}^N \Psi^\dagger_{\sigma_1}(\mathbf{r}_1)\cdots\left[\Psi^\dagger_\sigma(\mathbf{r})\Psi^\dagger_{\sigma'}(\mathbf{r}')\Psi_{\sigma'}(\mathbf{r}')\Psi_\sigma(\mathbf{r}), \Psi^\dagger_{\sigma_i}(\mathbf{r}_i)\right]\cdots\Psi^\dagger_{\sigma_N}(\mathbf{r}_N)|0\rangle.\end{aligned} \tag{1.73}$$

This implies

$$\frac{1}{2}\sum_{\sigma,\sigma'}\int d^3r\int d^3r'\ V_2(\mathbf{r},\mathbf{r}')\Psi^\dagger_\sigma(\mathbf{r})\Psi^\dagger_{\sigma'}(\mathbf{r}')\Psi_{\sigma'}(\mathbf{r}')\Psi_\sigma(\mathbf{r})|\mathbf{r}_1\sigma_1,\ldots,\mathbf{r}_N\sigma_N\rangle$$

$$=\sum_{i=1}^{N}\Psi^\dagger_{\sigma_1}(\mathbf{r}_1)\cdots\Psi^\dagger_{\sigma_i}(\mathbf{r}_i)\int d^3r\ V_2(\mathbf{r}_i,\mathbf{r})n(\mathbf{r})\Psi^\dagger_{\sigma_{i+1}}(\mathbf{r}_{i+1})\cdots\Psi^\dagger_{\sigma_N}(\mathbf{r}_N)|0\rangle\ , \quad (1.74)$$

where $n(\mathbf{r})=\sum_\sigma\Psi^\dagger_\sigma(\mathbf{r})\Psi_\sigma(\mathbf{r})$, and we have used the symmetry $V(\mathbf{r},\mathbf{r}')=V(\mathbf{r}',\mathbf{r})$. We thus arrive at the problem of applying external potentials on many-particle states, and we can use Eq. (1.61). This gives the desired result,

$$\frac{1}{2}\sum_{\sigma,\sigma'}\int d^3r\int d^3r'\ V_2(\mathbf{r},\mathbf{r}')\Psi^\dagger_\sigma(\mathbf{r})\Psi^\dagger_{\sigma'}(\mathbf{r}')\Psi_{\sigma'}(\mathbf{r}')\Psi_\sigma(\mathbf{r})|\mathbf{r}_1\sigma_1,\ldots,\mathbf{r}_N\sigma_N\rangle$$

$$=\sum_{\substack{i,j\\ i>j}}V_2(\mathbf{r}_i,\mathbf{r}_j)|\mathbf{r}_1\sigma_1,\ldots,\mathbf{r}_N\sigma_N\rangle\ . \quad (1.75)$$

The momentum space representation for the two-body interaction (1.70) is obtained by inserting the relation (1.33) for the quantum fields. One finds

$$V_2=\frac{1}{2}\sum_{\sigma,\sigma'}\sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4}\langle\mathbf{k}_1,\mathbf{k}_2|V_2|\mathbf{k}_4,\mathbf{k}_3\rangle\ a^\dagger_{\mathbf{k}_1,\sigma}a^\dagger_{\mathbf{k}_2,\sigma'}a_{\mathbf{k}_3,\sigma'}a_{\mathbf{k}_4,\sigma} \quad (1.76)$$

with matrix elements

$$\langle\mathbf{k}_1,\mathbf{k}_2|V_2|\mathbf{k}_4,\mathbf{k}_3\rangle\ =\frac{1}{V^2}\int d^3r\int d^3r'\ e^{-i(\mathbf{k}_1-\mathbf{k}_4)\cdot\mathbf{r}}e^{-i(\mathbf{k}_2-\mathbf{k}_3)\cdot\mathbf{r}'}V_2(\mathbf{r},\mathbf{r}')\ . \quad (1.77)$$

For a homogeneous system the interaction depends only on the difference $\mathbf{r}-\mathbf{r}'$, $V_2(\mathbf{r},\mathbf{r}')=V_2(\mathbf{r}-\mathbf{r}')$. Moreover, assuming periodic boundary conditions for $V_2(\mathbf{r})$, we have the Fourier series

$$V_2(\mathbf{r})=\frac{1}{V}\sum_{\mathbf{q}}e^{i\mathbf{q}\cdot\mathbf{r}}\ \tilde{V}_2(\mathbf{q}) \quad (1.78)$$

with $\mathbf{q}=\frac{2\pi}{L}(\nu_1,\nu_2,\nu_3),\ \nu_i\in\mathbb{Z}$. The matrix elements are then simplified as follows,

$$\langle\mathbf{k}_1,\mathbf{k}_2|V_2|\mathbf{k}_4,\mathbf{k}_3\rangle=\frac{1}{V}\tilde{V}_2(\mathbf{q})\ \delta_{\mathbf{q},\mathbf{k}_1-\mathbf{k}_4}\ \delta_{\mathbf{q},-\mathbf{k}_2+\mathbf{k}_3}\ . \quad (1.79)$$

With $\mathbf{k}_1=\mathbf{k},\ \mathbf{k_2}=\mathbf{k}',\ \mathbf{k_3}=\mathbf{k}'+\mathbf{q}$ and $\mathbf{k}_4=\mathbf{k}-\mathbf{q}$, the two-particle interaction becomes

$$V_2=\frac{1}{2V}\sum_{\substack{\mathbf{k},\mathbf{k}',\mathbf{q}\\ \sigma,\sigma'}}\tilde{V}_2(\mathbf{q})\ a^\dagger_{\mathbf{k},\sigma}a^\dagger_{\mathbf{k}',\sigma'}a_{\mathbf{k}'+\mathbf{q},\sigma'}a_{\mathbf{k}-\mathbf{q},\sigma}\ . \quad (1.80)$$

It can be viewed as a scattering process, where two particles with initial momenta $\hbar\mathbf{k}$ and $\hbar\mathbf{k}'$ interact and go out with final momenta $\hbar(\mathbf{k}-\mathbf{q})$ and $\hbar(\mathbf{k}'+\mathbf{q})$ as illustrated in Fig. 2. Thereby the total momentum is conserved.

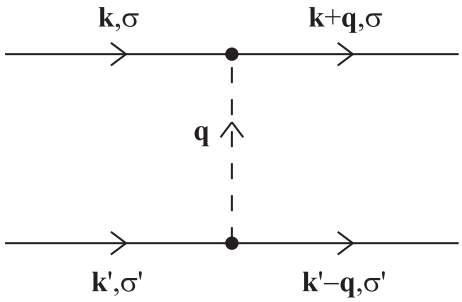

Figure 2: Diagram illustrating the two-particle interaction.

For an arbitrary single-particle basis $\{|\phi_n\rangle\}$ a two-body operator is written as

$$V_2 = \frac{1}{2} \sum_{m,m',n,n'} V_{m,m';n,n'}\ a_m^\dagger a_{m'}^\dagger a_{n'} a_n, \tag{1.81}$$

where $V_{m,m';n,n'} := \langle m, m'|V_2|n, n'\rangle$ is the matrix element between two-particle states $|m, m'\rangle = |\phi_m\rangle \otimes |\phi_{m'}\rangle$ and $|n, n'\rangle = |\phi_n\rangle \otimes |\phi_{n'}\rangle$. Note that the order of the last two operators in Eq. (1.81) is reversed relative to the order of indices in the matrix elements.

1.6 Wick's theorem

The solution of a typical problem in many-body theory often requires the calculation of expectation values of operator products with respect to the vacuum state $|0\rangle$. This step is greatly facilitated by Wick's theorem. Before formulating the theorem we introduce two definitions. Let each of the operators $A_1, A_2, ..., A_n$ be either a creation or annihilation operator. The *normal-ordered* product (already mentioned previously) $: A_1 A_2 ... A_n :$ is the product reordered in such a way that all creation operators are to the left and all annihilation operators to the right, multiplied in the case of fermions by the sign of the permutation needed to produce the normal order. Thus

$$: a_1 a_2^\dagger : \ = \ \begin{cases} a_2^\dagger a_1 & \text{for bosons,} \\ -a_2^\dagger a_1 & \text{for fermions} \end{cases} \tag{1.82}$$

$$: a_1^\dagger a_2 a_3^\dagger a_4 : \ = \ a_1^\dagger a_3^\dagger a_4 a_2. \tag{1.83}$$

The *contraction* $\langle A_1 A_2\rangle$ of a pair of operators is the vacuum expectation value,

$$\langle A_1 A_2\rangle := \langle 0|A_1 A_2|0\rangle\ . \tag{1.84}$$

The following contraction is non-zero,

$$\langle a_m a_m^\dagger\rangle = 1 = [a_m, a_m^\dagger]_\pm, \tag{1.85}$$

where the upper sign (the anticommutator) applies to fermions, while the lower sign (the commutator) is for bosons. All other contractions vanish,

$$\begin{aligned} \langle a_m a_{m'}\rangle = \langle a_m^\dagger a_{m'}^\dagger\rangle = \langle a_m^\dagger a_{m'}\rangle &= 0 \text{ for arbitrary } m, m', \\ \langle a_m a_{m'}^\dagger\rangle &= 0 \text{ for } m \neq m'. \end{aligned} \tag{1.86}$$

We can now state *Wick's theorem*:

An ordinary product of any finite number of creation and annihilation operators is equal to the sum of normal products from which 0,1,2,... contractions have been removed in all possible ways.

For $n = 2$ this means:

$$A_1 A_2 = : A_1 A_2 : + \langle A_1 A_2 \rangle . \tag{1.87}$$

This is clearly true if both operators are creation operators or if both are annihilation operators. It also applies if A_1 is a creation operator and A_2 an annihilation operator. In the remaining case where $A_1 = a_1$ and $A_2 = a_2^\dagger$ we can write the product as

$$a_1 a_2^\dagger = \mp a_2^\dagger a_1 + [a_1, a_2^\dagger]_\pm . \tag{1.88}$$

In view of Eqs. (1.82) and (1.85) this is identical to Eq. (1.87). Wick's theorem is therefore proven for $n = 2$. For $n = 4$ it asserts

$$\begin{aligned} A_1 A_2 A_3 A_4 &= : A_1 A_2 A_3 A_4 : \\ &+ : A_1 A_2 : \langle A_3 A_4 \rangle \mp : A_1 A_3 : \langle A_2 A_4 \rangle + : A_2 A_3 : \langle A_1 A_4 \rangle \\ &+ : A_1 A_4 : \langle A_2 A_3 \rangle \mp : A_2 A_4 : \langle A_1 A_3 \rangle + : A_3 A_4 : \langle A_1 A_2 \rangle \\ &+ \langle A_1 A_2 \rangle \langle A_3 A_4 \rangle \mp \langle A_1 A_3 \rangle \langle A_2 A_4 \rangle + \langle A_1 A_4 \rangle \langle A_2 A_3 \rangle , \end{aligned} \tag{1.89}$$

where the upper sign refers to fermions, the lower to bosons.

The following relation is very useful for proving Wick's theorem:

$$\begin{aligned} : A_1 \cdots A_n : B &= \sum_{m=1}^{n} (\mp)^s \langle A_m B \rangle : A_1 A_2 \cdots A_{m-1} A_{m+1} \cdots A_n : \\ &+ : A_1 \cdots A_n B : , \end{aligned} \tag{1.90}$$

where s counts the number of pairwise permutations that are necessary to realize the indicated sequence of operators. This relation is trivially fulfilled if B is an annihilation operator. If B is a creation operator, the contraction $\langle A_m B \rangle$ vanishes if A_m is also a creation operator, and therefore we can limit ourselves to the case where all A_i, $i = 1 \ldots n$, are annihilation operators, *i.e.* we have to prove the relation

$$\begin{aligned} A_1 \cdots A_n B &= \sum_{m=1}^{n} (\mp)^s \langle A_m B \rangle A_1 A_2 \cdots A_{m-1} A_{m+1} \cdots A_n \\ &+ (\mp 1)^n B A_1 \cdots A_n . \end{aligned} \tag{1.91}$$

We do this by induction. For $n = 1$ the relation simply corresponds to Eq. (1.87) with $A_2 = B$. Suppose now Eq. (1.91) is proven for a certain n. Multiplying from the left by the annihilation operator A_0 and using Eq. (1.87) for $A_0 B$ we get

$$\begin{aligned} A_0 A_1 \cdots A_n B &= \sum_{m=1}^{n} (\mp 1)^s \langle A_m B \rangle A_0 A_1 \cdots A_{m-1} A_{m+1} \cdots A_n \\ &+ (\mp 1)^n (\langle A_0 B \rangle \mp B A_0) A_1 \cdots A_n . \end{aligned} \tag{1.92}$$

This expression can readily be casted into the form (1.91) with n replaced by $n+1$. Therefore the relation (1.90) is proven.

To prove Wick's theorem, we again proceed by induction. We have already verified the theorem for $n = 2$. We assume it to be true for a certain n, *i.e.*

$$\begin{aligned} A_1 A_2 \cdots A_n &= :A_1 A_2 \cdots A_n: \\ &+ \sum_{1 \le m_1 < m_2 \le n} (\mp)^s \langle A_{m_1} A_{m_2} \rangle : A_1 \cdots A_{m_1 - 1} A_{m_1 + 1} \cdots A_{m_2 - 1} A_{m_2 + 1} \cdots A_n : \\ &+ \ \ldots \ . \end{aligned} \tag{1.93}$$

Multiplying from the right by A_{n+1} and applying the relation (1.90) to the first term, we have

$$\begin{aligned} :A_1 \cdots A_n : A_{n+1} &= \sum_{m=1}^{n} (\mp)^s \langle A_m A_{n+1} \rangle : A_1 A_2 \cdots A_{m-1} A_{m+1} \cdots A_n : \\ &+ \ :A_1 \cdots A_n A_{n+1}: \ . \end{aligned} \tag{1.94}$$

Doing the same for the second term, we arrive at

$$\begin{aligned} &\sum_{1 \le m_1 < m_2 \le n} (\mp)^s \langle A_{m_1} A_{m_2} \rangle : A_1 \cdots A_{m_1 - 1} A_{m_1 + 1} \cdots A_{m_2 - 1} A_{m_2 + 1} \cdots A_n : A_{n+1} \\ &= \sum_{1 \le m_1 < m_2 \le n} (\mp)^s \langle A_{m_1} A_{m_2} \rangle : A_1 \cdots A_{m_1 - 1} A_{m_1 + 1} \cdots A_{m_2 - 1} A_{m_2 + 1} \cdots A_n A_{n+1} : \\ &+ \sum_{\substack{1 \le m_1 < m_2 \le n \\ m \ne m_1, m_2}} (\mp)^s \langle A_{m_1} A_{m_2} \rangle \langle A_m A_{n+1} \rangle : A_1 \cdots \ \cdots A_n : , \end{aligned} \tag{1.95}$$

where in the last normal-ordered product the operators $A_{m_1},\ A_{m_2},\ A_m,\ A_{n+1}$ are omitted. We see that in this way we reproduce the first two terms in the Wick decomposition of $A_1 A_2 \cdots A_{n+1}$. Continuing in the same way one generates the full decomposition. This completes the proof of Wick's theorem.

We consider as a simple application the vacuum expectation value of an arbitrary product of operators $A_1 A_2 \cdots A_n$. The expectation value of any normal-ordered product with respect to the vacuum state $|0\rangle$ vanishes. Therefore the only contribution comes from the fully contracted terms,

$$\langle 0 | A_1 A_2 \cdots A_n | 0 \rangle = \sum_{\substack{m_1 < m_2 \\ n_1 < n_2 \\ \cdots \\ r_1 < r_2 \\ m_1 < n_1 < \cdots < r_1}} (\mp 1)^s \langle A_{m_1} A_{m_2} \rangle \langle A_{n_1} A_{n_2} \rangle \cdots \langle A_{r_1} A_{r_2} \rangle \ . \tag{1.96}$$

This expression is non-zero only if half of the operators A_i are creation operators and the other half annihilation operators.

2 Many-boson systems

In 1938 superfluidity was discovered by Peter Kapitza in liquid ^{4}He below 2.18K. Soon after these experiments, Bose-Einstein condensation was advocated for explaining the transition to the superfluid phase. For several decades superfluid helium represented the canonical many-boson system. Unfortunately, helium atoms interact strongly and therefore a completely satisfactory microscopic theory, especially concerning the connection between superfluidity and Bose-Einstein condensation, is still missing. Thus it came as a relief when with the trapping of atomic gases at ultralow temperatures a new system became available where the interaction effects are much smaller. In 1995 bosonic alkali atoms were found to show Bose-Einstein condensation around $1\mu K$. Subsequently the field of trapped atomic gases has become extremely active and many new results are still expected to come. For instance, in a similar way as in helium where the fermionic counterpart ^{3}He has first to pair up before becoming superfluid (below 3mK, as observed first in 1972), fermionic gases also have first to bind as composite bosons before they can make a transition to a superfluid state (evidence for such a transition has been provided in 2006 in gases of ^{6}Li isotopes at about 100nK).

2.1 Bose-Einstein condensation in a trap

In an ideal Bose gas with N particles in a cubic box of volume $V = L^3$ the one-particle states have energies $\epsilon_{\mathbf{k}} = \frac{\hbar^2|\mathbf{k}|^2}{2m}$. Quantum effects of Bose statistics are important when the thermal de Broglie wavelength $\Lambda_T = (2\pi\hbar^2/mk_BT)^{\frac{1}{2}}$, *i.e.* the typical wavelength of an atom in an ideal gas at temperature T, is larger than the interparticle distance $n^{-\frac{1}{3}}$, where $n = N/V$. The condition $\Lambda_T \approx n^{-\frac{1}{3}}$ gives an estimate of the critical temperature for Bose-Einstein condensation, in good agreement with the exact result (obtained in the thermodynamic limit)

$$T_c = 3.313\frac{\hbar^2}{k_B m}n^{\frac{2}{3}}. \tag{2.1}$$

For ^{4}He with $m \approx 6.646 \times 10^{-24}$g and $n \approx 2.186 \times 10^{22}$cm^{-3} this formula predicts $T_c \approx 3.13K$, in surprisingly good agreement with the so-called λ-temperature where superfluidity sets in. For $T < T_c$ the uniform ideal Bose gas has a macroscopic number of particles occupying the lowest one-particle energy-level $\epsilon_{\mathbf{k}=0}$, and for $T \to 0$ all particles condense into the state with $\mathbf{k} = 0$.

In the recent experiments with atomic gases an external potential is used to confine the atoms, and as a consequence the Bose gas has a non-uniform density. We have to deal with an inhomogeneous system with typically 10^4 to 10^7 atoms. We consider a harmonic external potential for the trap,

$$V_{tr}(\mathbf{r}) = \frac{1}{2}m\omega_0^2|\mathbf{r}|^2. \tag{2.2}$$

In this potential an atom of mass m has a Gaussian ground state

$$\psi_0(\mathbf{r}) = \frac{1}{\pi^{\frac{3}{4}}d_0^{\frac{3}{2}}}\exp\left(-\frac{1}{2}\frac{|\mathbf{r}|^2}{d_o^2}\right), \quad d_0 = \left(\frac{\hbar}{m\omega_0}\right)^{\frac{1}{2}}. \tag{2.3}$$

In the absence of interactions the ground state of N atoms in the trap is obtained by putting all particles into this state (we consider spin zero particles),

$$|\Psi_0\rangle = \frac{\left(a_0^\dagger\right)^N}{\sqrt{N!}}|0\rangle \tag{2.4}$$

and in coordinate representation we have the normalized, totally symmetric N-particle wave function

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) = \psi_0(\mathbf{r}_1)\psi_0(\mathbf{r}_2)\cdots\psi_0(\mathbf{r}_N). \tag{2.5}$$

The density profile of the condensate in the ground state is given by

$$\begin{aligned}&\int d\mathbf{r}_1 \ldots \int d\mathbf{r}_N \left(\sum_{i=1}^{N}\delta(\mathbf{r}-\mathbf{r}_i)\right)|\psi_0(\mathbf{r}_1)\psi_0(\mathbf{r}_2)\cdots\psi_0(\mathbf{r}_N)|^2 \\ &= N|\psi_0(\mathbf{r})|^2 = \frac{N}{\pi^{\frac{3}{2}}d_0^3}\exp\left(-\frac{|\mathbf{r}|^2}{d_0^2}\right).\end{aligned} \tag{2.6}$$

This defines an effective volume d_0^3 for the condensate at $T = 0$. The velocity distribution of the condensate can be found from the Fourier transform

$$\tilde{\psi}_0(\mathbf{k}) \sim \exp\left(-\frac{d_0^2}{2}|\mathbf{k}|^2\right) \tag{2.7}$$

and is of the form $N\exp(-d_0^2k^2)$. For anisotropic traps one has anisotropic profiles for the density and velocity distributions. In actual experiments, spherical, cigar shaped and disk shaped condensates have been realized. Both the density profile and the velocity profile have been observed. They depend strongly on temperature. A clear experimental signature of the transition to a condensed state is an abrupt change of the velocity distribution at a well defined temperature T_c. Above T_c, we have an isotropic rather broad Maxwellian distribution of width $\sqrt{mk_BT}/\hbar$. Below T_c, a sharp peak develops and has a width of the order of $1/d_0$.

In order to estimate T_c we take a typical set-up with $N = 10^6$ sodium atoms and a condensate size of $d_0 = 10^{-3}$ cm, *i.e.* a density $n \approx Nd_0^{-3} \approx 10^{15}\text{cm}^{-3}$. With a mass $m \approx 3.8\times10^{-23}$ g for sodium, Eq. (2.1) yields a critical temperature $T_c \approx 7\mu K$, as typically observed for such parameter values.

2.2 The weakly interacting Bose gas

The interactions in atomic gases are usually very weak, but nevertheless they can have important effects. For instance superfluidity does not occur in an ideal Bose gas, but it exists in the weakly interacting Bose system. To simplify the analysis we consider a homogeneous case, *i.e.* N spinless bosons in a cubic volume $V = L^3$, in the absence of an external potential, and we assume periodic boundary conditions. With respect to the plane-wave basis the Hamiltonian reads

$$H = \sum_{\mathbf{k}}\varepsilon_{\mathbf{k}}a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \frac{1}{2V}\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}}\tilde{V}(\mathbf{q})a_{\mathbf{k}}^\dagger a_{\mathbf{k}'}^\dagger a_{\mathbf{k}'+\mathbf{q}}a_{\mathbf{k}-\mathbf{q}}, \tag{2.8}$$

where

$$\varepsilon_{\mathbf{k}} = \frac{(\hbar|\mathbf{k}|)^2}{2m}. \tag{2.9}$$

For neutral atoms we can assume the two-body potential to be short-ranged and repulsive. For a dilute system most of the particles occupy the zero-momentum state at zero temperature and only collisions with small momentum transfer are important. In this case we can replace $\tilde{V}(\mathbf{q})$ by $g := \tilde{V}(0)$. In the absence of interactions only the $\mathbf{k} = 0$ single-particle state would be occupied, *i.e.* $n_{\mathbf{k}} = 0$ for $\mathbf{k} \neq 0$ and $n_0 = N$. For weak interactions we expect this to remain approximately true and $|N - n_0| \ll N$. This implies that the commutator $[a_0, a_0^\dagger] = 1$ can be neglected as compared to $a_0^\dagger a_0 = n_0$. Therefore we approximate the operators $a_0, a_0^\dagger$ as numbers,

$$a_0 \approx a_0^\dagger \approx \sqrt{n_0} \tag{2.10}$$

and keep only the interaction terms of highest order in n_0,

$$H \approx \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \frac{g}{2V}\left\{ n_0^2 + n_0 \sum_{\mathbf{k}\neq 0} \left(4a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + a_{-\mathbf{k}} a_{\mathbf{k}} + a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger \right) \right\}. \tag{2.11}$$

Using the same argument we may replace n_0^2 by

$$[N - (N - n_0)]^2 \approx N^2 - 2N(N - n_0) = N^2 - 2N \sum_{\mathbf{k}\neq \mathbf{0}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \tag{2.12}$$

as well as n_0 by N in the terms that are linear in n_0. Therefore we get

$$H \approx N\frac{ng}{2} + \sum_{\mathbf{k}\neq 0} \left\{ (\varepsilon_{\mathbf{k}} + ng) a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \frac{ng}{2}(a_{-\mathbf{k}} a_{\mathbf{k}} + a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger) \right\}, \tag{2.13}$$

where $n = N/V$ is the particle density. This is a quadratic form in the operators $a_{\mathbf{k}}, a_{\mathbf{k}}^\dagger$ and can be diagonalized by a so-called Bogoliubov transformation

$$\alpha_{\mathbf{k}} = u_{\mathbf{k}} a_{\mathbf{k}} - v_{\mathbf{k}} a_{-\mathbf{k}}^\dagger, \tag{2.14}$$

where $u_{\mathbf{k}}, v_{\mathbf{k}}$ are real coefficients. This transformation is canonical if the new operators satisfy the commutation relations

$$\begin{aligned} [\alpha_{\mathbf{k}}, \alpha_{\mathbf{k}'}] &= \left[\alpha_{\mathbf{k}}^\dagger, \alpha_{\mathbf{k}'}^\dagger\right] = 0, \\ \left[\alpha_{\mathbf{k}}, \alpha_{\mathbf{k}'}^\dagger\right] &= \delta_{\mathbf{k},\mathbf{k}'}. \end{aligned} \tag{2.15}$$

This is achieved if the coefficients satisfy the relation

$$u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2 = 1. \tag{2.16}$$

With the choice $u_{\mathbf{k}} = u_{-\mathbf{k}},\ v_{\mathbf{k}} = v_{-\mathbf{k}}$ we have

$$\alpha_{-\mathbf{k}}^\dagger = u_{\mathbf{k}} a_{-\mathbf{k}}^\dagger - v_{\mathbf{k}} a_{\mathbf{k}}, \tag{2.17}$$

which together with Eq. (2.14) yields the inverse transformation

$$a_{\mathbf{k}} = u_{\mathbf{k}} \alpha_{\mathbf{k}} + v_{\mathbf{k}} \alpha_{-\mathbf{k}}^\dagger. \tag{2.18}$$

We insert now this transformation into the Hamiltonian (2.13) and find

$$\begin{aligned} H &\approx N\frac{ng}{2} + \sum_{\mathbf{k}\neq 0}\left[(\varepsilon_{\mathbf{k}}+ng)v_{\mathbf{k}}^2 + ngu_{\mathbf{k}}v_{\mathbf{k}}\right] \\ &+ \sum_{\mathbf{k}\neq 0}\left[(\varepsilon_{\mathbf{k}}+ng)(u_{\mathbf{k}}^2+v_{\mathbf{k}}^2) + 2ngu_{\mathbf{k}}v_{\mathbf{k}}\right]\alpha_{\mathbf{k}}^\dagger\alpha_{\mathbf{k}} \\ &+ \sum_{\mathbf{k}\neq 0}\left[(\varepsilon_{\mathbf{k}}+ng)u_{\mathbf{k}}v_{\mathbf{k}} + \frac{ng}{2}(u_{\mathbf{k}}^2+v_{\mathbf{k}}^2)\right]\left(\alpha_{-\mathbf{k}}\alpha_{\mathbf{k}} + \alpha_{\mathbf{k}}^\dagger\alpha_{-\mathbf{k}}^\dagger\right). \end{aligned} \tag{2.19}$$

This expression can be brought into the form of an uncoupled collection of bosons if the last term vanishes. This can be achieved by choosing the coefficients such that

$$(\varepsilon_{\mathbf{k}}+ng)u_{\mathbf{k}}v_{\mathbf{k}} + \frac{ng}{2}(u_{\mathbf{k}}^2+v_{\mathbf{k}}^2) = 0. \tag{2.20}$$

The solution is

$$\begin{aligned} u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 &= \frac{\varepsilon_{\mathbf{k}}+ng}{E_{\mathbf{k}}} \\ 2u_{\mathbf{k}}v_{\mathbf{k}} &= -\frac{ng}{E_{\mathbf{k}}}, \end{aligned} \tag{2.21}$$

where

$$E_{\mathbf{k}} = \sqrt{\varepsilon_{\mathbf{k}}(\varepsilon_{\mathbf{k}}+2ng)}. \tag{2.22}$$

The final form of the Hamiltonian is

$$H \approx E_0 + \sum_{\mathbf{k}\neq 0} E_{\mathbf{k}}\alpha_{\mathbf{k}}^\dagger\alpha_{\mathbf{k}}, \tag{2.23}$$

where the zero-point energy E_0 is given by

$$E_0 = N\frac{ng}{2} + \frac{1}{2}\sum_{\mathbf{k}\neq 0}(E_{\mathbf{k}} - \varepsilon_{\mathbf{k}} - ng). \tag{2.24}$$

In the long-wavelength limit the spectrum is that of a sound wave,

$$E_{\mathbf{k}} \sim \hbar s|\mathbf{k}| \quad \text{for} \quad |\mathbf{k}| \to 0, \quad s = \sqrt{\frac{ng}{m}}, \tag{2.25}$$

as actually observed in superfluid helium. This linear relation can also be derived within the so-called two-fluid hydrodynamics. It plays a crucial role in Landau's argument for superfluidity, which should be distinguished from Bose-Einstein condensation.

The number of particles in the condensate at zero temperature is given by the equation

$$n_0 = N - \sum_{\mathbf{k}\neq 0}\langle\Psi_0|a_{\mathbf{k}}^\dagger a_{\mathbf{k}}|\Psi_0\rangle, \tag{2.26}$$

where the ground state $|\Psi_0\rangle$ is defined by $\alpha_{\mathbf{k}}|\Psi_0\rangle = 0$. It is the vacuum of quasi-particles. The momentum distribution function for $\mathbf{k} \neq 0$ is then easily obtained using Eqs. (2.16),(2.18) and (2.21),

$$\langle\Psi_0|a_{\mathbf{k}}^\dagger a_{\mathbf{k}}|\Psi_0\rangle = v_{\mathbf{k}}^2 = \frac{1}{2}\left(\frac{\varepsilon_{\mathbf{k}}+ng}{E_{\mathbf{k}}} - 1\right). \tag{2.27}$$

Replacing the sum over $\mathbf{k}$ by an integral in the usual way and introducing the integration variable $\varepsilon = (\hbar^2 k^2)/(2m)$, we get

$$\begin{aligned}\sum_{\mathbf{k}\neq 0}\langle\Psi_0|a_{\mathbf{k}}^\dagger a_{\mathbf{k}}|\Psi_0\rangle &= \frac{V}{2(2\pi)^3}\int d^3k\ \left(\frac{\varepsilon_{\mathbf{k}}+ng}{E_{\mathbf{k}}}-1\right)\\ &= \frac{V}{4\pi^2}\sqrt{2}\left(\frac{m}{\hbar^2}\right)^{3/2}\int_0^\infty d\varepsilon\ \left(\frac{\varepsilon+ng}{\sqrt{\varepsilon+2ng}}-\sqrt{\varepsilon}\right)\\ &= \frac{V}{4\pi^2}\sqrt{2}\left(\frac{m}{\hbar^2}\right)^{3/2}\frac{1}{3}(2ng)^{3/2}\ . \end{aligned} \tag{2.28}$$

For our contact potential $V(\mathbf{r}) = g\delta(\mathbf{r})$ the total scattering cross section for the elastic collision between two particles in Born approximation is given by

$$\sigma = 4\pi\left(\frac{mg}{4\pi\hbar^2}\right)^2\ . \tag{2.29}$$

Identifying this expression with $\sigma = 4\pi a^2$, where a is the scattering length, we get

$$\frac{mg}{4\pi\hbar^2} = a\ . \tag{2.30}$$

Inserting this relation into Eq. (2.28), we obtain a very simple result for the number of particles in the condensate, Eq. (2.26),

$$n_0 = N\left(1-\frac{8}{3\sqrt{\pi}}(na^3)^{1/2}\right)\ . \tag{2.31}$$

This shows that the interaction between the bosons reduces the condensate fraction in the ground state, as compared to the ideal gas. Consistency with the initial assumption ($n_0 \approx N$) requires $na^3 \ll 1$, *i.e.* the system has to be both dilute (small density n) and weakly interacting (small coupling constant g).

2.3 The Gross-Pitaevskii equation

For a system of cold bosonic atoms in a trap one has to take into account both the trap potential (2.2) and the two-particle interaction $V(\mathbf{r})$, which we take as a contact potential

$$V(\mathbf{r}) = g\delta(\mathbf{r})\ , \tag{2.32}$$

corresponding to $\tilde{V}(\mathbf{q}) = g$, as in the previous section. In second quantization the Hamiltonian for spinless bosons takes the form

$$H = \int d\mathbf{r}\ \left\{\Psi^\dagger(\mathbf{r})\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{tr}(\mathbf{r})\right)\Psi(\mathbf{r}) + \frac{g}{2}\left(\Psi^\dagger(\mathbf{r})\right)^2\left(\Psi(\mathbf{r})\right)^2\right\}\ . \tag{2.33}$$

The field operators for bosons satisfy the commutation relations (1.25). For the homogeneous case, treated in the previous section ($V_{tr} = 0$), Bogoliubov's prescription corresponds to the decomposition

$$\Psi(\mathbf{r}) = \sqrt{\frac{n_0}{V}} + \underbrace{\frac{1}{\sqrt{V}}\sum_{\mathbf{k}\neq 0} e^{i\mathbf{k}\cdot\mathbf{r}}a_{\mathbf{k}}}_{\chi(\mathbf{r})} \tag{2.34}$$

into a "classical contribution" $\sqrt{n_0/V}$ and a quantum part $\chi(\mathbf{r})$ which is a field operator. The field $\chi(\mathbf{r})$ is small in the sense that

$$\int d\mathbf{r}\, \chi^\dagger(\mathbf{r})\chi(\mathbf{r}) = N - n_0 \ll N \ . \tag{2.35}$$

For the inhomogeneous case one generalizes Bogoliubov's prescription as

$$\Psi(\mathbf{r}) = \Phi(\mathbf{r}) + \chi(\mathbf{r}) \ , \tag{2.36}$$

where $\Phi(\mathbf{r})$ is a classical field and $\chi(\mathbf{r})$ is a quantum field. The classical field is interpreted as the macroscopic wave function of the condensate, $|\Phi(\mathbf{r})|^2$ being its density profile. The quantum part $\chi(\mathbf{r})$ is treated as a perturbation of the classical part. We limit ourselves on the ground state in mean-field approximation, where the energy is just that of the condensate. Replacing $\Psi(\mathbf{r})$ in the Hamiltonian (2.33) by the classical field $\Phi(\mathbf{r})$, we obtain the Gross-Pitaevskii functional

$$E[\Phi] = \int d^3r \ \left\{ \Phi^*(\mathbf{r}) \left(-\frac{\hbar^2}{2m}\nabla^2 + V_{tr}(\mathbf{r}) \right) \Phi(\mathbf{r}) + \frac{g}{2}|\Phi(\mathbf{r})|^4 \right\} \ . \tag{2.37}$$

The macroscopic wave function of the condensate is adjusted such as to minimize this energy functional under the constraint

$$\int d^3r \ \Phi^*(\mathbf{r})\Phi(\mathbf{r}) = N \ . \tag{2.38}$$

Thus we introduce the chemical potential μ and search for a field $\Phi(\mathbf{r})$ satisfying the relation

$$\frac{\delta}{\delta\Phi^*(\mathbf{r})} \left\{ E[\Phi] - \mu \int d^3r \ \Phi^*(\mathbf{r})\Phi(\mathbf{r}) \right\} = 0 \ . \tag{2.39}$$

This yields the (time-independent) Gross-Pitaevskii equation

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{tr}(\mathbf{r}) - \mu \right) \Phi(\mathbf{r}) + g|\Phi(\mathbf{r})|^2\Phi(\mathbf{r}) = 0 \ . \tag{2.40}$$

Its solution gives both the wave function $\Phi(\mathbf{r})$ and the density profile $|\Phi(\mathbf{r})|^2$ of the condensate.

The theory is readily extended to take into account quantum fluctuations to lowest order, in a similar way as we did in the case of the homogeneous system. This yields, on the one hand, a quantum correction to the ground state energy. On the other hand, one also obtains equations for the energy eigenvalues and eigenfunctions of elementary excitations, which depend both on the trap potential $V_{tr}(\mathbf{r})$ and on the condensate density $|\Phi(\mathbf{r})|^2$.

An alternative route to obtain an approximate wave function for the ground state uses Eq. (2.5) as a variational ansatz, *i.e.* we write the trial ground state as

$$\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N) = \prod_{i=1}^{N} \ \varphi(\mathbf{r}_i) \tag{2.41}$$

without *a priori* specifying the single-particle wave function, except that it has to be normalized,

$$\int_V d^3r \; |\varphi(\mathbf{r})|^2 = 1 \; . \tag{2.42}$$

The expectation value of the Hamiltonian (2.33) is

$$\begin{aligned} E[\varphi] &= N \int d^3r \; \varphi^*(\mathbf{r}) \left(-\frac{\hbar^2}{2m}\nabla^2 + V_{tr}(\mathbf{r}) \right) \varphi(\mathbf{r}) \\ &+ \frac{N(N-1)}{2} g \int d^3r \; |\varphi(\mathbf{r})|^4 \; . \end{aligned} \tag{2.43}$$

In the thermodynamic limit ($N \to \infty$, $V \to \infty$, $n = N/V = \text{constant}$) Eqs. (2.43) and (2.42) are the same as Eqs. (2.37) and (2.38) if we make the identification

$$\Phi(\mathbf{r}) = \sqrt{N} \; \varphi(\mathbf{r}) \; . \tag{2.44}$$

Applying the variational principle using the ansatz (2.41) therefore leads again to the Gross-Pitaevskii equation (2.40).

Literature

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3 Many-electron systems

A wealth of phenomena in solids results from an interplay between (Fermi) statistics and electron-electron interactions. Superconductivity, magnetic order, the (Mott) metal-insulator transition, charge- and spin-density waves or the fractional quantum Hall effect are prominent examples. But also the physics of nuclei or of neutron stars can only be understood as (strongly) interacting many-fermion systems. In this short chapter we can get at most a glimpse of this still rapidly evolving field.

3.1 The jellium model

Electric charge has a natural tendency of spreading in such a way that the system is both neutral and homogeneous. Consider a (classical) charge density $\rho(\mathbf{r})$ with Coulomb energy

$$E = \frac{1}{2}\int_V d^3r \int_V d^3r' \; \rho(\mathbf{r}) \frac{1}{4\pi\varepsilon_0|\mathbf{r}-\mathbf{r}'|}\rho(\mathbf{r}'). \tag{3.1}$$

or, in Fourier space,

$$E = \frac{1}{2V}\sum_{\mathbf{q}} \frac{1}{\varepsilon_0|\mathbf{q}|^2}|\tilde{\rho}(\mathbf{q}|^2. \tag{3.2}$$

Clearly this energy is a minimum if $\tilde{\rho}(\mathbf{q})$ vanishes, i.e. if the system is both neutral ($\tilde{\rho}(0) = 0$) and homogeneous ($\tilde{\rho}(\mathbf{q}) = 0$ for $\mathbf{q} \neq 0$). In an actual solid, consisting of positively charged ions and negatively charged (delocalized) electrons, charge neutrality is achieved if ions and electrons are equal in number, whereas homogeneity is reached on a length scale exceeding the distance between ions. The specific nature and geometric arrangement of ions gives rise to complicated electronic energy bands, which is the cause for the electronic diversity of the different materials. In the jellium model these complications are avoided by smearing out uniformly the ionic charge. The Coulomb energy is therefore given by

$$E = \frac{1}{2}\int d^3r \int d^3r' \; n(\mathbf{r})V(\mathbf{r}-\mathbf{r}')n(\mathbf{r}'), \tag{3.3}$$

where

$$V(\mathbf{r}) = \frac{e^2}{4\pi\varepsilon_0|\mathbf{r}|} \tag{3.4}$$

and $n(\mathbf{r}) = n_e(\mathbf{r}) - n_i$ is the difference between the electronic density $n_e(\mathbf{r})$ and the ionic density n_i. The Fourier transform of $n(\mathbf{r})$ is given by

$$\tilde{n}(\mathbf{q}) = \int_V d^3r \; e^{-i\mathbf{q}\cdot\mathbf{r}} \, (n_e(\mathbf{r}) - n_i) = \begin{cases} \tilde{n}_e(\mathbf{q}), & \mathbf{q} \neq 0, \\ N_e - n_i V, & \mathbf{q} = 0. \end{cases} \tag{3.5}$$

For a neutral system ($N_e = n_i V$) the Coulomb energy can therefore be written as

$$E = \frac{1}{2V}\sum_{\mathbf{q}\neq\mathbf{0}} \tilde{V}(\mathbf{q})|\tilde{n}_e(\mathbf{q})|^2 \tag{3.6}$$

with $\tilde{V}(\mathbf{q}) = e^2/(\varepsilon_0|\mathbf{q}|^2)$. In second quantization the electronic Hamiltonian is then given by

$$H = \sum_{\mathbf{k},\sigma} \frac{|\hbar\mathbf{k}|^2}{2m} a^\dagger_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma} + \frac{1}{2V} \sum_{\sigma,\sigma'} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}\neq\mathbf{0}} \tilde{V}(\mathbf{q})\ a^\dagger_{\mathbf{k},\sigma} a^\dagger_{\mathbf{k}',\sigma'} a_{\mathbf{k}'+\mathbf{q},\sigma'} a_{\mathbf{k}-\mathbf{q},\sigma}\ . \tag{3.7}$$

3.2 Hartree-Fock approximation

Despite the rather drastic simplification of the jellium model it is hopeless to try to find the eigenstates of the Hamiltonian (3.7) without further approximations. A very widely used method consists in replacing the many-body Hamiltonian by an effective single-particle Hamiltonian. This is the Hartree-Fock approximation. It is based on the idea that each electron moves in a mean-field produced both by the external potential and by the interaction with all the other electrons. The effective potential is determined in such a way that the expectation value of the full many-body Hamiltonian with respect to the ground state of the effective single-particle Hamiltonian (a single Slater determinant in coordinate representation) is a minimum. For the jellium model, where the external potential (due to the ions) has been eliminated, we can hope that an ansatz without an effective single-particle potential will be acceptable, i.e. the Hartree-Fock ground state is simply the filled Fermi sea,

$$|\Psi_0\rangle = \prod_{\substack{\mathbf{k},|\mathbf{k}|<k_F \\ \sigma=\uparrow,\downarrow}} a^\dagger_{\mathbf{k}\sigma}|0\rangle. \tag{3.8}$$

The expectation value of the kinetic part of the Hamiltonian is readily obtained,

$$\sum_{\mathbf{k},\sigma} \frac{|\hbar\mathbf{k}|^2}{2m} \langle\Psi_0|a^\dagger_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma}|\Psi_0\rangle = \sum_{\substack{\mathbf{k},|\mathbf{k}|<k_F \\ \sigma=\uparrow,\downarrow}} \frac{|\hbar\mathbf{k}|^2}{2m}. \tag{3.9}$$

The expectation value of the interaction term can be calculated by adapting Wick's theorem to the present case,

$$\begin{aligned}
&\langle\Psi_0|\ a^\dagger_{\mathbf{k},\sigma} a^\dagger_{\mathbf{k}',\sigma'} a_{\mathbf{k}'+\mathbf{q},\sigma'} a_{\mathbf{k}-\mathbf{q},\sigma}|\Psi_0\rangle \\
&\quad = \langle\Psi_0|\ a^\dagger_{\mathbf{k},\sigma} a_{\mathbf{k}-\mathbf{q},\sigma}|\Psi_0\rangle \langle\Psi_0|a^\dagger_{\mathbf{k}',\sigma'} a_{\mathbf{k}'+\mathbf{q},\sigma'}|\Psi_0\rangle \\
&\quad -\langle\Psi_0|\ a^\dagger_{\mathbf{k},\sigma} a_{\mathbf{k}'+\mathbf{q},\sigma'}|\Psi_0\rangle \langle\Psi_0|a^\dagger_{\mathbf{k}',\sigma'} a_{\mathbf{k}-\mathbf{q},\sigma}|\Psi_0\rangle \\
&\quad = n_{\mathbf{k},\sigma} n_{\mathbf{k}',\sigma'} \delta_{\mathbf{q},0} - n_{\mathbf{k},\sigma} n_{\mathbf{k}',\sigma'} \delta_{\mathbf{k}',\mathbf{k}-\mathbf{q}} \delta_{\sigma,\sigma'},
\end{aligned} \tag{3.10}$$

where

$$n_{\mathbf{k},\sigma} = \langle\Psi_0|\ a^\dagger_{\mathbf{k},\sigma} a_{\mathbf{k},\sigma}|\Psi_0\rangle = \begin{cases} 1, & k < k_F, \\ 0, & k > k_F. \end{cases} \tag{3.11}$$

The first term in (3.10), the so-called Hartree term, does not contribute to the potential energy and therefore the only contribution is the so-called Fock or exchange term. The expectation value of the Hamiltonian is therefore

$$E = 2 \sum_{\mathbf{k},|\mathbf{k}|<k_F} \frac{|\hbar\mathbf{k}|^2}{2m} - \frac{1}{V} \sum_{\substack{\mathbf{k},\mathbf{k}',\mathbf{k}\neq\mathbf{k}' \\ |\mathbf{k}|<k_F,|\mathbf{k}'|<k_F}} \tilde{V}(\mathbf{k}-\mathbf{k}'). \tag{3.12}$$

In the thermodynamic limit, where $\frac{1}{V}\sum_{\mathbf{k}}$ is replaced by $\int d^3k/(2\pi)^3$, the integration can be carried out, and one finds

$$E = N\left(\frac{3}{5}\frac{\hbar^2 k_F^2}{2m} - \frac{3e^2 k_F}{16\pi^2\varepsilon_0}\right). \tag{3.13}$$

Here the Fermi wave vector k_F is related to the electron density through

$$\frac{N}{V} = \frac{1}{V}\sum_{\mathbf{k},|\mathbf{k}|<k_F,\sigma} \to \frac{k_F^3}{3\pi^2} \tag{3.14}$$

in the thermodynamic limit. The standard parametrization proceeds in terms of the dimensionless parameter r_s defined through the volume per particle,

$$\frac{V}{N} =: \frac{4\pi}{3}(r_s a_0)^3, \tag{3.15}$$

where $a_0 = 4\pi\varepsilon_0\hbar^2/(me^2)$ is the Bohr radius. Together with the Rydberg as characteristic energy scale, $\mathrm{Ry} = e^2/(8\pi\varepsilon_0 a_0)$, we can write the Hartree-Fock energy per particle as

$$\frac{E}{N} = \mathrm{Ry}\left[\frac{2.2099}{r_s^2} - \frac{0.91633}{r_s}\right]. \tag{3.16}$$

It consists of a positive kinetic energy and a negative exchange energy. Considered as a function of r_s, the total energy has a minimum at $r_s \approx 4.823$. This value is in surprisingly good agreement with alkali metals where the density of conduction electrons can be identified with the ionic density with values r_s between 3.3 and 5.6. The Hartree-Fock approximation thus gives an appealing picture for the metallic cohesion originating from the exchange energy of conduction electrons.

The Hartree-Fock approximation is not only a variational ansatz, but also the lowest-order term in a perturbation expansion of the ground state energy in powers of the Coulomb coupling strength. To find higher-order corrections one has to develop the machinery of many-body perturbation theory. Here we confine ourselves to give the leading terms,

$$\frac{E}{N} = \mathrm{Ry}\left[\frac{2.2099}{r_s^2} - \frac{0.91633}{r_s} - 0.094 + 0.0622\log r_s + \ldots\right]. \tag{3.17}$$

The first two terms are just the Hartree-Fock energy, while terms beyond Hartree-Fock are referred to as correlation energy. Eq. (3.17) indicates that the expansion parameter is r_s. Therefore perturbation theory is expected to be valid for large densities (small r_s). Unfortunately, even for simple metals this expansion is of doubtful validity because r_s is rather large.

3.3 The Wigner crystal

In the small-density limit the Coulomb energy becomes dominant and therefore it is more appropriate to start from the ground state of the interaction term than from that of the kinetic energy. We are then faced with a purely classical problem,

namely to calculate the lowest energy configuration of charged particles immersed into a homogeneous background of opposite charge. This problem was addressed by Wigner already in 1934 as that of an "inverted alkali metal", and he argued that at low enough densities the electrons would form a crystal. A consistent theory has of course to take into account the kinetic energy, which leads to zero-point fluctuations of the electrons around their equilibrium positions. As the lattice constant decreases, these fluctuations become more and more important until the Wigner crystal melts. Numerical simulations indicate that this happens for $r_s \approx 100$.

A two-dimensional Wigner crystal with a triangular structure has actually been observed for a very low-density electron system ($r_s \approx 10^4$) dispersed over the surface of liquid helium.

3.4 The Hubbard model

The jellium model is expected to be applicable if effects due to the periodic lattice are negligible, *i.e.* if the electron energy bands close to the Fermi energy are nearly-free-electron-like and if the Fermi surface is off the Brillouin zone borders. Clearly there are materials where this assumption is not valid, for instance transition metal compounds where the region close to the Fermi energy is dominated by narrow bands. For simplicity we assume that we have only to take into account a single energy band. The many-electron Hamiltonian consisting of kinetic energy, periodic potential and two-body interaction can then be related to a basis of Bloch functions $\psi_{\mathbf{k}}(\mathbf{r})$, where $\mathbf{k}$ belongs to the first Brillouin zone and the band index has been dropped. The Hamiltonian is

$$H = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} a^\dagger_{\mathbf{k},\sigma} a_{\mathbf{k},\sigma} + \frac{1}{2} \sum_{\substack{\mathbf{k}_1,\cdots,\mathbf{k}_4 \\ \sigma,\sigma'}} \langle \mathbf{k}_1, \mathbf{k}_2 | V_2 | \mathbf{k}_4, \mathbf{k}_3 \rangle \; a^\dagger_{\mathbf{k}_1,\sigma} a^\dagger_{\mathbf{k}_2,\sigma'} a_{\mathbf{k}_3,\sigma'} a_{\mathbf{k}_4,\sigma} \; , \tag{3.18}$$

where the $\mathbf{k}$ sums are restricted to the first Brillouin zone and

$$\varepsilon_{\mathbf{k}} = \langle \mathbf{k} | \frac{\mathbf{p}^2}{2m} + U(\mathbf{r}) | \mathbf{k} \rangle \tag{3.19}$$

is the single-particle spectrum of the Bloch band. An equivalent representation can be given in terms of Wannier orbitals

$$\varphi(\mathbf{r} - \mathbf{R_i}) := \frac{1}{\sqrt{N_c}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R_i}} \psi_{\mathbf{k}}(\mathbf{r}), \tag{3.20}$$

where the $\mathbf{R}_i$ are the vectors of the Bravais lattice and N_c is the number of unit cells in the volume V (N_c is also the number of wave vectors $\mathbf{k}$ in the first Brillouin zone). Correspondingly, we introduce the operator

$$a^\dagger_{i,\sigma} = \frac{1}{\sqrt{N_c}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R_i}} a^\dagger_{\mathbf{k},\sigma}, \tag{3.21}$$

which creates an electron in the Wannier orbital i with spin σ. The following relations will be useful,

$$\begin{aligned} \frac{1}{N_c}\sum_i e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_i} &= \delta_{\mathbf{k},\mathbf{k}'}, \\ \frac{1}{N_c}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)} &= \delta_{i,j}, \end{aligned} \tag{3.22}$$

for instance for establishing the anticommutation relations,

$$\begin{aligned} \{a_{i,\sigma}, a_{j,\sigma'}\} &= \left\{a^\dagger_{i,\sigma}, a^\dagger_{j,\sigma'}\right\} = 0, \\ \left\{a_{i,\sigma}, a^\dagger_{j,\sigma'}\right\} &= \delta_{i,j}\delta_{\sigma,\sigma'}, \end{aligned} \tag{3.23}$$

or for proving the inverse transformation

$$a^\dagger_{\mathbf{k},\sigma} = \frac{1}{\sqrt{N_c}}\sum_i e^{i\mathbf{k}\cdot\mathbf{R}_i} a^\dagger_{i,\sigma}. \tag{3.24}$$

The Hamiltonian in Wannier representation is then found to be

$$H = \sum_{i,j,\sigma}\langle i|\frac{\mathbf{p}^2}{2m} + U(\mathbf{r})|j\rangle\ a^\dagger_{i,\sigma}a_{j,\sigma} + \frac{1}{2}\sum_{\substack{i,j,i',j' \\ \sigma,\sigma'}}\langle i,j|V_2|i',j'\rangle\ a^\dagger_{i,\sigma}a^\dagger_{j,\sigma'}a_{j',\sigma'}a_{i',\sigma}\ , \tag{3.25}$$

as expected. This representation has no advantages with respect to the Bloch representation (3.18) except if certain simplifying assumptions are made for the matrix elements. This can be done if the Wannier functions resemble well localized atomic wave functions. In this *tight-binding limit* we may use the parametrization

$$\langle i|\frac{\mathbf{p}^2}{2m} + U(\mathbf{r})|j\rangle = \begin{cases} \varepsilon, & i = j, \\ -t, & i,j \text{ nearest-neighbor sites}, \\ 0, & \text{otherwise}. \end{cases} \tag{3.26}$$

Since the diagonal term gives simply a constant energy shift $N\varepsilon$, we may discard it by choosing the zero of energy accordingly. The most drastic simplification of the two-body term consists in neglecting all matrix elements but the fully diagonal one,

$$\langle i,j|V_2|i',j'\rangle = \begin{cases} U, & i = j = i' = j', \\ 0, & \text{otherwise}. \end{cases} \tag{3.27}$$

With these simplifications we arrive at the Hubbard Hamiltonian

$$H = -t\sum_{\langle i,j\rangle,\sigma}\left(a^\dagger_{i,\sigma}a_{j,\sigma} + a^\dagger_{j,\sigma}a_{i,\sigma}\right) + U\sum_i n_{i\uparrow}n_{i\downarrow}, \tag{3.28}$$

where $\sum_{\langle i,j\rangle}$ means summation over all links (bonds) between nearest-neighbor sites and $n_{i\sigma} := a^\dagger_{i,\sigma}a_{i,\sigma}$. These severe approximations are usually justified by the small overlap between (well-localized) Wannier functions attached to different

sites. However, one has to keep in mind that this argument is of no use for the matrix elements

$$\langle i,j|V_2|i,j\rangle = \int d^3r \int d^3r' \; |\varphi(\mathbf{r}-\mathbf{R}_i)|^2 \, V(\mathbf{r},\mathbf{r}') \, |\varphi(\mathbf{r}'-\mathbf{R}_j)|^2. \tag{3.29}$$

If $V(\mathbf{r},\mathbf{r}')$ is taken as the bare Coulomb interaction, this matrix element decreases as $|\mathbf{R}_i-\mathbf{R}_j|^{-1}$, *i.e.* much slower than those involving overlap between different Wannier functions, such as

$$\langle i,i|V_2|j,j\rangle = \int d^3r \int d^3r' \varphi^*(\mathbf{r}-\mathbf{R}_i)\varphi(\mathbf{r}-\mathbf{R}_j)V(\mathbf{r},\mathbf{r}')\varphi^*(\mathbf{r}'-\mathbf{R}_i)\varphi(\mathbf{r}'-\mathbf{R}_j). \tag{3.30}$$

Therefore one needs an additional argument for discarding the terms $\langle i,j|V_2|i,j\rangle$, such as screening due to mobile charges, which leads to an effective interaction potential of the Yukawa type, $V(\mathbf{r},\mathbf{r}') \sim |\mathbf{r}-\mathbf{r}'|^{-1}\exp(-\kappa_0|\mathbf{r}-\mathbf{r}'|)$. These mobile charges are not available in insulators, where the applicability of the Hubbard model must be questioned.

Despite of these reservations, the Hubbard model is very often advocated as describing the essential physics of strongly correlated electron systems. The model is in fact widely used for describing quantum antiferromagnets, the metal-insulator transition induced by strong correlations and even (high-temperature) superconductivity. More recently it has also been applied to atoms in optical lattices. Clearly the Hubbard Hamiltonian represents a fascinating many-body problem, and therefore it is not surprising that a huge literature exists on analytical and numerical studies of this model. Unfortunately, an exact solution has been found so far only in one dimension (in terms of the Bethe ansatz).

With the transformation (3.21) the Hubbard Hamiltonian can be readily expressed in terms of the Bloch basis. To be specific, we consider a simple cubic lattice with lattice constant a, where the 6 neighboring lattice vectors of $\mathbf{R}_i$ are given by $\mathbf{R}_j = \mathbf{R}_i \pm a\mathbf{e}_\alpha$, $\mathbf{e}_\alpha$ being the unit vectors parallel to the x, y and z axes. We get

$$\begin{aligned}
\sum_{\langle i,j\rangle}\left(a^\dagger_{i,\sigma}a_{j,\sigma} + a^\dagger_{j,\sigma}a_{i,\sigma}\right) &= \sum_{\mathbf{k},\mathbf{k}'}\left[a^\dagger_{\mathbf{k},\sigma}a_{\mathbf{k}',\sigma}\frac{1}{N_c}\sum_{\langle i,j\rangle} e^{i(\mathbf{k}\cdot\mathbf{R}_i - \mathbf{k}'\cdot\mathbf{R}_j)} + \text{h.c.}\right] \\
&= \sum_{\mathbf{k},\mathbf{k}'}\left[a^\dagger_{\mathbf{k},\sigma}a_{\mathbf{k}',\sigma}\frac{1}{N_c}\sum_{i} e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_i}\sum_{\alpha=1}^{3} e^{ia\mathbf{k}'\cdot\mathbf{e}_\alpha} + \text{h.c.}\right] \\
&= 2\sum_{\mathbf{k}} a^\dagger_{\mathbf{k},\sigma}a_{\mathbf{k},\sigma}(\cos k_x a + \cos k_y a + \cos k_z a)\,.
\end{aligned} \tag{3.31}$$

The Hubbard Hamiltonian then reads

$$H = \sum_{\mathbf{k},\sigma}\varepsilon_{\mathbf{k}}a^\dagger_{\mathbf{k},\sigma}a_{\mathbf{k},\sigma} + \frac{U}{N_c}\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} a^\dagger_{\mathbf{k}\uparrow}a_{\mathbf{k}-\mathbf{q}\uparrow}a^\dagger_{\mathbf{k}'\downarrow}a_{\mathbf{k}'+\mathbf{q}\downarrow}\,, \tag{3.32}$$

with the tight-binding spectrum

$$\varepsilon_{\mathbf{k}} = -2t(\cos k_x a + \cos k_y a + \cos k_z a)\,. \tag{3.33}$$

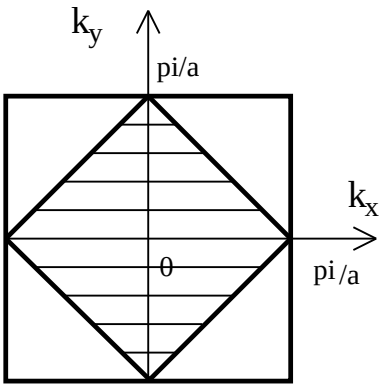

Figure 3: Occupied states of the half-filled tight-binding band for the square lattice.

This result is very similar to the Hamiltonian of the jellium model, Eq. (3.7), except that here the wave vectors are restricted to the first Brillouin zone, $-\pi/a < k_\alpha \leq \pi/a$, $\alpha = x, y, z$, the spectrum has a different form and the coupling does not depend on $\mathbf{q}$. Moreover, the interaction involves only electrons with different spins, due to the fact that $n_{i\sigma}n_{i\sigma}$ is in reality a single-particle term for fermions, $n_{i\sigma}n_{i\sigma} = a^\dagger_{i\sigma}a_{i\sigma}a^\dagger_{i\sigma}a_{i\sigma} = a^\dagger_{i\sigma}\{a_{i\sigma}, a^\dagger_{i\sigma}\}a_{i\sigma} = n_{i\sigma}$. This does not remain true if interactions between nearest-neighbor sites are included, proportional to $n_i n_j$. In this case, referred to as extended Hubbard model, the coupling becomes $\mathbf{q}$-dependent and electrons with the same spin interact.

We consider as an example the so-called half-filled band case, where the number of electrons N is equal to the number of sites (or the number of cells N_c). For small values of U we may use the Hartree-Fock approximation (3.8), which is handled as in the case of the jellium model. For simplicity we choose a square lattice with a tight-binding spectrum, $\varepsilon_{\mathbf{k}} = -2t(\cos k_x a + \cos k_y a)$. At half filling the Fermi surface is a square with corners at $(\pm\pi/a, 0)$ and $(0, \pm\pi/a)$, as illustrated in Fig. 3. One easily verifies the relation

$$\langle\Psi_0|n_{i\uparrow}n_{i\downarrow}|\Psi_0\rangle = \langle\Psi_0|n_{i\uparrow}|\Psi_0\rangle\ \langle\Psi_0|n_{i\downarrow}|\Psi_0\rangle = \frac{1}{4}. \tag{3.34}$$

It can be interpreted as the probability of a site being doubly occupied. The probability of a site being unoccupied is also 1/4, as is the probability of having a single electron with spin up (or one with spin down). We obtain the Hartree-Fock energy

$$\langle\Psi_0|H|\Psi_0\rangle = 2\sum_{\mathbf{k},\varepsilon_{\mathbf{k}}<0}\varepsilon_{\mathbf{k}} + \frac{1}{4}NU = N\left(-\frac{16t}{\pi^2} + \frac{U}{4}\right). \tag{3.35}$$

In the opposite limit of large U, where it costs a lot of energy to put two electrons onto the same site, it is more appropriate to start from the "dual" ansatz, *i.e.* the Hartree-Fock state made up of Wannier orbitals,

$$|\Psi_\infty\rangle = \prod_i a^\dagger_{i,\sigma_i}|0\rangle, \tag{3.36}$$

where $(\sigma_1, \sigma_2, \ldots, \sigma_N)$ is an arbitrary spin configuration. It is easy to see that the expectation values both of the hopping term (the single-particle term) and of

the two-body interaction vanish, and therefore we get

$$\langle \Psi_\infty | H | \Psi_\infty \rangle = 0. \tag{3.37}$$

Comparing the two variational results we conclude that the Bloch point of view leads to a lower energy for $U < U_c := 64t/\pi^2$, while for $U > U_c$ the Wannier picture prevails. One can show that $|\Psi_0\rangle$ is a metallic state, while $|\Psi_\infty\rangle$ is insulating. Therefore our simple variational procedure predicts a metal-insulator transition as a function of U at a critical value U_c of the order of the bandwidth ($8t$). This is referred to as the Mott metal-insulator transition. That $|\Psi_0\rangle$ is a metallic state is clear since this is simply the ground state of a partially filled band of non-interacting electrons. That $|\Psi_\infty\rangle$ is an insulating state appears also to be obvious if one imagines to move a particle from its site to a neighboring site. This leads to double occupancy of the new site and requires an energy U. It reminds us of conduction in an intrinsic semiconductor, which can only be produced by promoting an electron from the valence to the conduction band, *i.e.* by providing the energy difference between the bottom of the conduction band and the top of the valence band. The main difference is that in the present case the energy gap U results from the occupation of neighboring sites by other electrons – it is a *correlation gap* – while a semiconductor has a *band gap*, generated by the periodic potential.

Literature

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4 Magnetism

The field of magnetism covers a wide range of important topics, such as the nature of magnetic moments in crystals, Pauli paramagnetism and Landau diamagnetism of conduction electrons, magnetic ordering at low temperatures, the nature of domains and domain walls, complex magnetic structures (spin-density waves, spiral phases, ferrimagnetism). Magnetic impurities play an intricate role both in metals (Kondo effect) and in superconductors (breaking of Cooper pairs). Spin glasses are formed in dilute alloys (such as Cu:Mn) as a result of a competition between disorder and frustration. Subtle phenomena occur in low-dimensional systems where strong fluctuations may prevent ordering at finite temperatures.

Magnetic moments are generated both by the orbital motion of charged particles and by the spin (of electrons, protons and neutrons). In solids the electronic contribution is by far the largest, and in many cases the spin dominates, for instance in transition metals where the orbital moment of d electrons can be quenched by crystal-field effects. Therefore we will concentrate our attention on the Heisenberg model, which consists of spins coupled by the exchange interaction. It is worth mentioning that the spin, introduced *ad hoc* in non-relaticistic quantum mechanics to deal both with the anomalous Zeeman effect and with the Stern-Gerlach experiment, arises naturally in Dirac's relativistic quantum mechanics.

4.1 Exchange

Magnetic order (in insulators) occurs because of the interaction between magnetic moments. The most obvious coupling is purely electromagnetic. A magnetic moment $\boldsymbol{\mu}_1$ generates a magnetic field which acts on a second moment $\boldsymbol{\mu}_2$ a distance $\mathbf{r}$ apart. The result is the dipole-dipole interaction

$$H_{int} = \frac{\mu_0}{4\pi r^3}\left(\boldsymbol{\mu}_1 \cdot \boldsymbol{\mu}_2 - \frac{\mathbf{r}\cdot\boldsymbol{\mu}_1 \quad \mathbf{r}\cdot\boldsymbol{\mu}_2}{r^2}\right) \ . \tag{4.1}$$

This coupling is too weak to explain the ordering in magnetic materials. Nevertheless, due to its long-range nature, the dipole-dipole interaction plays an important role in ferromagnets, where it is responsible for the appearance of magnetic domains.

The origin of magnetic order is exchange, a cooperative effect of Coulomb interaction and Fermi statistics. We consider two electrons for two different situations. In the first case, the two electrons can occupy two different degenerate d orbitals of a single atom, in the second case they can hop between two Wannier states associated with two neighboring sites of a lattice. We number the two single-particle states by the index $i = 1, 2$ in both cases. We use the parameter U for the on-site Coulomb interaction, as in Eq. (3.27), together with

$$V = \langle i, j|V_2|i, j\rangle, \qquad J = \langle i, j|V_2|j, i\rangle \tag{4.2}$$

for $i \neq j$. We neglect the other terms, therefore the Coulomb interaction of Eq. (3.25) is reduced to

$$H_{int} = U(n_{1\uparrow}n_{1\downarrow} + n_{2\uparrow}n_{2\downarrow}) + Vn_1n_2 - J\sum_{\sigma,\sigma'} a^\dagger_{1\sigma}a_{1\sigma'}a^\dagger_{2\sigma'}a_{2\sigma} \ , \tag{4.3}$$

where $n_{i\sigma} = a^\dagger_{i\sigma} a_{i\sigma},\ n_i = n_{i\uparrow} + n_{i\downarrow}$. Introducing the (dimensionless) spin operators

$$\begin{aligned} S_{i+} &= a^\dagger_{i\uparrow} a_{i\downarrow}\,, \\ S_{i-} &= a^\dagger_{i\downarrow} a_{i\uparrow}\,, \\ S_{iz} &= \frac{1}{2}(n_{i\uparrow} - n_{i\downarrow})\,, \end{aligned} \tag{4.4}$$

we can rewrite the last term in Eq. (4.3) as $-J(\frac{1}{2} n_1 n_2 + 2\mathbf{S}_1 \cdot \mathbf{S}_2)$. We set the diagonal contribution of the single-particle term (3.26) equal to zero, by choosing the zero of energy accordingly, and therefore are left with the Hamiltonian

$$H = -t \sum_\sigma (a^\dagger_{1\sigma} a_{2\sigma} + a^\dagger_{2\sigma} a_{1\sigma}) + U(n_{1\uparrow} n_{1\downarrow} + n_{2\uparrow} n_{2\downarrow}) + (V - \frac{J}{2}) n_1 n_2 - 2J\, \mathbf{S}_1 \cdot \mathbf{S}_2\,, \tag{4.5}$$

where $t = 0$ for the case of two d orbitals on a single atom and $t \neq 0$ for the two-site problem.

To calculate the eigenstates of the Hamiltonian (4.5), we use the fact that H commutes with both S_z and $\mathbf{S}^2$, where

$$\mathbf{S} = \mathbf{S}_1 + \mathbf{S}_2 \tag{4.6}$$

is the total spin. There are three singlet states ($S = 0$)

$$|0,0\rangle_1 = a^\dagger_{1\uparrow} a^\dagger_{1\downarrow} |0\rangle,\ |0,0\rangle_2 = a^\dagger_{2\uparrow} a^\dagger_{2\downarrow} |0\rangle,\ |0,0\rangle_3 = \frac{1}{\sqrt{2}} (a^\dagger_{1\uparrow} a^\dagger_{2\downarrow} - a^\dagger_{1\downarrow} a^\dagger_{2\uparrow}) |0\rangle, \tag{4.7}$$

and three triplet states ($S = 1$)

$$|1,1\rangle = a^\dagger_{1\uparrow} a^\dagger_{2\uparrow} |0\rangle,\ |1,-1\rangle = a^\dagger_{1\downarrow} a^\dagger_{2\downarrow} |0\rangle,\ |1,0\rangle = \frac{1}{\sqrt{2}} (a^\dagger_{1\uparrow} a^\dagger_{2\downarrow} + a^\dagger_{1\downarrow} a^\dagger_{2\uparrow}) |0\rangle\,. \tag{4.8}$$

The triplet states are eigenstates of the Hamiltonian (4.5),

$$H|1,m\rangle = (V - J)|1,m\rangle\,. \tag{4.9}$$

In the singlet subspace the Hamiltonian is represented by the 3×3 matrix

$$H \to \begin{pmatrix} U & 0 & -\sqrt{2}t \\ 0 & U & -\sqrt{2}t \\ -\sqrt{2}t & -\sqrt{2}t & V + \frac{3}{2}J \end{pmatrix}\,. \tag{4.10}$$

It is readily diagonalized, giving the three eigenvalues

$$E_s = \begin{cases} U \\ \frac{1}{2}\left(U + V + \frac{3}{2}J \pm \sqrt{(U - V - \frac{3}{2}J)^2 + 16t^2} \right)\,. \end{cases} \tag{4.11}$$

We consider first the case of two electrons on the same atom ($t = 0$). The largest parameter is usually the term U, in this case the Coulomb energy for two electrons with the same wave function. Then the lowest singlet energy, $V + \frac{3}{2}J$, is higher than the triplet energy, $V - J$. Thus the *direct exchange*, the last term

in Eq. (4.3), is responsible for Hund's first rule, according to which the total spin of electrons in a partially filled shell has its maximum possible value.

For the two-site problem we have to take into account the hopping between sites. The on-site Coulomb term U is again much larger than the other parameters, including t, at least for typical transition metals. Therefore the lowest singlet energy is well approximated by

$$E_{s,min} \approx V + \frac{3}{2}J - \frac{4t^2}{U}\,. \tag{4.12}$$

The eigenstate is essentially $|0,0\rangle_3$, with a small admixture of the states $|0,0\rangle_1$ and $|0,0\rangle_2$ (of the order of t/U). Restricting ourselves to this lowest singlet state and to the three triplet states, we arrive at four states which are to a good approximation the eigenstates of the *Heisenberg Hamiltonian*

$$H = E_0 - J_{eff}\,\mathbf{S}_1 \cdot \mathbf{S}_2\,, \tag{4.13}$$

where E_0 is a constant and

$$J_{eff} = \frac{5}{2}J - \frac{4t^2}{U}\,. \tag{4.14}$$

Thus the hopping produces a *kinetic exchange* $-4t^2/U$, which counteracts the direct exchange $\frac{5}{2}J$. In fact, while the direct exchange tends to align the spins in a triplet state, the kinetic exchange favors a singlet state. In order to get a rough idea of the orders of magnitude of the two competing terms, we use the parameters estimated by Hubbard for transition metals: $U \approx 10$ eV, $J \approx 0.025$ eV. With t of the order of 1 eV we find that the kinetic exchange, $4t^2/U \approx 0.4$ eV, exceeds by far the direct exchange $\frac{5}{2}J$. Therefore we expect a strong tendency towards antiferromagnetic ordering among neighboring transition metal ions.

The kinetic exchange can also be obtained from the Hubbard model (where the direct exchange has been neglected), for $U \gg t$ and for an average density of one electron per site. In the limit $(t/U) \to 0$ there are 2^N different spin configurations (for N electrons on N sites) all of which have energy zero. For small values of (t/U) one uses degenerate perturbation theory to calculate the energy splitting due to the hopping term. One again arrives at the Heisenberg Hamiltonian with exchange constant $J = -4t^2/U$.

4.2 Magnetic order in the Heisenberg model

The Heisenberg Hamiltonian

$$H = -J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \tag{4.15}$$

plays an important role for magnetic insulators, both ferromagnetic ($J > 0$) and antiferromagnetic ($J < 0$). We have seen above how to arrive at such an expression with spin $\frac{1}{2}$ operators. Other values of localized spins occur in many materials, due to Hund's first rule. Thus the ion Ni^{2+} has $S = 1$, while Cr^{3+} has $S = \frac{3}{2}$. An important example is the ion Cu^{2+}, which does have a spin $\frac{1}{2}$. It occurs

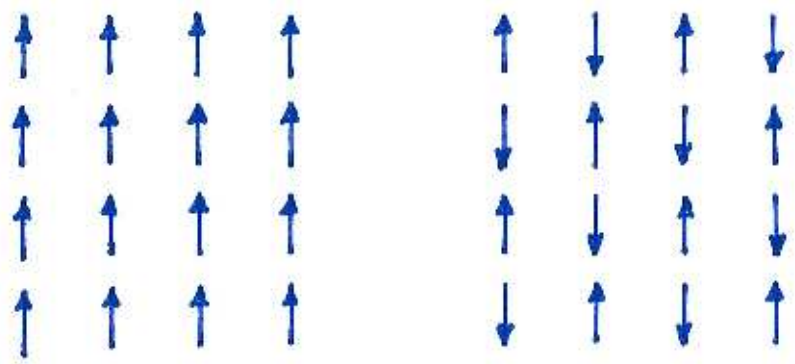

Figure 4: Ferromagnetic and Néel states on a square lattice.

for instance in the layered compound La_2CuO_4, which is very well described by the (quasi-two-dimensional) Heisenberg model with antiferromagnetic exchange (and spin $\frac{1}{2}$).

The Hamiltonian (4.15) has also been extensively studied for classical vectors $\mathbf{S}_i$, especially for discussing thermodynamic properties, for instance the transition from a paramagnetic to a ferromagnetic phase as a function of temperature. It is worthwhile to mention that neither the one-dimensional nor the two-dimensional Heisenberg Hamiltonians admit long-range magnetic order at any finite temperature, due to large statistical fluctuations associated with low-energy spin wave excitations (Mermin-Wagner theorem). Therefore the observed antiferromagnetic order below a Néel temperature of the order of 300 K in the layered (undoped) cuprates is due to a (very small, but finite) exchange coupling between the layers.

A negative value of J leads to antiparallel ordering of neighboring spins in the ground state. Hovewer, in contrast to the fully saturated ferromagnetic state which is an eigenstate of the Heisenberg Hamiltonian (4.15), the Néel state, where the spins are $\uparrow$ on half of the lattice sites and $\downarrow$ on the other sites, as illustrated in Fig. 4, is not an eigenstate. Nevertheless, the ground state for $J < 0$ is antiferromagnetic in the sense that there is a preference for spins $\uparrow$ on one sublattice and for spins $\downarrow$ on the other (except in one dimension where there is no broken symmetry, even at zero temperature).

The low-lying excitations are spin waves or magnons, which correspond to small deviations from the ground state configuration, characterized by a wave vector $\mathbf{q}$ and an excitation spectrum $\omega_{\mathbf{q}}$. For ferromagnets one finds $\omega_{\mathbf{q}} \sim |\mathbf{q}|^2$, while one obtains a linear law, $\omega_{\mathbf{q}} \sim |\mathbf{q}|$, for antiferromagnets. Inelastic neutron scattering experiments confirm these predictions.

Literature

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5 Electrons and phonons

Until now, whenever we used the word crystal, we assumed the atoms to sit on a perfectly periodic lattice. In reality, atoms oscillate around their equilibrium positions, even at zero temperature. The quantum of vibration is a *phonon*. Phonons contribute to the specific heat of crystals, to the thermal expansion and to the melting of a crystal (through anharmonicities), and they give rise to the electrical resistance via the electron-phonon interaction. Last but not least, the exchange of phonons between two electrons may provide an effective attraction and lead to superconductivity. In this short chapter, we limit ourselves to three topics, the phonons in a harmonic crystal, the origin of the electron-phonon interaction and the effective electron-electron attraction resulting from phonon exchange.

5.1 The harmonic crystal

The theory of lattice dynamics is based on the assumption that the atomic displacements are small. In the harmonic approximation, the expansion of the potential energy in powers of the displacements is carried out up to the second order. For simplicity, we consider the case of one atom per unit cell. The atomic positions are given by $\mathbf{R} + \mathbf{u}(\mathbf{R})$, where the vectors $\mathbf{R}$ span a three-dimensional Bravais lattice and the vectors $\mathbf{u}(\mathbf{R})$ are the atomic displacements away from equilibrium. Every atom has three degrees of freedom described by the three components of the displacement vector $u_\alpha(\mathbf{R})$, $\alpha = x, y, z$. In the harmonic approximation the Hamiltonian is given by

$$H = \frac{1}{2M} \sum_{\mathbf{R},\alpha} p_\alpha^2(\mathbf{R}) + \frac{1}{2} \sum_{\substack{\mathbf{R},\mathbf{R}' \\ \alpha,\beta}} D_{\alpha,\beta}(\mathbf{R} - \mathbf{R}') u_\alpha(\mathbf{R}) u_\beta(\mathbf{R}') \,, \tag{5.1}$$

where $p_\alpha(\mathbf{R})$ are the components of the atomic momentum at $\mathbf{R}$ and $D(\mathbf{R} - \mathbf{R}')$ is the *dynamical matrix*, the second derivative of the potential energy with respect to the atomic displacements at $\mathbf{R}$ and $\mathbf{R}'$. There is no linear term since we assume to start from equilibrium, where there is no force acting on the atoms. The transformation

$$\begin{aligned} \mathbf{u}(\mathbf{R}) &= \frac{1}{\sqrt{NM}} \sum_{\mathbf{k},\lambda} q_{\mathbf{k},\lambda}\, \mathbf{e}_{\mathbf{k},\lambda}\, e^{i\mathbf{k}\cdot\mathbf{R}} \,, \\ \mathbf{p}(\mathbf{R}) &= \sqrt{\frac{M}{N}} \sum_{\mathbf{k},\lambda} p_{\mathbf{k},\lambda}\, \mathbf{e}_{\mathbf{k},\lambda}\, e^{i\mathbf{k}\cdot\mathbf{R}} \,, \end{aligned} \tag{5.2}$$

where N is the number of unit cells, $\mathbf{e}_{\mathbf{k}\lambda}\,(\lambda = 1, 2, 3)$ are the three orthonormal eigenvectors of the Fourier transform $\tilde{D}(\mathbf{k})$ of the dynamical matrix with eigenvalues $M\omega_{\mathbf{k},\lambda}^2$, leads to

$$H = \frac{1}{2} \sum_{\mathbf{k},\lambda} \left(p_{\mathbf{k},\lambda} p_{-\mathbf{k},\lambda} + \omega_{\mathbf{k},\lambda}^2\, q_{\mathbf{k},\lambda} q_{-\mathbf{k},\lambda} \right) . \tag{5.3}$$

To quantize the theory, we replace the canonical variables $\mathbf{u}(\mathbf{R})$ and $\mathbf{p}(\mathbf{R})$ by operators satisfying the commutation relations

$$\begin{aligned} [u_\alpha(\mathbf{R}), u_\beta(\mathbf{R}')] &= [p_\alpha(\mathbf{R}), p_\beta(\mathbf{R}')] = 0, \\ [u_\alpha(\mathbf{R}), p_\beta(\mathbf{R}')] &= i\hbar\, \delta_{\mathbf{R},\mathbf{R}'}\, \delta_{\alpha,\beta}\,. \end{aligned} \tag{5.4}$$

This leads to

$$\begin{aligned} [q_{\mathbf{k},\lambda}, q_{\mathbf{k}',\lambda'}] &= [p_{\mathbf{k},\lambda}, p_{\mathbf{k}',\lambda'}] = 0, \\ [q_{\mathbf{k},\lambda}, p_{\mathbf{k}',\lambda'}] &= i\hbar\, \delta_{\lambda,\lambda'}\, \delta_{\mathbf{k},-\mathbf{k}'}\,. \end{aligned} \tag{5.5}$$

Finally, introducing phonon creation and annihilation operators $b^\dagger_{\mathbf{k},\lambda}$ and $b_{\mathbf{k},\lambda}$, respectively,

$$\begin{aligned} q_{\mathbf{k},\lambda} &= \sqrt{\frac{\hbar}{2\omega_{\mathbf{k},\lambda}}}\left(b_{\mathbf{k},\lambda} + b^\dagger_{-\mathbf{k},\lambda}\right) \\ p_{\mathbf{k},\lambda} &= -i\sqrt{\frac{\hbar\omega_{\mathbf{k},\lambda}}{2}}\left(b_{\mathbf{k},\lambda} - b^\dagger_{-\mathbf{k},\lambda}\right), \end{aligned} \tag{5.6}$$

with commutation relations

$$\begin{aligned} [b_{\mathbf{k},\lambda}, b_{\mathbf{k}',\lambda'}] &= \left[b^\dagger_{\mathbf{k},\lambda}, b^\dagger_{\mathbf{k}',\lambda'}\right] = 0\,, \\ \left[b_{\mathbf{k},\lambda}, b^\dagger_{\mathbf{k}',\lambda'}\right] &= \delta_{\mathbf{k}',\mathbf{k}}\delta_{\lambda,\lambda'}\,, \end{aligned} \tag{5.7}$$

we obtain the familiar Hamiltonian of a collection of independent bosons

$$H = \sum_{\mathbf{k},\lambda} \hbar\omega_{\mathbf{k},\lambda}\left(b^\dagger_{\mathbf{k},\lambda} b_{\mathbf{k},\lambda} + \frac{1}{2}\right)\,. \tag{5.8}$$

The dynamical matrix has both inversion symmetry,

$$D_{\alpha\beta}(\mathbf{R} - \mathbf{R}') = D_{\alpha\beta}(\mathbf{R}' - \mathbf{R}) \tag{5.9}$$

and continuous translational symmetry,

$$\sum_{\mathbf{R}} D_{\alpha\beta}(\mathbf{R}) = 0\,. \tag{5.10}$$

Its Fourier transform $\tilde{D}(\mathbf{k})$ can therefore be rewritten as

$$\tilde{D}(\mathbf{k}) = \frac{1}{2}\sum_{\mathbf{R}} \left(e^{-i\mathbf{k}\cdot\mathbf{R}} + e^{i\mathbf{k}\cdot\mathbf{R}} - 2\right) D(\mathbf{R}) = -2\sum_{\mathbf{R}} \sin^2\frac{\mathbf{k}\cdot\mathbf{R}}{2}\; D(\mathbf{R})\,. \tag{5.11}$$

It follows that $\tilde{D}(\mathbf{k}) \sim k^2$ for $k \to 0$ (provided that $D(\mathbf{R})$ decreases sufficiently fast for $R \to \infty$). Therefore the eigenvalues of $\tilde{D}(\mathbf{k})$ have dispersion relations

$$\omega^2_{\mathbf{k},\lambda} \sim c^2_\lambda k^2 \text{ for } k \to 0,\ \lambda = 1, 2, 3\,, \tag{5.12}$$

corresponding to acoustic phonons, two "transverse" modes and one "longitudinal" mode, with sound velocities c_λ .

5.2 Electron-phonon interaction

To describe the coupling between an electron and the acoustic phonons, we use a simple "rigid ion" model. Each ion represents for the electron a potential V_a, which depends on the distance between the position $\mathbf{r}$ of the electron and the ionic position $\mathbf{R}+\mathbf{u}(\mathbf{R})$. Assuming these contributions to add up, we obtain the potential $V(\mathbf{r})$ acting on the electron

$$V(\mathbf{r}) = \sum_{\mathbf{R}} V_a(\mathbf{r}-\mathbf{R}-\mathbf{u}(\mathbf{R})) \approx \sum_{\mathbf{R}} V_a(\mathbf{r}-\mathbf{R}) - \sum_{\mathbf{R}} \nabla V_a(\mathbf{r}-\mathbf{R})\cdot\mathbf{u}(\mathbf{R})\,. \quad (5.13)$$

The first term of the Taylor expansion is a periodic potential leading to Bloch eigenstates for the electron, the second term represents the electron-phonon interaction

$$V_{ep}(\mathbf{r}) := -\sum_{\mathbf{R}} \nabla V_a(\mathbf{r}-\mathbf{R})\cdot\mathbf{u}(\mathbf{R})\,. \quad (5.14)$$

In order to treat a many-electron system (the partially filled conduction band of a metal), we write $V_{ep}(\mathbf{r})$ in second-quantized representation, using the Bloch states as single-particle basis. For simplicity, we restrict ourselves to a single band with (Bloch) wave function

$$\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}}(\mathbf{r})\,, \quad (5.15)$$

where $\mathbf{k}$ is a vector of the first Brillouin zone and $u_{\mathbf{k}}(\mathbf{r}) = u_{\mathbf{k}}(\mathbf{r}+\mathbf{R})$. Using the Fourier transform,

$$V_a(\mathbf{r}) = \frac{1}{V}\sum_{\mathbf{q}} \tilde{V}_a(\mathbf{q})\, e^{i\mathbf{q}\cdot\mathbf{r}} \quad (5.16)$$

together with Eqs. (5.2) and (5.6), we get

$$\begin{aligned}\langle \mathbf{k}|V_{ep}|\mathbf{k}'\rangle = -\tfrac{1}{V}\textstyle\sum_{\mathbf{q},\mathbf{q}',\lambda} \tilde{V}_a(\mathbf{q})\sqrt{\tfrac{\hbar}{2NM\omega_{\mathbf{q}'\lambda}}}\, i\mathbf{q}\cdot\mathbf{e}_{\mathbf{q}'\lambda} \\ \textstyle\sum_{\mathbf{R}} e^{-i(\mathbf{q}-\mathbf{q}')\cdot\mathbf{R}}(b_{\mathbf{q}'\lambda} + b^\dagger_{-\mathbf{q}'\lambda}) \int_V d^3r\; e^{-i(\mathbf{k}-\mathbf{k}'-\mathbf{q})\cdot\mathbf{r}}\, u^*_{\mathbf{k}}(\mathbf{r})\, u_{\mathbf{k}'}(\mathbf{r})\,. \end{aligned} \quad (5.17)$$

We use the relation

$$\sum_{\mathbf{R}} e^{-i(\mathbf{q}-\mathbf{q}')\cdot\mathbf{R}} = N\Delta(\mathbf{q}-\mathbf{q}')\,, \quad (5.18)$$

where

$$\Delta(\mathbf{q}) = \begin{cases} 1, & \text{if } \mathbf{q} \text{ is a reciprocal lattice vector} \\ 0, & \text{otherwise.} \end{cases} \quad (5.19)$$

Similarly, the matrix elements $\int_V d^3r\; e^{-i(\mathbf{k}-\mathbf{k}'-\mathbf{q})\cdot\mathbf{r}}\, u^*_{\mathbf{k}}(\mathbf{r})\, u_{\mathbf{k}'}(\mathbf{r})$ are only non-zero if $\mathbf{k}-\mathbf{k}'-\mathbf{q}$ is a reciprocal lattice vector. We neglect Umklapp processes which involve finite reciprocal lattice vectors. Moreover, the acoustic modes consist (approximately) of one longitudinal and two transverse modes, among which only the longitudinal mode contributes, with $\mathbf{q}\cdot\mathbf{e}_{\mathbf{q}} = |\mathbf{q}|$, $\omega_{\mathbf{q}} = sq$. With these simplifications we obtain ($\mathbf{k}' = \mathbf{k}-\mathbf{q}$)

$$\langle \mathbf{k}|V_{ep}|\mathbf{k}-\mathbf{q}\rangle = g_{\mathbf{k},\mathbf{q}}(b_{\mathbf{q}} + b^\dagger_{-\mathbf{q}})\,, \quad (5.20)$$

where the electron-phonon coupling constant is

$$g_{\mathbf{k},\mathbf{q}} = -\frac{i}{V}\tilde{V}_a(\mathbf{q})\sqrt{\frac{\hbar N q}{2Ms}}\int_V d^3r\; u^*_{\mathbf{k}}(\mathbf{r})\, u_{\mathbf{k}-\mathbf{q}}(\mathbf{r})\,. \quad (5.21)$$

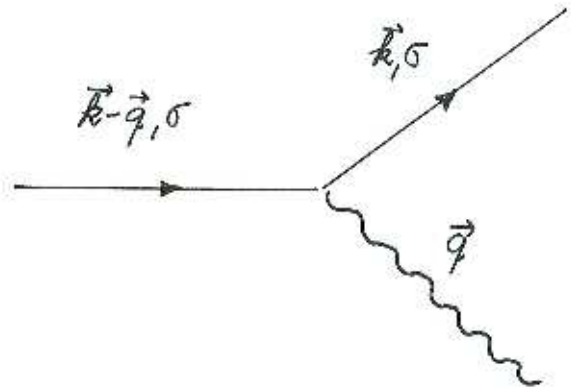

Figure 5: Electron-phonon scattering process.

The second-quantized representation of the electron-phonon interaction is then given by

$$H_{ep} = \sum_{\mathbf{k},\mathbf{q},\sigma} g_{\mathbf{k},\mathbf{q}} (b_{\mathbf{q}} + b^{\dagger}_{-\mathbf{q}}) a^{\dagger}_{\mathbf{k}\sigma} a_{\mathbf{k}-\mathbf{q}\sigma} \,, \tag{5.22}$$

where $a^{\dagger}_{\mathbf{k}\sigma}$ and $a_{\mathbf{k}\sigma}$ are, respectively, creation and annihilation operators of electrons with wavevector $\mathbf{k}$ and spin σ. H_{ep} corresponds to the scattering process depicted in Fig. 5.

5.3 Phonon-induced attraction

The fundamental interactions in metals are the Coulomb interaction between electrons and the electron-phonon interaction. A thorough treatment of both interactions would require advanced techniques, such as the Green function formalism. These techniques are able to show that the Coulomb interaction, which decays very slowly in an insulator, not only is screened in a metal and thus becomes short ranged, but it even may be "overscreened" due to the electron-phonon interaction and change sign. Here we use a plausibility argument for the origin of an effective attraction, as proposed by H. Fröhlich several years before the BCS theory. We consider the Hamiltonian of (conduction) electrons coupled to (longitudinal acoustic) phonons,

$$H = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} a^{\dagger}_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma} + \sum_{\mathbf{q}} \hbar\omega_{\mathbf{q}} b^{\dagger}_{\mathbf{q}} b_{\mathbf{q}} + \sum_{\mathbf{k},\mathbf{q},\sigma} g_{\mathbf{k},\mathbf{q}} (b_{\mathbf{q}} + b^{\dagger}_{-\mathbf{q}}) a^{\dagger}_{\mathbf{k}\sigma} a_{\mathbf{k}-\mathbf{q}\sigma} \,. \tag{5.23}$$

We use stationary state perturbation theory in powers of the electron-phonon coupling, starting from the bare ground state,

$$|\Psi_0\rangle = \prod_{\substack{\mathbf{k},\sigma \\ \varepsilon_{\mathbf{k}} < \varepsilon_F}} a^{\dagger}_{\mathbf{k}\sigma} |0\rangle_e \otimes |0\rangle_p \,, \tag{5.24}$$

where the electronic levels are filled up to the Fermi level and there is no phonon. The first order contribution to the energy vanishes. The second order contribution

can be written as

$$\Delta E = 2\sum_{\mathbf{k},\mathbf{k}'}(1-f_{\mathbf{k}})f_{\mathbf{k}'}\,\frac{|g_{\mathbf{k},\mathbf{k}-\mathbf{k}'}|^2}{\varepsilon_{\mathbf{k}'}-\varepsilon_{\mathbf{k}}-\hbar\omega_{\mathbf{k}-\mathbf{k}'}}\,, \tag{5.25}$$

where $f_{\mathbf{k}}$ is the Fermi-Dirac function at zero temperature,

$$f_{\mathbf{k}} = \begin{cases} 1, & \varepsilon_{\mathbf{k}} < \varepsilon_F \\ 0, & \varepsilon_{\mathbf{k}} > \varepsilon_F\,. \end{cases} \tag{5.26}$$

The symmetry $|g_{\mathbf{k},\mathbf{k}-\mathbf{k}'}|^2 = |g_{\mathbf{k}',\mathbf{k}'-\mathbf{k}}|^2$ allows us to rewrite Eq. (5.25) as

$$\begin{aligned}\Delta E &= 2\sum_{\mathbf{k}} f_{\mathbf{k}} \sum_{\mathbf{k}'} \frac{|g_{\mathbf{k},\mathbf{k}-\mathbf{k}'}|^2}{\varepsilon_{\mathbf{k}}-\varepsilon_{\mathbf{k}'}-\hbar\omega_{\mathbf{k}'-\mathbf{k}}} \\ &+ 2\sum_{\mathbf{k},\mathbf{k}'} f_{\mathbf{k}} f_{\mathbf{k}'}\,\frac{|g_{\mathbf{k},\mathbf{k}-\mathbf{k}'}|^2\hbar\omega_{\mathbf{k}-\mathbf{k}'}}{(\hbar\omega_{\mathbf{k}-\mathbf{k}'})^2-(\varepsilon_{\mathbf{k}}-\varepsilon_{\mathbf{k}'})^2}\,.\end{aligned} \tag{5.27}$$

This expression can be interpreted as arising from a purely electronic Hamiltonian

$$H = \sum_{\mathbf{k}\sigma}(\varepsilon_{\mathbf{k}}+\Delta\varepsilon_{\mathbf{k}})a^\dagger_{\mathbf{k}\sigma}a_{\mathbf{k}\sigma} + \frac{1}{2V}\sum_{\substack{\mathbf{k},\mathbf{k}',\mathbf{q}\\ \sigma,\sigma'}} \Delta v(\mathbf{k},\mathbf{k}',\mathbf{q})\; a^\dagger_{\mathbf{k}\sigma}a^\dagger_{\mathbf{k}'\sigma'}a_{\mathbf{k}'+\mathbf{q}\sigma'}a_{\mathbf{k}-\mathbf{q}\sigma}\;, \tag{5.28}$$

where the single particle spectrum has been renormalized, $\varepsilon_{\mathbf{k}} \to \varepsilon_{\mathbf{k}} + \Delta\varepsilon_{\mathbf{k}}$ with

$$\Delta\varepsilon_{\mathbf{k}} = \sum_{\mathbf{k}'}\frac{|g_{\mathbf{k},\mathbf{k}-\mathbf{k}'}|^2}{\varepsilon_{\mathbf{k}}-\varepsilon_{\mathbf{k}'}-\hbar\omega_{\mathbf{k}'-\mathbf{k}}}\,, \tag{5.29}$$

and an effective electron-electron interaction has been induced by phonon exchange, with coupling

$$\Delta v(\mathbf{k},\mathbf{k}',\mathbf{q}) = 2V\frac{|g_{\mathbf{k},\mathbf{q}}|^2\hbar\omega_{\mathbf{q}}}{(\varepsilon_{\mathbf{k}}-\varepsilon_{\mathbf{k}'})^2-(\hbar\omega_{\mathbf{q}})^2}\,. \tag{5.30}$$

In fact, first order perturbation theory with respect to $\Delta\varepsilon$ and Δv gives

$$\begin{aligned}\Delta E &= 2\sum_{\mathbf{k}} f_{\mathbf{k}}\Delta\varepsilon_{\mathbf{k}} \\ &+ \frac{1}{V}\sum_{\mathbf{k},\mathbf{k}'} f_{\mathbf{k}}f_{\mathbf{k}'}\left[2\Delta v(\mathbf{k},\mathbf{k}',0) - \Delta v(\mathbf{k},\mathbf{k}',\mathbf{k}-\mathbf{k}')\right].\end{aligned} \tag{5.31}$$

The Hartree term with momentum transfer zero vanishes since $g(\mathbf{k},\mathbf{q}=\mathbf{0}) = 0$. Therefore we recover indeed Eq. (5.27). The crucial point is that the effective coupling function (5.30) is attractive for $|\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}'}| < \hbar\omega_{\mathbf{k}-\mathbf{k}'}$. A more elaborate treatment using the technique of Green functions confirms that close to the Fermi surface the electron-phonon interaction leads to an effective attraction.

6 Superconductivity: BCS theory

The aim of this chapter is to present the BCS theory, the probably most successful microscopic description of a collective quantum phenomenon. Another important theory, the Ginzburg-Landau theory, does not depend on microscopic details but rather establishes a general phenomenological framework for the transition from the normal to the superconducting phase. We will limit ourselves to the microscopic BCS theory.

6.1 Cooper pairs

From now on it will be assumed that the electron-phonon interaction (or possibly also the exchange of another type of boson, for instance a magnon) can produce an effective attraction beween electrons. If the attractive interaction is strong enough, two electrons may form a bound state or composite boson. In such a case it is tempting to develop a model for superconductivity in terms of a Bose-Einstein condensation of electron pairs. However, for ordinary superconductors the attraction is not strong enough to produce a two-electron bound state (except in one and two dimensions). The reason is that in three dimensions the single-particle density of states

$$N(\varepsilon) = \frac{1}{V}\sum_{\mathbf{k}} \delta(\varepsilon - \varepsilon_{\mathbf{k}}) \tag{6.1}$$

tends to zero for $\varepsilon \to 0$ (in the case of a parabolic spectrum). Cooper realized that the situation is different if we add two electrons to the filled Fermi sea (and not to the vacuum).

For simplicity, we limit ourselves on that part of the Hamiltonian which is relevant for both the Cooper problem and the BCS theory, the so-called reduced Hamiltonian

$$H_{red} = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} a^+_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma} + \frac{1}{V}\sum_{\mathbf{k},\mathbf{k}'} \tilde{v}(\mathbf{k},\mathbf{k}')\ a^+_{\mathbf{k}\uparrow} a^+_{-\mathbf{k}\downarrow} a_{-\mathbf{k}'\downarrow} a_{\mathbf{k}'\uparrow}\ . \tag{6.2}$$

For the Cooper problem we assume $\tilde{v}(\mathbf{k},\mathbf{k}')$ to be attractive in a finite strip above the Fermi energy,

$$\tilde{v}(\mathbf{k},\mathbf{k}') = \begin{cases} -g & , \quad \varepsilon_F < \varepsilon_{\mathbf{k}}, \varepsilon_{\mathbf{k}'} < \varepsilon_F + \hbar\omega_D\ , \\ 0 & , \quad \text{otherwise,} \end{cases} \tag{6.3}$$

where the Debye frequency ω_D is the characteristic scale of acoustic phonons. An added pair with total momentum zero and $S_z = 0$ is described by the state

$$|\Psi\rangle = \sum_{\mathbf{k}} \varphi(\mathbf{k}) a^+_{\mathbf{k}\uparrow} a^+_{-\mathbf{k}\downarrow} |\mathrm{F}\rangle\,. \tag{6.4}$$

We look for an eigenstate of energy E. Applying the reduced Hamiltonian on the pair state we get

$$H_{red}|\Psi\rangle = \sum_{\mathbf{k}} \varphi(\mathbf{k})(E_0 + 2\varepsilon_{\mathbf{k}}) a^+_{\mathbf{k}\uparrow} a^+_{-\mathbf{k}\downarrow}|\mathrm{F}\rangle + \frac{1}{V}\sum_{\mathbf{k},\mathbf{k}'} \varphi(\mathbf{k})\tilde{v}(\mathbf{k}',\mathbf{k}) a^+_{\mathbf{k}'\uparrow} a^+_{-\mathbf{k}'\downarrow}|\mathrm{F}\rangle\,, \tag{6.5}$$

where E_0 is the energy of the filled Fermi sea. Multiplying from the left by $\langle \mathrm{F}|a_{-\mathbf{k}'\downarrow}a_{\mathbf{k}'\uparrow}$, we obtain the eigenvalue equation

$$\varphi(\mathbf{k}')(E_0 + 2\varepsilon_{\mathbf{k}'} - E) + \frac{1}{V}\sum_{\mathbf{k}} \varphi(\mathbf{k})\tilde{v}(\mathbf{k}', \mathbf{k}) = 0. \tag{6.6}$$

Using Eq. (6.3) and summing over $\mathbf{k}'$ we arrive at the relation

$$1 = \frac{g}{V}\sum_{\mathbf{k}'}{}' \frac{1}{E_0 + 2\varepsilon_{\mathbf{k}'} - E}\ , \tag{6.7}$$

where the sum is restricted to the energy strip defined above. In the absence of interactions the lowest possible energy for a filled Fermi sea plus two additional electrons is $E = E_0 + 2\varepsilon_F$. Therefore the quantity $\varepsilon_b := E - E_0 - 2\varepsilon_F$ defines the binding energy due to the attractive coupling. With the density of states (6.1) Eq. (6.7) can be rewritten as

$$1 = g\int_{\varepsilon_F}^{\varepsilon_F + \hbar\omega_D} \frac{N(\varepsilon)}{2(\varepsilon - \varepsilon_F) - \varepsilon_b} \approx gN(\varepsilon_F)\int_{\varepsilon_F}^{\varepsilon_F + \hbar\omega_D} \frac{1}{2(\varepsilon - \varepsilon_F) - \varepsilon_b}\ , \tag{6.8}$$

where we have assumed that $N(\varepsilon)$ does not change appreciably on the scale $\hbar\omega_D \ll \varepsilon_F$. The integration is elementary and we obtain the interesting relation for the binding energy

$$\varepsilon_b \approx 2\hbar\omega_D e^{-\frac{2}{gN(\varepsilon_F)}}. \tag{6.9}$$

This is a non-analytic function, which cannot be obtained by a finite-order perturbation expansion.

6.2 BCS ground state

For a very low density of electrons and strong attraction we expect the system to consist of bound (bosonic) pairs, which may undergo a Bose-Einstein condensation at low temperatures. Eq. (6.4) is then a good starting point and we can consider the operator

$$b^+_{q=0} := \sum_{\mathbf{k}} \varphi(\mathbf{k}) a^+_{\mathbf{k}\uparrow} a^+_{-\mathbf{k}\downarrow} \tag{6.10}$$

approximately as a bosonic creation operator with momentum zero. Neglecting the residual interaction between the pairs we can write down the ground state of $\frac{N}{2}$ pairs as a Bose condensate

$$|\mathrm{BEC}\rangle = \frac{1}{\sqrt{(N/2)!}}\left(b^+_{q=0}\right)^{\frac{N}{2}}|0\rangle\,. \tag{6.11}$$

In the weak coupling limit (high density and weak attraction) the BCS state, which describes the instability of the Fermi surface with respect to a coherent pairing, is more appropriate. It is defined as

$$|\mathrm{BCS}\rangle = \prod_{\mathbf{k}}\left(u_{\mathbf{k}} + v_{\mathbf{k}} a^\dagger_{\mathbf{k}\uparrow} a^\dagger_{-\mathbf{k}\downarrow}\right)|0\rangle\,, \tag{6.12}$$

where the coefficients $u_{\mathbf{k}}, v_{\mathbf{k}}$ are variational parameters. The BCS state is normalized if

$$u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 = 1. \tag{6.13}$$

In this state the number of particles is not fixed, but this is not a problem in the thermodynamic limit (as in statistical mechanics, where the grand canonical ensemble produces the same thermodynamics as the canonical ensemble). We can obtain the projection of the BCS state onto the subspace with a fixed (even) number N of electrons as follows. We observe that $(a_{\mathbf{k}\uparrow}^\dagger a_{-\mathbf{k}\downarrow}^\dagger)^n$ vanishes for $n \geq 2$. Therefore we can write

$$u_{\mathbf{k}} + v_{\mathbf{k}} a_{\mathbf{k}\uparrow}^\dagger a_{-\mathbf{k}\downarrow}^\dagger = u_{\mathbf{k}} \left(1 + \frac{v_{\mathbf{k}}}{u_{\mathbf{k}}} a_{\mathbf{k}\uparrow}^+ a_{-\mathbf{k}\downarrow}^+\right) = u_{\mathbf{k}} \exp\left(\frac{v_{\mathbf{k}}}{u_{\mathbf{k}}} a_{\mathbf{k}\uparrow}^+ a_{-\mathbf{k}\downarrow}^+\right) . \tag{6.14}$$

The BCS state then reads

$$|\mathrm{BCS}\rangle = \text{const } \exp\left(\sum_{\mathbf{k}} \frac{v_{\mathbf{k}}}{u_{\mathbf{k}}} a_{\mathbf{k}\uparrow}^+ a_{-\mathbf{k}\downarrow}^+\right) |0\rangle . \tag{6.15}$$

Its projection onto the subspace with N electrons,

$$|\mathrm{BCS}\rangle_N = \text{const'} \left(\sum_{\mathbf{k}} \frac{v_{\mathbf{k}}}{u_{\mathbf{k}}} a_{\mathbf{k}\uparrow}^+ a_{-\mathbf{k}\downarrow}^+\right)^{\frac{N}{2}} |0\rangle , \tag{6.16}$$

is equal to Eq. (6.11) except that the wave function $\varphi(\mathbf{k})$ has been replaced by $\frac{v_{\mathbf{k}}}{u_{\mathbf{k}}}$. The calculations are much simpler for the full BCS state (6.12) than for the projected state.

We have to minimize the expectation value of the reduced Hamiltonian (6.2), $\langle \mathrm{BCS}|H_{\mathrm{red}}|\mathrm{BCS}\rangle$, for a given average number of electrons

$$\bar{N} = \langle \mathrm{BCS}|N|\mathrm{BCS}\rangle, \quad \text{where } N = \sum_{\mathbf{k},\sigma} a_{\mathbf{k}\sigma}^+ a_{\mathbf{k}\sigma} . \tag{6.17}$$

This is carried out by introducing the chemical potential μ as a Lagrange multiplier. Thus we have to minimize first the expression

$$W := \langle \mathrm{BCS}|H_{red} - \mu N|\mathrm{BCS}\rangle \tag{6.18}$$

and at the end fix μ by solving Eq. (6.17).

We use a similar model for the attraction as in the Cooper problem and restrict the coupling to a strip of width $2\hbar\omega_D$ around the chemical potential μ (which is approximately equal to the Fermi energy ε_F in the weak-coupling limit).

$$\tilde{v}(\mathbf{k}, \mathbf{k}') = \begin{cases} -g, & \mu - \hbar\omega_D < \varepsilon_{\mathbf{k}}, \varepsilon_{\mathbf{k}'} < \mu + \hbar\omega_D , \\ 0, & \text{otherwise.} \end{cases} \tag{6.19}$$

The single-particle states outside this strip are not affected and we have

$$u_{\mathbf{k}} = \begin{cases} 0, & \varepsilon_{\mathbf{k}} < \mu - \hbar\omega_D , \\ 1, & \varepsilon_{\mathbf{k}} > \mu + \hbar\omega_D . \end{cases} \qquad v_{\mathbf{k}} = \begin{cases} 1, & \varepsilon_{\mathbf{k}} < \mu - \hbar\omega_D , \\ 0, & \varepsilon_{\mathbf{k}} > \mu + \hbar\omega_D . \end{cases} \tag{6.20}$$

With the parametrization

$$u_{\mathbf{k}} = \cos\vartheta_{\mathbf{k}}\,, \quad v_{\mathbf{k}} = \sin\vartheta_{\mathbf{k}} \tag{6.21}$$

the relation (6.13) is automatically satisfied.

It is straightforward to calculate the expectation value (6.18). One finds

$$\begin{aligned} W &= 2\sum_{\mathbf{k}} \xi_{\mathbf{k}} v_{\mathbf{k}}^2 - \frac{g}{V}\sum_{\mathbf{k},\mathbf{k}'} u_{\mathbf{k}} v_{\mathbf{k}} u_{\mathbf{k}'} v_{\mathbf{k}'} \\ &= \sum_{\mathbf{k}} \xi_{\mathbf{k}}(1-\cos 2\vartheta_{\mathbf{k}}) - \frac{g}{4V}\left(\sum_{\mathbf{k}} \sin 2\vartheta_{\mathbf{k}}\right)^2 , \end{aligned} \tag{6.22}$$

where $\xi_{\mathbf{k}} := \varepsilon_{\mathbf{k}} - \mu$. (The diagonal term of the interaction energy, $\mathbf{k} = \mathbf{k}'$, is not correct, but this error is negligible in the thermodynamic limit.) The signs have to be chosen such as to render this expression as small as possible. The sign of $\sin 2\vartheta_{\mathbf{k}}$ is arbitrary (we choose $\sin 2\vartheta_{\mathbf{k}} > 0$), but not that of $\cos 2\vartheta_{\mathbf{k}}$ which has to fulfill

$$\mathrm{sign}(\cos 2\vartheta_{\mathbf{k}}) = \mathrm{sign}(\xi_{\mathbf{k}}) \tag{6.23}$$

because W is required to be a minimum. Moreover, the equation $\partial W/\partial\vartheta_{\mathbf{k}} = 0$ leads to

$$\xi_{\mathbf{k}} \tan 2\vartheta_{\mathbf{k}} = \frac{g}{2V}\sum_{\mathbf{k}'} \sin 2\vartheta_{\mathbf{k}'}\,, \tag{6.24}$$

where both $\mathbf{k}$ and $\mathbf{k}'$ are in the region of $\mathbf{k}$-space defined above. Introducing the (positive) gap parameter

$$\Delta_{\mathbf{k}} := \xi_{\mathbf{k}} \tan 2\vartheta_{\mathbf{k}}\,, \tag{6.25}$$

we can write Eq. (6.24) as

$$\Delta_{\mathbf{k}} = \frac{g}{2V}\sum_{\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}}{E_{\mathbf{k}'}}, \tag{6.26}$$

where

$$E_{\mathbf{k}} := \sqrt{\xi_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}\,. \tag{6.27}$$

With

$$\Delta_{\mathbf{k}} = \begin{cases} \Delta_0 & , \quad |\xi_{\mathbf{k}}| < \hbar\omega_D\,, \\ 0 & , \quad \text{otherwise}\,, \end{cases} \tag{6.28}$$

and the replacement

$$\frac{1}{V}\sum_{\mathbf{k}} f(\xi_{\mathbf{k}'}) \to N(\varepsilon_F)\int_{-\hbar\omega_D}^{\hbar\omega_D} d\xi\ f(\xi) \tag{6.29}$$

the *gap equation* (6.26) becomes

$$1 = \frac{g}{2}N(\varepsilon_F)\int_{-\hbar\omega_D}^{\hbar\omega_D} d\xi\ \frac{1}{\sqrt{\xi^2+\Delta_0^2}}\,. \tag{6.30}$$

This equation is readily solved, we get

$$\Delta_0 = \hbar\omega_D \frac{1}{\sinh\frac{1}{gN(\varepsilon_F)}} \approx 2\hbar\omega_D e^{-\frac{1}{N(\varepsilon_F)g}}\,, \tag{6.31}$$

where the approximate expression is valid in the weak-coupling limit, $gN(\varepsilon_F) \ll 1$. This result resembles the binding energy of a Cooper pair, Eq. (6.9), it is again a non-analytic function of the coupling strength.

In the strong-coupling limit one can show that the gap equation (6.26) is nothing but the eigenvalue equation (6.6) "in disguise" (A. J. Leggett, Proc. 16th Karpacz Winter School, Lecture Notes in Physics **115**, Springer 1980, p. 13). The BCS state describes in fact a smooth crossover from a coherent many-electron bound state (with "pair size" larger than the interpair distance and a chemical potential $\mu \approx \varepsilon_F$) for weak coupling to a Bose condensate of bound pairs (with $\mu < 0$) for strong coupling.

The physical meaning of $E_{\mathbf{k}}$ can be understood by calculating the energy required for adding an electron with momentum $\hbar\mathbf{k}$ to the system. This *quasi-particle* energy is just equal to $E_{\mathbf{k}}$ (see J. R. Schrieffer, *Theory of Superconductivity*, Section 2.5).

6.3 Thermodynamics

It is straightforward to generalize the BCS theory to finite temperatures T, using a self-consistent field method. Here we simply quote the main results and use them to calculate the specific heat.

For $T > 0$ the gap parameter becomes temperature dependent. Eq. (6.26) is replaced by ($\beta = \frac{1}{k_B T}$)

$$\Delta_{\mathbf{k}} = \frac{g}{2V} \sum_{\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}}{E_{\mathbf{k}'}} \tanh \frac{\beta E_{\mathbf{k}'}}{2} \,, \tag{6.32}$$

which goes over into Eq. (6.26) for $T \to 0$. Proceeding as above we obtain the finite temperature gap equation

$$1 = \frac{g}{2} N(\varepsilon_F) \int_{-\hbar\omega_D}^{\hbar\omega_D} d\xi \; \frac{1}{\sqrt{\xi^2 + \Delta^2}} \; \tanh \left(\frac{\beta}{2} \sqrt{\xi^2 + \Delta^2} \right) . \tag{6.33}$$

The r.h.s. is a decreasing function of both T and Δ. It follows that the solution of Eq. (6.33), $\Delta(T)$, decreases with increasing temperature until it vanishes at a critical temperature T_c. For weak coupling ($k_B T_c \ll \hbar\omega_D$) the function $\Delta(T)$, depicted in Fig. 6, is universal. For $T = 0$ the solution of the gap equation is given by Eq. (6.31). For $T = T_c$ partial integration gives

$$\begin{aligned} 1 &= gN(\varepsilon_F) \int_0^{\beta_c \hbar\omega_D} dy \, \frac{1}{y} \, \tanh \frac{y}{2} \\ &= gN(\varepsilon_F) \left[\log(\beta_c \hbar\omega_D) \, \tanh \, \frac{\beta_c \hbar\omega_D}{2} \, - \frac{1}{2} \int_0^{\beta_c \hbar\omega_D} dy \, \log y \, \operatorname{sech}^2 \, \frac{y}{2} \right] . \end{aligned}$$

In the last term we can replace $\beta_c \hbar\omega_D$ by ∞ (in the weak coupling limit) and use

$$-\frac{1}{2} \int_0^{\infty} dy \, \log y \, \operatorname{sech}^2 \frac{y}{2} = \log \left(\frac{2\gamma}{\pi} \right) ,$$

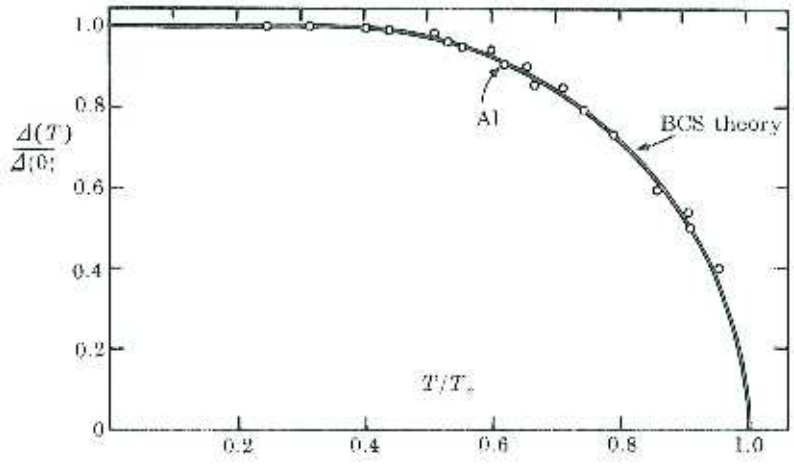

Figure 6: Temperature dependence of the gap parameter (after Schrieffer).

where γ is Euler's constant, i.e. $\frac{2\gamma}{\pi} \approx 1.13$. Thus we get

$$k_B T_c \approx 1.13 \hbar\omega_D \, e^{-\frac{1}{gN(\varepsilon_F)}} \,. \tag{6.34}$$

Comparing Eqs. (6.31) and (6.34) we obtain an interesting relation between the energy gap at $T = 0$, $E_g = 2\Delta(0)$, and the critical temperature

$$\frac{E_g}{k_B T_c} \approx 3.53 \,. \tag{6.35}$$

This relation, often used to check whether a superconducting material is BCS-like, is well satisfied in elemental superconductors:

Al	Cd	Ga	Hg	In	La	Nb	Pb	Sn	Ta	Tl	V	Zn
3.53	3.44	3.5	3.95	3.65	3.72	3.65	3.95	3.6	3.63	3.63	3.50	3.44

(after R. Meservey and B. B. Schwartz, in the book of Parks).

With $\Delta(T)$ given, the excitation energies

$$E_{\mathbf{k}}(T) = \sqrt{\xi_{\mathbf{k}}^2 + \Delta^2(T)} \tag{6.36}$$

are fixed and determine the quasi-particle occupation numbers

$$f_{\mathbf{k}} = \frac{1}{e^{\beta E_{\mathbf{k}}} + 1} \,. \tag{6.37}$$

One can show that the electronic entropy is simply given by that of a free fermion gas with spin $\frac{1}{2}$ and with the excitation spectrum (6.36), namely

$$S = -2k_B \sum_{\mathbf{k}} [(1 - f_{\mathbf{k}}) \log(1 - f_{\mathbf{k}}) + f_{\mathbf{k}} \log f_{\mathbf{k}}] \,. \tag{6.38}$$

The presence of the gap implies that in the superconducting phase the entropy is lower than it would be for $\Delta = 0$ (see Fig. 7). The superconducting phase has a higher degree of order than the normal phase. The specific heat per unit volume is given by

$$\begin{aligned} \frac{C_V}{V} &= \frac{T}{V}\frac{\partial S}{\partial T} = \frac{2}{V}\sum_{\mathbf{k}} E_{\mathbf{k}} \frac{\partial f_{\mathbf{k}}}{\partial E_{\mathbf{k}}} \left(\frac{\Delta}{E_{\mathbf{k}}} \frac{d\Delta}{dT} - \frac{E_{\mathbf{k}}}{T} \right) \\ &\approx 2N(\varepsilon_F) \int_{-\infty}^{\infty} d\xi \left(\frac{1}{2} \frac{d\Delta^2}{dT} - \frac{E^2}{T} \right) \frac{\partial f}{\partial E} , \end{aligned} \tag{6.39}$$

where $E = \sqrt{\xi^2 + \Delta^2}$. Close to T_c, where

$$\frac{\Delta(T)}{\Delta(0)} \sim 1.74 \left(\frac{T_c - T}{T_c} \right)^{\frac{1}{2}} , \tag{6.40}$$

the derivative $\frac{d\Delta^2}{dT}$ is finite when approaching T_c from below and it vanishes for $T > T_c$, where the specific heat is given by the usual expression

$$\frac{C_V^{(n)}}{V} = \gamma T = \frac{2\pi^2}{3} N(\varepsilon_F) k_B^2 T .$$

It follows that there is a step at T_c

$$\frac{C_V^{(s)} - C_V^{(n)}}{C_V^{(n)}} \approx 1.43 , \tag{6.41}$$

in quite good agreement with experiments on elemental superconductors:

Al	Cd	Ga	Hg	In	La	Nb	Pb	Sn	Ta	Tl	V	Zn
1.4	1.4	1.4	2.37	1.73	1.5	1.9	2.71	1.60	1.59	1.50	1.49	1.3

(after R. Meservey and B. B. Schwartz, in the book of Parks). The BCS prediction for the specific heat is illustrated in Fig. 7.

We did not discuss the most striking phenomena of superconductivity, such as persistent currents, Meissner effect, flux quantization or Josephson tunneling. This would require to extend BCS theory by adding the coupling to an electromagnetic field. We do not present this extension here, but simply mention that this coupling can be readily obtained in BCS theory in terms of the standard replacement (see, for instance, Chapter 8 of Schrieffer's book)

$$\mathbf{p} \to \mathbf{p} + e\mathbf{A}, \quad i\hbar\frac{\partial}{\partial t} \to i\hbar\frac{\partial}{\partial t} - e\Phi. \tag{6.42}$$

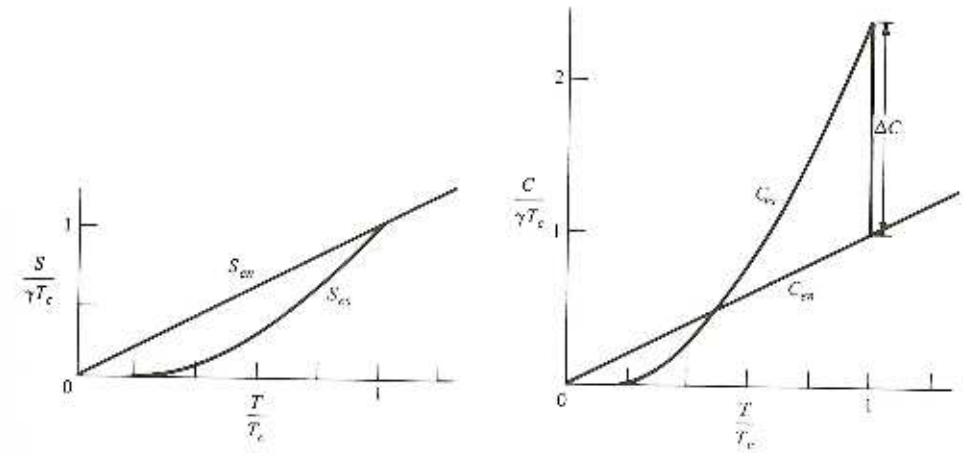

Figure 7: Entropy and specific heat according to BCS (from Tinkham).

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