1. Second quantization in quantum field theory

1.1   Fock space in quantum theory

■ **Evolution equations of a many-particle system.** Consider the N-particle Hamilton operator of identical particles with a pair interaction

$$\widehat{H} = \sum_{k=1}^{N} \widehat{T}(x_k) + \frac{1}{2} \sum_{\substack{k,l=1 \\ k \neq l}} \widehat{V}(x_k, x_l) \,. \tag{1.1}$$

This Hamilton operator generates the dynamics of the system through the Schrödinger equation

$$i\hbar \frac{\partial \Psi}{\partial t} = \widehat{H}\Psi \,, \tag{1.2}$$

for the wave function Ψ of the system, if the system is in a pure state. The other possibility is the von Neumann equation for the density operator $\widehat{\rho}$

$$i\hbar \frac{\partial \widehat{\rho}}{\partial t} = \left[\widehat{H}, \widehat{\rho} \right] \,. \tag{1.3}$$

This equation reduces to the Schrödinger equation for the density operator of the pure state $\widehat{\rho} = |\,\Psi\,\rangle\langle\,\Psi\,|$.

For systems with a variable number of particles the explicit dependence on the particle number is inconvenient. Evolution of quantum system may be represented in a form independent of the particle number in a *Fock space* with operators in their *second-quantized* form. The price to pay for this is less mathematical rigour, since the Fock space is not a Hilbert space anymore: its basis is uncountable.

■ **Many-particle systems.** It is convenient to express wave functions of many-particle systems as linear combinations of products of one-particle wave functions of the form

$$\psi_{\ell_1}(\xi_1)\psi_{\ell_2}(\xi_2)\cdots\psi_{\ell_N}(\xi_N) \,,$$

where $\xi_i = (\boldsymbol{x}_i, s_i)$ (s_i is the spin of the particle) and ψ_n are eigenfunctions of the one-particle Hamiltonian enumerated by the quantum number ℓ. This allows to introduce the *occupation number* representation for identical particles: the number of occurrences n_ℓ of one-particle functions of a particular

quantum number ℓ is the number of particles in this state. This is an illustrative way of speaking only: in a many-particle quantum system the very notion of one particle in a given state is actually meaningless.

For identical particles symmetry conditions are imposed on the physical wave functions. The particles are either bosons of fermions. The former obey Bose–Einstein statistics and the wave function must be completely symmetric with respect to all permutations of the particle arguments. The latter obey Fermi–Dirac statistics, requiring complete antisymmetry (change of sign) in any permutation of a pair of particle arguments of the wave functions. These requirements have a profound effect on the statistical mechanics.

■ **Basis vectors of a Fock space.** From the point of view of statistical physics, the quantum mechanics of many-particle systems is most conveniently formulated in the *Fock space*, which allows to treat systems with variable number of particles. The Fock space is a direct sum of all properly (anti)symmetrized N-particle Hilbert spaces. In the coordinate representation a state vector of a Fock space may be written as column vector with an infinite number of elements

$$
\Phi = \begin{pmatrix} \zeta \\ \psi_1(\xi_1) \\ \psi_2(\xi_1, \xi_2) \\ \dots \\ \psi_N(\xi_1, \dots, \xi_N) \\ \dots \end{pmatrix}, \tag{1.4}
$$

where ζ is a complex number, $\xi_i = (\boldsymbol{x}_i, s_i)$ and $\psi_N(\xi_1, \dots, \xi_N)$ is a completely (anti)symmetric wave function of an N-particle system.

The basis elements of the Fock space are obtained with the use of all possible properly normalized (anti)symmetric linear combinations of one-particle wave functions (i.e. the one-particle basis functions of the Hilbert space of the N-particle system) as the N-particle elements of the Fock-space vector (1.4). The coordinate (configuration-space) representation of a basis vector contains a single nonvanishing element on the "row" number $N+1$ which may be expressed as

$$
\langle \xi_1, \dots, \xi_N | \{n_\ell\} \rangle = \sqrt{\frac{1}{N! \prod_\ell n_\ell!}} \sum_{P(\xi_1, \dots, \xi_N)} \varepsilon_P \langle \xi_1 | \ell_1 \rangle \cdots \langle \xi_N | \ell_N \rangle, \tag{1.5}
$$

where $\ell_1, \ell_2, \dots, \ell_N$ are labels of the one-particle states and the summation goes over all $N!$ permutations of the argument permutations and ε_P is a sign factor, which for bosons is always 1, whereas for fermions ± 1 according to the parity of the permutation (in the fermionic case this is a $N \times N$ Slater determinant).

The normalization factor in (1.5) may by calculated by the traditional "box-filling" procedure, in which "boxes" corresponding to one-particle

states are filled by enumerated balls in all possible ways to count the number of linearly independent terms in the sum on the right-hand side of (1.5). Let us start by putting a ball in the first box. There are N possibilities to do this. For the second ball there are $N - 1$ possibilities for all initial N cases, thus $N(N - 1)$. After having the required number n_1 of balls in the first box, we notice that we have counted each different term $n_1!$ times, since the order of casting the balls does not make any difference. Restore the correct relative weight of each term by dividing by $n_1!$. So far $N(N - 1)\ldots(N - n_1 + 1)/n_1!$ different terms with n_1 particles have been obtained. For the second box, the starting number of possibilities is $N - n_1$. After completing the filling of all boxes, we arrive at the number of

$$\frac{N!}{n_1! n_2! \cdots n_\ell! \cdots}, \qquad \sum_\ell n_\ell = N$$

of linearly independent terms involved in the basis vector (1.5). In the normalization factor it should be taken into account that the coefficient of each linearly independent term in the (anti)symmetrized expression is $n_1! n_2! \cdots n_\ell! \cdots$. These terms are orthonormal, so that

$$\int d\xi_1 \cdots \int d\xi_N \sum_{P(\xi_1,\ldots,\xi_N)} \varepsilon_P \langle \ell_1 | \xi_1 \rangle \cdots \langle \ell_N | \xi_N \rangle \sum_{P(\xi_1,\ldots,\xi_N)} \varepsilon_P \langle \xi_1 | \ell_1 \rangle \cdots \langle \xi_N | \ell_N \rangle$$
$$= (n_1! n_2! \cdots n_\ell! \cdots)^2 \frac{N!}{n_1! n_2! \cdots n_\ell! \cdots},$$

which gives rise to the normalization of (1.5).

In (1.5) the notation refers to a Dirac state vector determined by the set of occupation numbers: N-particle states may be enumerated as

$$|\{n_\ell\}\rangle \equiv |n_1, \ldots, n_\ell, \ldots\rangle, \tag{1.6}$$

where $n_1, \ldots, n_\ell$ are the occupation numbers of the one-particle states $\{\ell\} = \{1, 2, 3, \ldots\}$. In an N-particle state obviously $\sum_\ell n_\ell = N$. This notation is very convenient for calculations with the use of creation and annihilation operators. Its connection with the Fock space in the configuration-space form spanned by (1.4) is not obvious, however.

■ **Creation and annihilation operators.** In a Fock space spanned by the occupation-number basis states (1.6) hermitian conjugated creation and annihilation operators a_ℓ^+ and a_ℓ are defined in the occupation-number representation by the rules

$$a_\ell | n_1, \ldots, n_\ell, \ldots \rangle = (-1)^{P_\ell(\{n\})} \sqrt{n_\ell}\, | n_1, \ldots, n_\ell - 1, \ldots \rangle, \tag{1.7}$$
$$a_\ell^+ | n_1, \ldots, n_\ell, \ldots \rangle = (-1)^{P_\ell(\{n\})} \sqrt{1 \pm n_\ell}\, | n_1, \ldots, n_\ell + 1, \ldots \rangle. \tag{1.8}$$

Here, the upper and lower sign refer to bosons and fermions, respectively. The sign factor $(-1)^P$ is equal to the unity for bosons, while for fermions it

may be defined through relation

$$P_\ell(\{n\}) = \sum_{k(<\ell)} n_k.$$

Here, it is implied that for the state-numbering subscript $\{\ell\}$ some ordering rule has been chosen. From the definitions and symmetry properties of the basis states it follows that bosonic operators obey the *commutation rules*

$$\left[a_\ell, a_{\ell'}\right] = \left[a_\ell^+, a_{\ell'}^+\right] = 0; \qquad \left[a_\ell, a_{\ell'}^+\right] = \delta_{\ell\ell'}, \tag{1.9}$$

where δ is the Kronecker symbol, whereas fermionic operators obey the *anticommutation rules*

$$\left[a_\ell, a_{\ell'}\right]_+ = \left[a_\ell^+, a_{\ell'}^+\right]_+ = 0; \qquad \left[a_\ell, a_{\ell'}^+\right]_+ = \delta_{\ell\ell'}. \tag{1.10}$$

Here, $[A, B]_+ \equiv AB + BA$. The eigenvalues of the *occupation-number operator* of the state $|\ell\rangle$

$$\widehat{n}_\ell = a_\ell^+ a_\ell \tag{1.11}$$

n_ℓ are all natural numbers $0, 1, 2, \ldots$ for bosons, but only 0 and 1 for fermions. The latter conclusion follows immediately from the relation $\widehat{n}_\ell^2 = \widehat{n}_\ell$, which is readily checked by the anticommutation rules. This is a formal explanation of the *Pauli exclusion principle* stating that no more than one fermion can occupy a one-particle state.

■ **Ground state and occupation-number basis.** To construct the basis states (1.6) explicitly in terms of the operators $\widehat{a}^+$ and $\widehat{a}$, introduce the *ground state* (vacuum) $|0\rangle$ with the properties

$$\widehat{a}|0\rangle = 0, \qquad \langle 0|0\rangle = 1. \tag{1.12}$$

The properly normalized basis vectors may then be written as

$$|\{n_\ell\}\rangle = |n_1, \ldots, n_\ell, \ldots\rangle$$
$$= \sqrt{\frac{1}{n_1! n_2! \cdots n_\ell! \cdots}} \left(\widehat{a}_1^+\right)^{n_1} \left(\widehat{a}_2^+\right)^{n_2} \cdots \left(\widehat{a}_\ell^+\right)^{n_\ell} \cdots |0\rangle. \tag{1.13}$$

Note that there is no explicit N here anymore. The ground-state vector for bosons may be visualized as a direct product of infinite-dimensional column vectors (one for each one-particle state) of the form

$$|0_\ell\rangle = \begin{pmatrix} 1 \\ 0 \\ \vdots \end{pmatrix}_\ell. \tag{1.14}$$

The action of the creation operator on this vacuum state is given by the usual rules of matrix multiplication with the matrix

$$\widehat{a}_\ell^+ = \begin{pmatrix} 0 & 0 & 0 & \dots\dots\dots & 0 & \dots \\ 1 & 0 & 0 & \dots\dots\dots & 0 & \dots \\ 0 & \sqrt{2} & 0 & \dots\dots\dots & 0 & \dots \\ \dots\dots\dots\dots\dots\dots\dots\dots\dots \\ 0 & 0 & 0 & \dots & 0 & 0 & \dots \\ 0 & 0 & 0 & \dots & \sqrt{n_\ell} & 0 & \dots \\ \dots\dots\dots\dots\dots\dots\dots\dots\dots \end{pmatrix}. \tag{1.15}$$

acting on the ℓth column vector only. Since the annihilation operator $\widehat{a}_\ell$ is the Hermitian conjugate to the creation operator, from here it immediately follows that :

$$\widehat{a}_\ell = \begin{pmatrix} 0 & 1 & 0 & \dots\dots & 0 & \dots \\ 0 & 0 & \sqrt{2} & \dots\dots & 0 & \dots \\ 0 & 0 & 0 & \dots\dots & 0 & \dots \\ \dots\dots\dots\dots\dots\dots\dots\dots \\ 0 & 0 & 0 & \dots & 0 & \sqrt{n_\ell} & \dots \\ 0 & 0 & 0 & \dots & 0 & 0 & \dots \\ \dots\dots\dots\dots\dots\dots\dots\dots \end{pmatrix}. \tag{1.16}$$

■ **Schrödinger equation in the occupation-number representation.** In terms of the creation and annihilation operators the Hamilton operator (1.1) of the many-particle system assumes the form

$$\widehat{H} = \sum_{k,l} \langle\, k\,|\widehat{T}|\, l\,\rangle \widehat{a}_k^+ \widehat{a}_l + \frac{1}{2} \sum_{i,j,k,l} \langle\, ij\,|\widehat{V}|\, kl\,\rangle \widehat{a}_i^+ \widehat{a}_j^+ \widehat{a}_l \widehat{a}_k \,, \tag{1.17}$$

where $\langle\, k\,|\widehat{T}|\, l\,\rangle$ and $\langle\, i,j\,|\widehat{V}|\, k,l\,\rangle$ are the matrix elements of the respective operators in the one-particle state basis, e.g.

$$\langle\, ij\,|\widehat{V}|\, kl\,\rangle = \int d\xi \int d\xi'\, \psi_i^*(\xi)\psi_j^*(\xi')\widehat{V}(\xi,\xi')\psi_k(\xi)\psi_l(\xi')\,.$$

Note that in (1.17) sums are taken over all *one-particle states* instead of the sums over the particle numbers in the configuration-space Hamiltonian (1.1). Thus, there is no explicit number of particles in the system in Hamiltonian (1.17).

To construct the Schrödinger equation in the occupation-number representation, expand first the wave function Ψ from (1.1) in the set (1.5):

$$\Psi(t,\xi_1,\dots,\xi_N) = \sum_{\{n_\ell\}} \langle\, \xi_1,\dots,\xi_N\,|\,\{n_\ell\}\,\rangle \langle\, \{n_\ell\}\,|\,\Psi\,\rangle\,,$$

where the set of coefficient functions $\langle\, \{n_\ell\}\,|\,\Psi\,\rangle$ is the wave function in the occupation-number basis. Note that the set (1.5) consists of stationary one-particle functions, therefore the time dependence of the wave function is

solely in $\langle\,\{n_\ell\}\,|\,\Psi\,\rangle$. Substitution of this expansion in the Schrödinger equation (1.2) yields

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\langle\,\{n_\ell\}\,|\,\Psi\,\rangle$$
$$= \sum_{\{m_\ell\}}\int d\xi_1\ldots\int d\xi_N\,\langle\,\{n_\ell\}\,|\,\xi_1,\ldots,\xi_N\,\rangle\widehat{H}\langle\,\xi_1,\ldots,\xi_N\,|\,\{m_\ell\}\,\rangle\langle\,\{m_\ell\}\,|\,\Psi\,\rangle\,.$$

The matrix elements of the Hamiltonian here are written in the configuration-space basis (1.5) and the transition to the occupation number basis (1.13) boils down to demonstration that these matrix elements may be expressed with the aid of the Hamiltonian in the occupation-number basis (1.17), i.e. that

$$\int d\xi_1\ldots\int d\xi_N\,\langle\,\{n_\ell\}\,|\,\xi_1,\ldots,\xi_N\,\rangle\widehat{H}\langle\,\xi_1,\ldots,\xi_N\,|\,\{m_\ell\}\,\rangle$$
$$= \langle\,\{n_\ell\}\,|\widehat{H}|\,\{m_\ell\}\,\rangle\,,\quad(1.18)$$

where on the left-hand side the Hamiltonian stands in the configuration-space form (1.1), whereas on the right-hand side it stands in the occupation-number form (1.17). Reduction of the right-hand side requires calculation of matrix elements of operator monomials of the form (bosonic operators implied here)

$$\langle\,\{n_\ell\}\,|\widehat{a}_i^+\widehat{a}_j|\,\{m_\ell\}\,\rangle = \sqrt{n_i n_j}\,\delta_{n_1 m_1}\cdots\delta_{n_i-1 m_i}\cdots\delta_{n_j m_j-1}\cdots$$

Calculation of such matrix elements may be carried out straightforwardly with the use of the (anti)commutation rules and the explicit form of the basis vectors constructed with the aid of the creation and annihilation operators from the ground state. Expression of the matrix elements on the left-hand side of (1.18) in the same form and with the same sums requires some combinatorial manipulations and the use of the fact that most occupation numbers actually vanish. However, all this is a tedious effort to accomplish and utterly boring to look at, therefore, following classical textbooks, I leave this as an exercise for the student.

Taking relation (1.18) granted, the set of Schrödinger equations in the occupation-number representation may be conveniently expressed with the us of the *state vector*

$$|\,\Psi\,\rangle = \sum_{\{n_\ell\}}|\,\{n_\ell\}\,\rangle\langle\,\{n_\ell\}\,|\,\Psi\,\rangle$$

for which the Schrödinger equation assumes the form

$$i\hbar\frac{\mathrm{d}|\,\Psi\,\rangle}{\mathrm{d}t} = \widehat{H}|\,\Psi\,\rangle$$

with the Hamilton operator in the *second-quantized* form (1.17).

■ **Field operators.** Define now the *field operators* $\widehat{\psi}^+$ and $\widehat{\psi}$ as

$$\widehat{\psi}^+(\xi) = \sum_\ell \psi_\ell^*(\xi)\widehat{a}_\ell^+ , \qquad \widehat{\psi}(\xi) = \sum_\ell \psi_\ell(\xi)\widehat{a}_\ell . \tag{1.19}$$

The operator $\widehat{\psi}^+(\xi)$ creates a particle at ξ, the operator $\widehat{\psi}(\xi)$ destroys a particle at ξ. Relation (1.19) gives the name second quantization to this approach. The field operators obey the (anti)commutation relations

$$\left[\widehat{\psi}^+(\xi), \widehat{\psi}^+(\xi')\right]_\pm = \left[\widehat{\psi}(\xi), \widehat{\psi}(\xi')\right]_\pm = 0 , \quad \left[\widehat{\psi}(\xi), \widehat{\psi}^+(\xi')\right]_\pm = \delta(\xi - \xi') .$$

The *number density operator* is defined as

$$\widehat{n}(\xi) = \widehat{\psi}^+(\xi)\widehat{\psi}(\xi)$$

and gives rise to the *particle number operator*

$$\widehat{N} = \int d\xi \, \widehat{\psi}^+(\xi)\widehat{\psi}(\xi) .$$

In terms of the field operators the Hamilton operator (1.1) of the many particle system may be expressed in the suggestive form

$$\widehat{H} = \int d\xi \, \widehat{\psi}^+(\xi)\widehat{T}(\xi)\widehat{\psi}(\xi) + \frac{1}{2} \int d\xi \int d\xi' \, \widehat{\psi}^+(\xi)\widehat{\psi}^+(\xi')\widehat{V}(\xi,\xi')\widehat{\psi}(\xi')\widehat{\psi}(\xi) , \tag{1.20}$$

which allows to cast many-particle quantum mechanics into the form of a quantum field theory. The ordering of field operators in the interaction term is important for fermions. Nota that the explicit number of particles has disappeared both from the Hamilton operator and basis vectors of the Fock space.

The field operators are defined in (1.19) without any time dependence, i.e. in the Schrödinger picture. Their evolution in time is determined as the time evolution of any quantum-mechanical operator, let alone the density operator, by the Heisenberg picture. For a time-independent Hamilton operator this means

$$\widehat{\psi}^+(t,\xi) = e^{it\widehat{H}/\hbar}\widehat{\psi}^+(\xi)e^{-it\widehat{H}/\hbar} , \qquad \widehat{\psi}(t,\xi) = e^{it\widehat{H}/\hbar}\widehat{\psi}(\xi)e^{-it\widehat{H}/\hbar} .$$

■ **Noninteracting particles.** The Hamilton operator of a quantum system of noninteracting particles with the one-particle Hamilton operator $\widehat{H}(\xi)$ may be conveniently expressed in terms of the creation and annihilation operators and field operators

$$\widehat{H} = \sum_\ell \varepsilon_\ell \, \widehat{n}_\ell = \int d\xi \, \widehat{\psi}^+(\xi)\widehat{H}(\xi)\widehat{\psi}(\xi) , \tag{1.21}$$

when the one-particle states are eigenfunctions of a one-particle Hamilton operator (free particle or in some external field). The eigenvalue of the

energy of the system in the basis state $|n_1, \ldots, n_\ell, \ldots\rangle = |\{n_\ell\}\rangle$ of the Fock space is then

$$E = \sum_\ell \varepsilon_\ell n_\ell \,. \tag{1.22}$$

The sum in representations (1.21) and (1.22) goes over all one-particle states and there is no need to specify explicitly the number of particles in the system at hand.

It should be noted that in this case the field operator is a solution of the Schrödinger equation:

$$i\hbar \frac{\partial \widehat{\psi}(t,\xi)}{\partial t} = \widehat{H}(\xi)\widehat{\psi}(t,\xi) \,,$$

when the usual time dependence is included in the stationary-state wave functions of the field operator.

1.2   One-particle Green functions

In quantum field theory, *Green functions* are ground-state averages of *time-ordered products* (*chronological products*) of Heisenberg field operators, e.g. operators $\widehat{\psi}^+$ and $\widehat{\psi}$ in many-particle quantum mechanics. Let me introduce generic notation which covers both relativistic and nonrelativistic field theories and denote any field operator by $\widehat{\varphi}$. The time-ordered product of one field operator is the operator itself, in the more interesting case of two operators in the time ordered product the operators are put in the order of growing time arguments from the right to the left with the proper sign factor for fermionic operators:

$$T\left[\widehat{\varphi}(t_1,\xi_1)\widehat{\varphi}(t_2,\xi_2)\right] = \begin{cases} \widehat{\varphi}(t_1,\xi_1)\widehat{\varphi}(t_2,\xi_2), & t_1 > t_2 \,, \\ \kappa\,\widehat{\varphi}(t_2,\xi_2)\widehat{\varphi}(t_1,\xi_1), & t_1 < t_2 \,, \end{cases} \tag{1.23}$$

where $\kappa = 1$ for bosonic operators and $\kappa = -1$ for fermionic operators.

Note that the time-ordered product is not defined for coinciding time arguments. The way the definition (1.23) is amended for that case does affect the appearance of the mathematical description, although the physics is, of course, independent of that. It should also be noted that operators (anti)commute under the T-product sign. In a more compact – and suggestive for generalizations – form the T product of two field operators may be written as

$$\begin{aligned} T\left[\widehat{\varphi}(t_1,\xi_1)\widehat{\varphi}(t_2,\xi_2)\right] \\ = \theta(t_1 - t_2)\widehat{\varphi}(t_1,\xi_1)\widehat{\varphi}(t_2,\xi_2) + \kappa\,\theta(t_2 - t_1)\widehat{\varphi}(t_2,\xi_2)\widehat{\varphi}(t_1,\xi_1) \,. \end{aligned} \tag{1.24}$$

The Green function of a single field operator is the ground-state expectation value of the field operator itself. In a translation invariant system – which will be assumed if not stated otherwise – it is independent of position and time and in most cases (with a few important exceptions) simply vanishes.

On the contrary, the Green function of two field operators (the *one-particle Green function*, the *two-point function*)

$$G(t_1, \xi_1; t_2, \xi_2) = \langle T \left[\widehat{\varphi}(t_1, \xi_1) \widehat{\varphi}(t_2, \xi_2) \right] \rangle \qquad (1.25)$$

is one of the most important tools in the statistical analysis of many-particle systems.

For the field operators of second quantization of quantum mechanics $\widehat{\varphi}$ is a two-component quantity

$$\widehat{\varphi}(x) = \left(\begin{array}{c} \widehat{\psi}(x) \\ \widehat{\psi}^+(x) \end{array} \right) = \left(\begin{array}{c} \widehat{\psi}(x) \\ 0 \end{array} \right) + \left(\begin{array}{c} 0 \\ \widehat{\psi}^+(x) \end{array} \right)$$

and, correspondingly, the one-particle Green function is a 2×2 matrix (if the operators $\widehat{\psi}(x)$ and $\widehat{\psi}^+(x)$ are scalar quantities).

■ **One-particle Green functions of many-particle quantum mechanics.** The standard definition of the one-particle Green function of nonrelativistic field theory differs from the generic form (1.25) by the normalization factor $-i$:

$$G_{\alpha\beta}(x, x') = -i \left\langle T \left[\widehat{\psi}_{H\alpha}(x) \widehat{\psi}_{H\beta}^+(x') \right] \right\rangle, \qquad (1.26)$$

where α and β are spin-component indices and $x = (t, \boldsymbol{x})$. The time-dependent field operators in (1.26) are taken in the Heisenberg picture and the expectation value calculated in the ground state of the full Hamilton operator of the system. Expectation values of time-ordered operator products are usually not directly observable quantities and in a sense contain some superfluous information about the physical system. For instance, thermodynamic properties of many-body systems are often calculated with the use of the Green functions, which at first sight appear excessively complex tools for that task. The main point of using Green functions in the analysis of interacting many-particle systems is that for them relatively simple rules for perturbation theory have been constructed. It should also be noted that some technical problems related to the thermodynamic limit in direct calculation of the partition function may be circumvented within the Green function approach.

For instance, with the aid of the one-particle Green function ground-state expectation values of any one-particle operator (i.e. an operator acting on separate particles) $\widehat{A}$ may be calculated. Indeed, the second-quantized form of such an operator (for simplicity, consider operators including the sum over spin variables but independent of them; the trace in the following relations is then taken over the spin indices of the field operators)

$$\widehat{A} = \int d\boldsymbol{x} \operatorname{Tr} \widehat{\psi}^+(t, \boldsymbol{x}) \widehat{A}(\boldsymbol{x}) \widehat{\psi}(t, \boldsymbol{x})$$

yields for the expectation value

$$\left\langle \widehat{A} \right\rangle = \int d\boldsymbol{x} \left\langle \operatorname{Tr} \widehat{\psi}^+(t, \boldsymbol{x}) \widehat{A}(\boldsymbol{x}) \widehat{\psi}(t, \boldsymbol{x}) \right\rangle$$

so that

$$\left\langle \widehat{A} \right\rangle = \kappa i \int d\boldsymbol{x}\, \widehat{A}(\boldsymbol{x}) \operatorname{Tr} G(t, \boldsymbol{x}, t', \boldsymbol{x}') \Big|_{\substack{\boldsymbol{x}' \to \boldsymbol{x} \\ t' \to t+0}},$$

where the sign factor $\kappa = 1$ for bosons and $\kappa = -1$ for fermions. For instance, for the expectation values of number density and particle flux density we obtain

$$n(x) = \kappa i \lim_{\substack{\boldsymbol{x}' \to \boldsymbol{x} \\ t' \to t+0}} \operatorname{Tr} G(x, x'), \tag{1.27}$$

$$\boldsymbol{j}(x) = \kappa \frac{\hbar}{2m} \lim_{\substack{\boldsymbol{x}' \to \boldsymbol{x} \\ t' \to t+0}} (\nabla - \nabla') \operatorname{Tr} G(x, x'). \tag{1.28}$$

■ **Particles and holes.** The ground state of a free fermion system is the *Fermi sea*, in which all states with the wave number $k < k_F$ are occupied and states with $k > k_F$ empty. Let the field operator be (the spinor structure is implied)

$$\widehat{\psi}(\boldsymbol{x}) = \sum_{\boldsymbol{k},\sigma} \psi_{\boldsymbol{k},\sigma}(\boldsymbol{x}) \widehat{c}_{\boldsymbol{k},\sigma}.$$

Carry out a canonical transformation by introducing new creation and annihilation operators for particles (states $k > k_F$) and *holes* (states $k < k_F$) according to the rule

$$\widehat{c}_{\boldsymbol{k},\sigma} = \begin{cases} \widehat{a}_{\boldsymbol{k},\sigma}, & k > k_F, \\ \widehat{b}^+_{-\boldsymbol{k},\sigma}, & k < k_F. \end{cases} \tag{1.29}$$

Since the ground state $|\,0\,\rangle$ is the Fermi sea, it follows from the definitions that

$$\widehat{a}_{\boldsymbol{k},\sigma}|\,0\,\rangle = 0,$$

because all states with $k > k_F$ are empty and

$$\widehat{b}_{\boldsymbol{k},\sigma}|\,0\,\rangle = \widehat{c}^+_{-\boldsymbol{k},\sigma}|\,0\,\rangle = 0,$$

because all states in the Fermi sea are occupied. The anticommutation rules remain in the standard form for fermions and the Hamilton operator assumes the form

$$\widehat{H}_0 = \sum_{\boldsymbol{k},\sigma} \varepsilon_{\boldsymbol{k}} \widehat{c}^+_{\boldsymbol{k},\sigma} \widehat{c}_{\boldsymbol{k},\sigma}$$

$$= \sum_{|\boldsymbol{k}|>k_F,\sigma} \varepsilon_{\boldsymbol{k}} \widehat{a}^+_{\boldsymbol{k},\sigma} \widehat{a}_{\boldsymbol{k},\sigma} - \sum_{|\boldsymbol{k}|<k_F,\sigma} \varepsilon_{\boldsymbol{k}} \widehat{b}^+_{\boldsymbol{k},\sigma} \widehat{b}_{\boldsymbol{k},\sigma} + \sum_{|\boldsymbol{k}|<k_F,\sigma} \varepsilon_{\boldsymbol{k}}, \tag{1.30}$$

where the last term is the energy of the filled Fermi sea.

The time-dependent field operator in the new representation is (note that Heisenberg and Dirac pictures are identical for a free system)

$$\widehat{\psi}(t, \boldsymbol{x}) = \sum_{|\boldsymbol{k}|>k_F,\sigma} \psi_{\boldsymbol{k},\sigma}(\boldsymbol{x}) e^{-i\omega_k t} \widehat{a}_{\boldsymbol{k},\sigma} + \sum_{|\boldsymbol{k}|<k_F,\sigma} \psi_{\boldsymbol{k},\sigma}(\boldsymbol{x}) e^{-i\omega_k t} \widehat{b}^+_{-\boldsymbol{k},\sigma}. \tag{1.31}$$

◼ **Green function of electron gas.** Calculate the Green function of free electron gas. Consider particles in a box, whose wave functions are plane waves

$$\psi_{\boldsymbol{k},\sigma} = \chi_\sigma \frac{e^{i\boldsymbol{k}\cdot\boldsymbol{x}}}{\sqrt{V}}\,,$$

where χ_σ is a two-component spinor. Substitution of representation (1.31) in the definition of the one-particle Green function yields (note that α and β here are spin indices, i.e. they label components of spinors χ_σ, whereas σ enumerates spinors)

$$iG_{0\alpha\beta}(t,\boldsymbol{x},t',\boldsymbol{x}') = \left\langle 0 \left| T\left[\widehat{\psi}_\alpha(t,\boldsymbol{x})\widehat{\psi}_\beta^+(t',\boldsymbol{x}')\right] \right| 0 \right\rangle$$

$$= \frac{\delta_{\alpha\beta}}{V} \sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{x}')-i\omega_k(t-t')} \left[\theta(t-t')\theta(k-k_F) - \theta(t'-t)\theta(k_F-k)\right].$$

Passing to the thermodynamic limit and using the integral representation of the step function

$$\theta(t) = \frac{i}{2\pi} \int\limits_{-\infty}^{\infty} d\omega\, \frac{e^{-i\omega t}}{\omega + i\epsilon}\,, \qquad \epsilon \to 0+$$

we obtain

$$G_{0\alpha\beta}(t,\boldsymbol{x},t',\boldsymbol{x}')$$
$$= \int \frac{d\boldsymbol{k}}{(2\pi)^3} \int \frac{d\omega}{2\pi}\, e^{i\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{x}')-i\omega(t-t')} \delta_{\alpha\beta} \left[\frac{\theta(k-k_F)}{\omega-\omega_k+i\epsilon} + \frac{\theta(k_F-k)}{\omega-\omega_k-i\epsilon}\right].$$

From here it follows that the Fourier transform of the one-particle Green function of the free fermion gas is

$$G_{0\alpha\beta}(\omega,\boldsymbol{k}) = \delta_{\alpha\beta} \left[\frac{\theta(k-k_F)}{\omega-\omega_k+i\epsilon} + \frac{\theta(k_F-k)}{\omega-\omega_k-i\epsilon}\right]$$
$$= \frac{\delta_{\alpha\beta}}{\omega-\omega_k+i\epsilon\,\mathrm{sign}\,(k-k_F)}\,. \quad (1.32)$$

◼ **Retarded and advanced Green functions.** The one-particle Green function introduced above is also called the *causal Green function*. In the analysis of the dynamics of many-body quantum systems two other closely related Green functions, the *advanced Green function* G^A and the *retarded Green function* G^R are needed as well. The definitions are

$$G_{\alpha\beta}^A(x,x') = -\kappa i\theta(t'-t)\left\langle \left[\widehat{\psi}_{H\beta}^+(x'), \widehat{\psi}_{H\alpha}(x)\right]_\pm \right\rangle,$$

$$G_{\alpha\beta}^R(x,x') = -i\theta(t-t')\left\langle \left[\widehat{\psi}_{H\alpha}(x), \widehat{\psi}_{H\beta}^+(x')\right]_\pm \right\rangle, \qquad (1.33)$$

where commutator is chosen for bosons and the anticommutator for fermions. The main reason for introduction of the retarded and advanced Green functions is that – contrary to the causal Green function – they are analytic functions of ω.

For the free-fermion system calculation yields

$$G_{0\alpha\beta}^{A}(\omega, \boldsymbol{k}) = \frac{\delta_{\alpha\beta}}{\omega - \omega_k - i\epsilon},$$

$$G_{0\alpha\beta}^{R}(\omega, \boldsymbol{k}) = \frac{\delta_{\alpha\beta}}{\omega - \omega_k + i\epsilon}. \tag{1.34}$$

1.3 Problems

Problem 1.1. Basis vectors in the Hilbert space of an N-particle system may be presented also in the form

$$\langle \xi_1, \ldots, \xi_N | \{n_\ell\} \rangle = C \sum_{P'(\ell_1, \ldots, \ell_N)} \varepsilon_P \langle \xi_1 | \ell_1 \rangle \cdots \langle \xi_N | \ell_N \rangle,$$

where the sum goes over all permutations of *different* labels ℓ_i of the normalized one-particle state vectors. Determine the normalization coefficient C in this representation.

Problem 1.2. Construct a column-vector representation for the ground-state as well as matrix representations for the creation and annihilation operators for a one-particle state in case of fermions.

Problem 1.3. Evaluate the matrix elements $\langle \{n_\ell\} | \widehat{a}_i^+ \widehat{a}_j | \{m_\ell\} \rangle$ and $\langle \{n_\ell\} | \widehat{a}_i^+ \widehat{a}_j^+ \widehat{a}_k \widehat{a}_l | \{m_\ell\} \rangle$ in case of fermionic operators.

Problem 1.4. Show that the matrix elements of the Hamilton operator

$$\widehat{H} = \sum_{k=1}^{N} \widehat{T}(x_k) + \frac{1}{2} \sum_{\substack{k,l=1 \\ k \neq l}} \widehat{V}(x_k, x_l)$$

in the Fock space spanned by the N free particle states (here, $\langle \xi | \ell \rangle = \psi_\ell(\xi)$)

$$\langle \xi_1, \ldots, \xi_N | \{n_\ell\} \rangle = \sqrt{\frac{1}{N! \prod_\ell n_\ell!}} \sum_{P(\xi_1, \ldots, \xi_N)} \varepsilon_P \langle \xi_1 | \ell_1 \rangle \cdots \langle \xi_N | \ell_N \rangle$$

are equal to the matrix elements of the second-quantized Hamilton operator

$$\widehat{H} = \int d\xi \, \widehat{\psi}^+(\xi) \widehat{T}(\xi) \widehat{\psi}(\xi) + \frac{1}{2} \int d\xi \int d\xi' \, \widehat{\psi}^+(\xi) \widehat{\psi}^+(\xi') \widehat{V}(\xi, \xi') \widehat{\psi}(\xi') \widehat{\psi}(\xi)$$

in the occupation-number basis. Consider fermionic case.

Problem 1.5. The field operators of the second quantization are $\widehat{\psi}^+(t,x) = \sum_{n=1}^\infty \psi_n^+(x)e^{itE_n/\hbar}\widehat{a}_n^+$ and $\widehat{\psi}(t,x) = \sum_{n=1}^\infty \psi_n(x)e^{-itE_n/\hbar}\widehat{a}_n$, where $\psi_n(x)$ is the wave function of the stationary one-particle state number n [i.e. $\widehat{H}\psi_n(x) = E_n\psi_n(x)$] and $\widehat{a}_n^+$, $\widehat{a}_n$ are the creation and annihilation operators of this state. Calculate the single-time commutators/anticommutators of the field operators

$$\left[\widehat{\psi}(t,x), \widehat{\psi}^+(t,x')\right]_\mp , \quad \left[\widehat{\psi}(t,x), \widehat{\psi}(t,x')\right]_\mp .$$

Problem 1.6. The field operators of the second quantization are $\widehat{\psi}^+(t,x) = \sum_{n=1}^\infty \psi_n^+(x)e^{itE_n/\hbar}\widehat{a}_n^+$ and $\widehat{\psi}(t,x) = \sum_{n=1}^\infty \psi_n(x)e^{-itE_n/\hbar}\widehat{a}_n$, where $\psi_n(x)$ is the wave function of the stationary one-particle state number n [i.e. $\widehat{H}\psi_n(x) = E_n\psi_n(x)$] and $\widehat{a}_n^+$, $\widehat{a}_n$ are the creation and annihilation operators of this state. Show that

$$C_\mp(t,x;t',x') = \left[\widehat{\psi}(t,x), \widehat{\psi}^+(t',x')\right]_\mp$$

is the Green function of the Schrödinger equation, i.e. $\left(i\hbar\partial_t - \widehat{H}\right)C_\mp(t,x;t',x') = 0$ and $\lim_{t'\to t} C_\mp(t,x;t',x') = \delta(x-x')$.

Problem 1.7. Show that the field operator is a solution of the Schrödinger equation:

$$i\hbar\frac{\partial\widehat{\psi}(t,\xi)}{\partial t} = \widehat{H}(\xi)\widehat{\psi}(t,\xi) .$$

Problem 1.8. Show that $\left[\widehat{N}, \widehat{H}\right] = 0$, when $\widehat{H}$ is a Hamilton operator with pair interaction. Calculate also the commutator $\left[\widehat{n}(\boldsymbol{x}), \widehat{H}_I\right]$, where $\widehat{n}(\boldsymbol{x})$ is the particle density operator and $\widehat{H}_I$ the Hamilton operator of the interaction (i.e. $\widehat{H}$ without the one-particle part).

Problem 1.9. The time-dependent fermionic field operator in terms of particles and holes is

$$\widehat{\psi}(t,\boldsymbol{x}) = \sum_{|\boldsymbol{k}|>k_F,\sigma} \psi_{\boldsymbol{k},\sigma}(\boldsymbol{x})e^{-i\omega_k t}\widehat{a}_{\boldsymbol{k},\sigma} + \sum_{|\boldsymbol{k}|<k_F,\sigma} \psi_{\boldsymbol{k},\sigma}(\boldsymbol{x})e^{-i\omega_k t}\widehat{b}_{-\boldsymbol{k},\sigma}^+ .$$

Show by direct calculation that the two-point Green function may be cast in the form

$$G_{0\alpha\beta}(t,\boldsymbol{x},t',\boldsymbol{x}')$$
$$= -i\frac{\delta_{\alpha\beta}}{V}\sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{x}')-i\omega_k(t-t')}\left[\theta(t-t')\theta(k-k_F) - \theta(t'-t)\theta(k_F-k)\right] .$$

Hint. The diagonalization of the Green function in spin indices is most conveniently seen in the representation, where the spinors of the wave function are eigenvectors of the Pauli matrix

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} .$$

2. Correlation and response functions

2.1   Pair correlation functions

In the description of the microscopic properties of a many-particle system functions characterizing mutual dependences of the observables are fundamental quantities. The most important of these are the *correlation functions* and the *response functions*, with the aid of whose, e.g., the thermodynamic responses may be derived from the underlying microscopic Hamilton operator. They also allow to determine transport properties and kinetic coefficients (heat conductivity, viscosity etc.) of non-equilibrium systems.

■ **Particle density.** In quantum mechanics positions of particles are operators $\{\widehat{r}_i\} \equiv \{\widehat{r}_1, \widehat{r}_2, \ldots, \widehat{r}_N\}$. They are diagonal in the Schrï£¡dinger picture:

$$\widehat{r}_i \Psi(r_1 r_2 \ldots r_N) = r_i \Psi(r_1 r_2 \ldots r_N).$$

Number density is the operator-valued function

$$\boxed{\widehat{n}(r) = \sum_i \delta(r - \widehat{r}_i).} \tag{2.1}$$

For instance, in the pure quantum state $\Psi(r_1 r_2 \ldots r_N)$ we obtain

$$\langle \widehat{n}(r) \rangle = \sum_{i=1}^{N} \int d^3 r_1 \cdots \int d^3 r_{i-1} \int d^3 r_{i+1} \cdots \int d^3 r_N \, |\Psi(r_1 \ldots [r_i = r] \ldots r_N)|^2 .$$

If the particles are identical fermions or bosons, then $|\Psi|^2$ is symmetric under permutations and

$$\langle \widehat{n}(r) \rangle = N \int d^3 r_2 \cdots \int d^3 r_N \, |\Psi(r r_2 \ldots r_N)|^2 . \tag{2.2}$$

If the system is enclosed in the volume V and the state $|\Psi\rangle$ properly normalized, then the obvious normalization follows

$$\int_V d^3 r \langle \widehat{n}(r) \rangle = N \int d^3 r_1 \ldots \int d^3 r_N |\Psi(r_1 \ldots r_N)|^2 = N.$$

This may be generalized to systems with a variable number of particles. Since the equation

$$\int_V d^3 r \widehat{n}(r) = \sum_{i=1}^{N} \int_V d^3 r \, \delta(r - \widehat{r}_i) = \sum_{i=1}^{N} 1 = N$$

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holds for every N-particle system enclosed in the volume V (i.e. for every N-particle Hilbert space, in the Fock space the particle-number operator $\widehat{N}_V$ may be defined as the integral

$$\widehat{N}_V \equiv \int_V d^3 \boldsymbol{r}\, \widehat{n}(\boldsymbol{r}). \tag{2.3}$$

The eigenvalues of the operator $\widehat{N}_V$ are obviously $0, 1, 2, \ldots$. The definition volume V may also be a part of larger volume, in which case the its particle number may vary even if the total particle number is constant.

■ **Pair correlation function.** Define the (static) correlation function of two Hermitian operators $\widehat{A}$ and $\widehat{B}$ as the expectation value calculated with the use of a suitable density operator $\widehat{\rho}$

$$C_{AB} \equiv \frac{1}{2}\left\langle \Delta\widehat{A}\,\Delta\widehat{B} + \Delta\widehat{B}\,\Delta\widehat{A} \right\rangle = \frac{1}{2}\operatorname{Tr}\widehat{\rho}\left[\Delta\widehat{A}\,\Delta\widehat{B} + \Delta\widehat{B}\,\Delta\widehat{A}\right], \tag{2.4}$$

where $\Delta\widehat{A} = \widehat{A} - \langle\widehat{A}\rangle$ is the fluctuating part of the operator. If one of the operators commutes with the density operator, then

$$C_{AB} = \left\langle \Delta\widehat{A}\,\Delta\widehat{B} \right\rangle.$$

Consider correlations of the particle density in a uniform system $\langle\widehat{n}(\boldsymbol{r})\rangle = n(\boldsymbol{r}) = n$. Decompose the function

$$
\begin{aligned}
\langle\widehat{n}(\boldsymbol{r})\widehat{n}(\boldsymbol{r}')\rangle &\equiv \sum_i \langle\delta(\boldsymbol{r}-\widehat{\boldsymbol{r}}_i)\,\delta(\boldsymbol{r}'-\widehat{\boldsymbol{r}}_i)\rangle + \sum_{i\neq j}\langle\delta(\boldsymbol{r}-\widehat{\boldsymbol{r}}_i)\,\delta(\boldsymbol{r}'-\widehat{\boldsymbol{r}}_j)\rangle \\
&= \delta(\boldsymbol{r}-\boldsymbol{r}')\langle\widehat{n}(\boldsymbol{r})\rangle + \sum_{i\neq j}\langle\delta(\boldsymbol{r}-\widehat{\boldsymbol{r}}_i)\,\delta(\boldsymbol{r}'-\widehat{\boldsymbol{r}}_j)\rangle \\
&= n\delta(\boldsymbol{r}-\boldsymbol{r}') + n^2 g(\boldsymbol{r}-\boldsymbol{r}').
\end{aligned}
\tag{2.5a}
$$

The first term here is the *autocorrelation function* of the particles, whereas $g(\boldsymbol{r}-\boldsymbol{r}')$ is the *pair correlation function*. The *density-density correlation function* is thus

$$C_{nn}(\boldsymbol{r}-\boldsymbol{r}') = \langle\Delta\widehat{n}(\boldsymbol{r})\,\Delta\widehat{n}(\boldsymbol{r}')\rangle = n\delta(\boldsymbol{r}-\boldsymbol{r}') + n^2\left[g(\boldsymbol{r}-\boldsymbol{r}')-1\right]. \tag{2.5b}$$

It should be noted that the same argument about the structure of the density-density correlation function works in classical statistical mechanics as well, only the hats are omitted. In particular, it is readily seen that the pair correlation function $g(\boldsymbol{r}-\boldsymbol{r}') = 1$ in an ideal gas with the Maxwell distribution of velocities.

In a homogeneous system Fourier-transformed functions are useful. Use the definitions

$$
\begin{aligned}
f(\boldsymbol{q}) &= \int_V d^3\boldsymbol{r}\, \mathrm{e}^{-i\boldsymbol{q}\cdot\boldsymbol{r}} f(\boldsymbol{r}); \\
f(\boldsymbol{r}) &= \frac{1}{V}\sum_{\boldsymbol{q}} \mathrm{e}^{i\boldsymbol{q}\cdot\boldsymbol{r}} f(\boldsymbol{q}).
\end{aligned}
\tag{2.6}
$$

It is customary to express the correlation function of density fluctuations in terms of the static *structure factor*

$$S(\boldsymbol{r} - \boldsymbol{r}') \equiv \frac{1}{n}\langle \Delta\widehat{n}(\boldsymbol{r})\Delta\widehat{n}(\boldsymbol{r}')\rangle \, .$$

Its Fourier transform is

$$S(\boldsymbol{q}) \equiv \frac{1}{N}\langle \Delta\widehat{n}(\boldsymbol{q})\Delta\widehat{n}(-\boldsymbol{q})\rangle = 1 + n \int d^3\boldsymbol{r}\, e^{-i\boldsymbol{q}\cdot\boldsymbol{r}}[g(r) - 1]. \qquad (2.7)$$

Note that in a homogeneous system

$$\langle \Delta\widehat{n}(\boldsymbol{q})\Delta\widehat{n}(-\boldsymbol{q}')\rangle = 0, \quad \text{if } \boldsymbol{q} \neq \boldsymbol{q}' \, .$$

The function $S(\boldsymbol{q})$ is real-valued and non-negative.

Because simultaneous events taking place far away cannot be correlated, the expectation values factorize

$$\langle A(\boldsymbol{r})B(\boldsymbol{r}')\rangle \xrightarrow[|\boldsymbol{r}-\boldsymbol{r}'|\to\infty]{} \langle A(\boldsymbol{r})\rangle\langle B(\boldsymbol{r}')\rangle \, ,$$

where A, B are any variables localized in the vicinity of their respective position arguments. Thus, the pair correlation function is asymptotically

$$g(\boldsymbol{r} - \boldsymbol{r}') \xrightarrow[|\boldsymbol{r}-\boldsymbol{r}'|\to\infty]{} 1 \, . \qquad (2.8)$$

Sometimes the name pair correlation function is attributed to the function

$$h(\boldsymbol{r} - \boldsymbol{r}') = g(\boldsymbol{r} - \boldsymbol{r}') - 1 \, , \qquad (2.9)$$

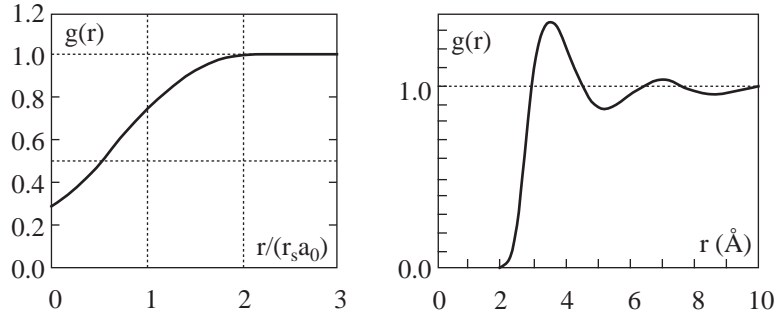vanishing at large separations, which is better in accord with the general definition of a correlation function.

Figure 2–1: Pair correlation functions. (a) Dense homogeneous electron gas, the density parameter $r_s = 1$. (b) ^{4}He liquid. The temperature $T = 1$ K

In the grand canonical ensemble

$$\frac{\partial}{\partial\mu}\langle\widehat{n}\rangle = \frac{\partial}{\partial\mu}\langle\widehat{n}(\boldsymbol{r})\rangle = \beta \int \left[\langle\widehat{n}(\boldsymbol{r})\widehat{n}(\boldsymbol{r}')\rangle - \langle\widehat{n}(\boldsymbol{r})\rangle\langle\widehat{n}(\boldsymbol{r}')\rangle\right] d\boldsymbol{r}' = \beta n S(0) \, .$$

Here,

$$\left(\frac{\partial n}{\partial \mu}\right)_T = \left(\frac{\partial n}{\partial p}\right)_T \left(\frac{\partial p}{\partial \mu}\right)_T = n \left(\frac{\partial n}{\partial p}\right)_T = n^2 \kappa_T \,.$$

Thus

$$Tn\kappa_T = 1 + n \int d^3 \boldsymbol{r} \left[g(\boldsymbol{r}) - 1\right]. \tag{2.10}$$

■ **Pair correlation function of ideal quantum gas.** In classical ideal gas the pair correlation function $h = g - 1$ vanishes, but a quantum ideal gas possesses a nontrivial pair correlation function. Consider free particles in a box, whose wave functions are plane waves

$$\psi_{\boldsymbol{k},\sigma} = \chi_\sigma \frac{e^{i\boldsymbol{k}\cdot\boldsymbol{x}}}{\sqrt{V}}\,,$$

where χ_σ is a two-component spinor for spin $\frac{1}{2}$ fermions. The number-density operator

$$\widehat{n}(\boldsymbol{x}) = \sum_{\boldsymbol{k},\sigma} \chi_\sigma^* \frac{e^{-i\boldsymbol{k}\cdot\boldsymbol{x}}}{\sqrt{V}} \widehat{a}_{\boldsymbol{k},\sigma}^+ \sum_{\boldsymbol{k}',\sigma'} \chi_{\sigma'} \frac{e^{i\boldsymbol{k}'\cdot\boldsymbol{x}}}{\sqrt{V}} \widehat{a}_{\boldsymbol{k}',\sigma'}$$

involves the inner product of the spinors, which for the properly normalized wave functions yields $\chi_\sigma^* \cdot \chi_{\sigma'} = \delta_{\sigma\sigma'}$. Therefore

$$\widehat{n}(\boldsymbol{x}) = \frac{1}{V} \sum_{\boldsymbol{k},\boldsymbol{k}',\sigma} \widehat{a}_{\boldsymbol{k},\sigma}^+ \widehat{a}_{\boldsymbol{k}',\sigma} e^{i\boldsymbol{x}\cdot(\boldsymbol{k}'-\boldsymbol{k})} \,. \tag{2.11}$$

Diagonal terms of the double sum give rise to the mean particle density, since

$$\frac{1}{V} \sum_{\boldsymbol{k},\boldsymbol{k}',\sigma} \widehat{a}_{\boldsymbol{k},\sigma}^+ \widehat{a}_{\boldsymbol{k},\sigma} = \frac{1}{V} \sum_{\boldsymbol{k},\boldsymbol{k}',\sigma} \widehat{n}_{\boldsymbol{k},\sigma} = \frac{\widehat{N}}{V} = n \,.$$

Therefore, the deviation of the particle-density operator from the mean is

$$\Delta\widehat{n}(\boldsymbol{x}) = \widehat{n}(\boldsymbol{x}) - n = \frac{1}{V} \sum_{\boldsymbol{k}\neq\boldsymbol{k}',\sigma} \widehat{a}_{\boldsymbol{k},\sigma}^+ \widehat{a}_{\boldsymbol{k},\sigma} e^{i\boldsymbol{x}\cdot(\boldsymbol{k}'-\boldsymbol{k})} \,.$$

In the grand canonical ensemble of nonrelativistic free particles

$$\widehat{\rho} = \frac{e^{-\beta(\widehat{H}-\mu\widehat{N})}}{Z_G}$$

with

$$\widehat{H} = \int d\boldsymbol{x}\, \widehat{\psi}^+(\boldsymbol{x}) \left(-\frac{\hbar^2 \nabla^2}{2m}\right) \widehat{\psi}(\boldsymbol{x})$$

$$= \frac{1}{V} \int d\boldsymbol{x} \sum_{\boldsymbol{k},\boldsymbol{k}',\sigma} \frac{\hbar^2 \boldsymbol{k}'^2}{2m} \widehat{a}_{\boldsymbol{k},\sigma}^+ \widehat{a}_{\boldsymbol{k}',\sigma} e^{i\boldsymbol{x}\cdot(\boldsymbol{k}'-\boldsymbol{k})} = \sum_{\boldsymbol{k},\sigma} \frac{\hbar^2 k^2}{2m} \widehat{n}_{\boldsymbol{k},\sigma} \,, \tag{2.12}$$

because the spinor structure is the same here as in the number-density (2.11).

Calculate the trace in the the correlation function (2.4) in the occupation-number basis. Then the expectation values $\langle \widehat{a}_{\boldsymbol{k},\sigma}^{+} \widehat{a}_{\boldsymbol{k}',\sigma} \widehat{a}_{\boldsymbol{p},\sigma'}^{+} \widehat{a}_{\boldsymbol{p}',\sigma'} \rangle$ vanish for all cases, in which any pair $\widehat{a}^{+}$, $\widehat{a}$ has different indices (note that by construction $\boldsymbol{k} \neq \boldsymbol{k}'$ and $\boldsymbol{p} \neq \boldsymbol{p}'$). In the nonvanishing matrix elements expectation values of pairs of $\widehat{a}^{+}$, $\widehat{a}$ factorize, thus

$$\langle \widehat{a}_{\boldsymbol{k},\sigma}^{+} \widehat{a}_{\boldsymbol{k}',\sigma} \widehat{a}_{\boldsymbol{k}',\sigma}^{+} \widehat{a}_{\boldsymbol{k},\sigma} \rangle = \langle \widehat{a}_{\boldsymbol{k},\sigma}^{+} \widehat{a}_{\boldsymbol{k},\sigma} \rangle \langle \widehat{a}_{\boldsymbol{k}',\sigma} \widehat{a}_{\boldsymbol{k}',\sigma}^{+} \rangle = \langle \widehat{n}_{\boldsymbol{k},\sigma} \rangle \langle 1 \mp \widehat{n}_{\boldsymbol{k}',\sigma} \rangle \,,$$

where the $+$ sign stands for bosons and the $-$ sign for fermions. Thus, the density-density correlation function for the quantum ideal gas assumes the form

$$C_{nn}(\boldsymbol{x} - \boldsymbol{x}') = \frac{1}{V^2} \sum_{\boldsymbol{k} \neq \boldsymbol{k}',\sigma} e^{i(\boldsymbol{x}-\boldsymbol{x}')\cdot(\boldsymbol{k}'-\boldsymbol{k})} \langle 1 \mp \widehat{n}_{\boldsymbol{k}',\sigma} \rangle \langle \widehat{n}_{\boldsymbol{k},\sigma} \rangle \,. \qquad (2.13)$$

In the thermodynamic limit

$$\frac{1}{V} \sum_{\boldsymbol{k}} \to \int \frac{d\boldsymbol{k}}{(2\pi)^3} \,.$$

The first term in (2.13) yields the δ function:

$$\frac{1}{V^2} \sum_{\boldsymbol{k} \neq \boldsymbol{k}',\sigma} e^{i(\boldsymbol{x}-\boldsymbol{x}')\cdot(\boldsymbol{k}'-\boldsymbol{k})} \langle \widehat{n}_{\boldsymbol{k},\sigma} \rangle$$

$$\to \int \frac{d\boldsymbol{k}'}{(2\pi)^3} e^{i(\boldsymbol{x}-\boldsymbol{x}')\cdot\boldsymbol{k}'} \int \frac{d\boldsymbol{k}}{(2\pi)^3} e^{-i(\boldsymbol{x}-\boldsymbol{x}')\cdot\boldsymbol{k}} \langle \widehat{n}_{\boldsymbol{k},\sigma} \rangle = \delta(\boldsymbol{x} - \boldsymbol{x}') n \,. \quad (2.14)$$

Therefore, the second term is the sought pair correlation function

$$h(\boldsymbol{x} - \boldsymbol{x}') = g(\boldsymbol{x} - \boldsymbol{x}') - 1 = \mp \frac{1}{n^2} \sum_{\sigma} \left| \int \frac{d\boldsymbol{k}}{(2\pi)^3} e^{i\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{x}')} \langle \widehat{n}_{\boldsymbol{k},\sigma} \rangle \right|^2 \,. \qquad (2.15)$$

In equilibrium the expectation value of the occupation number

$$\langle \widehat{n}_{\boldsymbol{k},\sigma} \rangle = \frac{1}{e^{\beta[\epsilon(\boldsymbol{k})-\mu]} \pm 1} \equiv \overline{n}_{\boldsymbol{k}}$$

and it is independent of the spin component, thus $\sum_{\sigma} \to g = 2S + 1$. In thermodynamic equilibrium we arrive at

$$h(\boldsymbol{r}) = \mp \frac{g}{n^2} \left| \int \frac{d\boldsymbol{k}}{(2\pi)^3} \frac{e^{i\boldsymbol{k}\cdot\boldsymbol{r}}}{e^{\beta[\epsilon(\boldsymbol{k})-\mu]} \pm 1} \right|^2 \,. \qquad (2.16)$$

Due to exclusion principle, the density-density correlation function is negative for fermions, whereas for bosons it is positive. Fourier transformation yields

$$\langle |\Delta \widehat{n}_{\boldsymbol{k}}|^2 \rangle = \frac{g}{V} \int \frac{d\boldsymbol{p}}{(2\pi)^3} \overline{n}_{\boldsymbol{p}} \left(1 \mp \overline{n}_{\boldsymbol{p}+\boldsymbol{k}}\right) \,, \qquad (2.17)$$

where

$$\Delta \widehat{n}_{\boldsymbol{k}} = \int d\boldsymbol{x} \, e^{-i\boldsymbol{k}\cdot\boldsymbol{x}} \Delta \widehat{n}(\boldsymbol{x}) \,.$$

From representation (2.16) it follows that the typical length scale (*correlation length* ξ) of an ideal quantum gas is proportional – not surprisingly – to the thermal de Broglie wavelength λ_T:

$$\xi = \frac{\hbar}{\sqrt{2mT}} = \frac{\lambda_T}{2\sqrt{\pi}} \,, \qquad \lambda_T = \frac{h}{\sqrt{2\pi mT}} \,.$$

■ **Effective free energy.** The pair correlation function $g(\boldsymbol{r} - \boldsymbol{r}')$ may usually be calculated only approximately. This is often carried out by the use of perturbation theory with a graphical representation of the terms of the expansion (diagrammatic expansion). It is also common to truncate at the level of the pair correlation function exact sets of equations connecting correlation functions of all orders. For the time being, however, let us take a look at a more phenomenological approach to the construction of the pair correlation function, which is especially well suited to description of correlations at large spatial separation.

Consider quantum-mechanical expressions for the partition function and the free energy

$$Z_N = e^{-\beta F_N} = \mathbf{Tr}_N e^{-\beta \widehat{H}} \,.$$

Divide the volume in elements ΔV_α, whose particle numbers may be $N_\alpha = 0, 1, 2, \ldots$. In the volume element α the following resolution of unity is then possible

$$\widehat{I}_\alpha = \sum_{N_\alpha=0}^{\infty} \widehat{P}(N_\alpha) \,,$$

where $\widehat{P}(N_\alpha)$ is the projection operator to the subspace with the particle number N_α in the volume element α. For the whole Hilbert (Fock) space the identity is

$$\widehat{I} = \prod_\alpha \widehat{I}_\alpha = \prod_\alpha \left[\sum_{N_\alpha=0}^{\infty} \widehat{P}(N_\alpha) \right] = \sum_{\{N_\alpha\}} \prod_\alpha \widehat{P}(N_\alpha).$$

With the aid of this resolution of unity the partition function may be expressed as

$$Z_N = e^{-\beta F_N} = \sum_{\{N_\alpha\}} e^{-\beta \widetilde{F}_N \{N_\alpha\}}, \qquad (2.18)$$

with the definition

$$e^{-\beta \widetilde{F}_N \{N_\alpha\}} \equiv \mathrm{Tr} \left\{ \prod_\alpha \widehat{P}(N_\alpha) e^{-\beta \widehat{H}} \right\} = \mathrm{Tr}_{\{N_\alpha\}} e^{-\beta \widehat{H}} \,. \qquad (2.19)$$

In this expression sum is taken over all microscopic degrees of freedom under the constraint that the semi-microscopic particle numbers $\{N_\alpha\}$ are

kept fixed. Since we are dealing with the canonical partition function, the condition $\sum_\alpha N_\alpha = N = const$ must be obeyed.

The function $\widetilde{F}_N(T, V, \{N_\alpha\})$ is the *reduced free energy* (or effective free energy) , i.e. the free energy of the configuration $\{N_\alpha\}$. The expression $\exp(-\beta\widetilde{F}_N)$ yields the unnormalized statistical probability of the configuration. This result reminds of Einstein's theory of fluctuations; here, the entropy maximum principle is replaced by the equivalent condition of minimum free energy, which takes into account the boundary conditions.

Calculation of the partial trace with some variables kept fixed is an example of *coarse graining* – a procedure, which is often necessary to extract macrophysically relevant information from a microscopic system.

Usually, the reduced free energy cannot be calculated exactly. In the following a simple phenomenological model is constructed for the functional $\widetilde{F}_N$. This is the local density approximation (LDA), in which the the free energy is a volume integral of the *free energy density*, which is assumed to be a local function of particle density and its low-order derivatives only (i.e. the *gradient expansion*). Thus

$$\widetilde{F}_N[n] = \int d^3\boldsymbol{r}\, f_N\left[n(\boldsymbol{r}), \nabla n(\boldsymbol{r}), \nabla\nabla n(\boldsymbol{r}), \cdots\right].$$

Consider, for brevity, small density fluctuations in a homogeneous system. Let the constant density be n and the deviation thereof $\delta n(\boldsymbol{r}) = n(\boldsymbol{r}) - n$, then the simplest physically meaningful model is of the form

$$\widetilde{F}_N[\delta n] = \int d^3\boldsymbol{r}\left\{ f_0 + \frac{1}{2}f_1[\delta n(\boldsymbol{r})]^2 + \frac{1}{2}f_2[\nabla\delta n(\boldsymbol{r})]^2 \right\}, \qquad (2.20)$$

where f_0, f_1 and f_2 are coefficients depending on the temperature T and the constant particle density n. There is no linear term, because it is assumed that the constant density n minimizes the free energy under given boundary conditions. Then the coefficients f_1 and f_2 must be positive. The gradient term $(\nabla\delta n)^2$ suppresses short wave-length fluctuations. Therefore, at close positions $\boldsymbol{r}$ and $\boldsymbol{r}'$ the deviations $\delta n(\boldsymbol{r})$ are $\delta n(\boldsymbol{r}')$ nearly equal with large probability.

Fourier transform yields

$$\widetilde{F} = \widetilde{F}^0 + \frac{1}{2V}\sum_{\boldsymbol{q}}{}' \left(f_1 + f_2\boldsymbol{q}^2\right)\delta n(\boldsymbol{q})\delta n(-\boldsymbol{q}), \qquad (2.21)$$

where the prime reminds that the term $\boldsymbol{q} = 0$ is absent (when N is constant, $\delta n(\boldsymbol{q} = 0) = \delta N = 0$). Since $\delta n(\boldsymbol{r})$ is real number, $\delta n(\boldsymbol{q})\delta n(-\boldsymbol{q}) = |\delta n(\boldsymbol{q})|^2$.

In the theory of thermodynamic fluctuations, the probability distribution of the fluctuation configuration is the Gaussian function

$$P[\delta n] \propto \mathrm{e}^{-\beta\widetilde{F}} \propto \exp\left[-\frac{1}{2TV}\sum_{\boldsymbol{q}}{}' \left(f_1 + f_2\boldsymbol{q}^2\right)\delta n(\boldsymbol{q})\delta n(-\boldsymbol{q})\right]. \qquad (2.22)$$

■ **Correlation length.** Since the distribution (2.22) is normal, the correlation function follows right away

$$\langle \delta n(\boldsymbol{q}) \delta n(-\boldsymbol{q}) \rangle = \frac{TV}{f_1 + f_2 q^2} = \frac{TV}{f_2} \cdot \frac{1}{q^2 + q_c^2} \,,$$

where $q_c^2 = f_1/f_2$. According to the definition (2.4), the density correlation function is thus

$$C_{nn}(\boldsymbol{q}) = \frac{1}{V} \langle \delta n(\boldsymbol{q}) \delta n(-\boldsymbol{q}) \rangle = \frac{T}{f_2} \cdot \frac{1}{q^2 + q_c^2}. \qquad (2.23)$$

Calculation of the inverse Fourier transform yields

$$C_{nn}(\boldsymbol{r}) = \frac{T}{f_2} \cdot \frac{1}{4\pi r} e^{-r/\xi} \,.$$

The parameters $\xi = 1/q_c = \sqrt{f_2/f_1}$ is the *correlation length*.

From relations (2.7) and (2.10) it follows that

$$\lim_{q \to 0} C_{nn}(\boldsymbol{q}) = T n^2 \kappa_T.$$

From here we see that the coefficients f_1, f_2 are

$$f_1 = \frac{1}{n^2 \kappa_T} \;;\quad f_2 = \frac{\xi^2}{n^2 \kappa_T} \qquad (2.24)$$

These results are of qualitative nature, because they have been derived from a model lacking sufficient microscopic foundation especially in the part of short-range correlations and interactions. In fact, this is a two-parameter (ξ and κ_T) classical model for density fluctuations. Expression (2.23) for the correlation function is of the *Ornstein–Zernicke* form (1917).

■ **Schwinger representation.** In the evaluation of the inverse Fourier transform of the correlation function (2.23) it is customary to use spherical coordinates with the direction of the third axis along the coordinate vector. In this case the angular integral is elementary, after which the integral over the radial variable reduces to a rather straightforward application of the calculus of residues. However, in modern statistical physics the dimension of space is sometimes considered a complex variable d instead of an integer. The calculation of the inverse Fourier transform according to the procedure just described is a bit cumbersome in the case of complex d. An alternative method circumventing the use of d-dimensional spherical coordinates is to express the correlation function in the Schwinger representation (α representation):

$$\frac{1}{(q^2 + q_c^2)^a} = \frac{1}{\Gamma(a)} \int_0^\infty d\alpha \, \alpha^{a-1} \, e^{-\alpha(q^2 + q_c^2)} \,, \qquad (2.25)$$

after which we arrive at a standard Gaussian integral over the wave-vector space. It then remains to identify the parametric integral with an elementary or a special function.

Example 2.1. Calculate the inverse Fourier transform of the Ornstein-Zernike correlation function with an infinite correlation length ($q_c = 0$) in a d-dimensional space.

Solution. Let us calculate a bit more general integral. The Schwinger representation yields

$$\int \frac{d\boldsymbol{q}}{(2\pi)^d} \frac{\mathrm{e}^{i\boldsymbol{q}\cdot\boldsymbol{r}}}{q^{2a}} = \frac{1}{\Gamma(a)} \int_0^\infty d\alpha\, \alpha^{a-1} \int \frac{d\boldsymbol{q}}{(2\pi)^d} e^{-\alpha q^2 + i\boldsymbol{q}\cdot\boldsymbol{r}}$$

$$= \frac{1}{(2\pi)^d \Gamma(a)} \int_0^\infty d\alpha\, e^{-r^2/4\alpha} \alpha^{a-1} \left(\frac{\pi}{\alpha}\right)^{d/2} .$$

With the change of variables $\frac{r^2}{4\alpha} = t$ we obtain the standard Euler integral for the Γ function

$$\frac{1}{(2\pi)^d} \int_0^\infty d\alpha\, e^{-r^2/4\alpha} \alpha^{a-1} \left(\frac{\pi}{\alpha}\right)^{d/2}$$

$$= \frac{1}{2^d \pi^{d/2}} \left(\frac{2}{r}\right)^{d-2a} \int_0^\infty dt\, e^{-t} t^{d/2-a-1} = \frac{\Gamma(d/2-a)}{2^{2a} \pi^{d/2} r^{d-2a}} .$$

Thus

$$\int \frac{d\boldsymbol{q}}{(2\pi)^d} \frac{\mathrm{e}^{i\boldsymbol{q}\cdot\boldsymbol{r}}}{q^{2a}} = \frac{\Gamma(d/2-a)}{2^{2a} \pi^{d/2} \Gamma(a) r^{d-2a}} . \tag{2.26}$$

The choice $a = 1$ yields the Ornstein-Zernike correlation function.

It should be noted, that the integral of the inverse Fourier transform (2.26) is convergent at $2a < d < 4a + 1$ only. The analytic continuation of the explicit expression obtained in this range is then accepted as the inverse Fourier transform for other complex d.

Example 2.2. Calculate the inverse Fourier transform of the Ornstein-Zernike correlation function in a d-dimensional space.

Solution. Proceeding as in the previous example we obtain

$$\int \frac{d\boldsymbol{q}}{(2\pi)^d} \frac{\mathrm{e}^{i\boldsymbol{q}\cdot\boldsymbol{r}}}{q^2 + q_c^2} = \int_0^\infty d\alpha\, e^{-\alpha q_c^2} \int \frac{d\boldsymbol{q}}{(2\pi)^d} e^{-\alpha q^2 + i\boldsymbol{q}\cdot\boldsymbol{r}}$$

$$= \frac{1}{2^d \pi^{d/2}} \int_0^\infty d\alpha\, e^{-r^2/4\alpha - \alpha q_c^2} \alpha^{-d/2} .$$

With a suitable change of variable the remaining integral may be cast into the form of the widely known integral representation of the modified Bessel function K_ν:

$$K_\nu(z) = \int_0^\infty e^{-z \cosh t} \cosh(\nu t)\, dt , \qquad |\arg z| < \frac{\pi}{2} . \tag{2.27}$$

To this end, first stretch the variable $\alpha = \dfrac{r}{2q_c}u$ to obtain

$$\frac{1}{2^d \pi^{d/2}} \int_0^\infty d\alpha \, e^{-r^2/4\alpha - \alpha q_c^2} \alpha^{-d/2}$$

$$= \frac{q_c^{d/2-1}}{2(2\pi)^{d/2} r^{d/2-1}} \int_0^\infty du \, e^{-(q_c r/2)(u+1/u)} u^{-d/2} = \frac{q_c^{d/2-1}}{2(2\pi)^{d/2} r^{d/2-1}}$$

$$\times \left[\int_1^\infty du \, e^{-(q_c r/2)(u+1/u)} u^{-d/2} + \int_0^1 du \, e^{-(q_c r/2)(u+1/u)} u^{-d/2} \right].$$

In the first integral of the last line, introduce a new variable $u = e^t$, whereas in the second $u = e^{-t}$. The result is the sum of two similar integrals, which may be written as

$$\int \frac{d\boldsymbol{q}}{(2\pi)^d} \frac{e^{i\boldsymbol{q}\cdot\boldsymbol{r}}}{q^2 + q_c^2} = \frac{q_c^{d/2-1}}{(2\pi)^{d/2} r^{d/2-1}} \int_0^\infty dt \, e^{-q_c r \cosh t} \cosh\left[(d/2-1)t\right].$$

Thus, the final result for the inverse Fourier transform of the Ornstein-Zernike correlation function is

$$\int \frac{d\boldsymbol{q}}{(2\pi)^d} \frac{e^{i\boldsymbol{q}\cdot\boldsymbol{r}}}{q^2 + q_c^2} = \frac{1}{(2\pi)^{d/2}} \left(\frac{q_c}{r}\right)^{d/2-1} K_{d/2-1}(q_c r). \qquad (2.28)$$

■ **Scattering of light and particles in isotropic medium.** Particle correlations and responses in a medium may be investigated with the aid of scattering experiments revealing both the spatial structure of matter and its elementary excitations. If interaction is small, as is often case in scattering of light or neutrons, it suffices to take into account the interaction in the linear approximation, i.e. in the linear response theory.

We do not intend to analyze details of scattering mechanisms. It is essential, however, that the external perturbation (particle, photon or electromagnetic field) couples to the particle density in the medium (sometimes to a current density) so that the relevant quantities are the density correlation and response functions.

The density correlation function (actually the structure factor) appears in the intensity of the scattered wave due to interference. Let the wave vector of the incident electromagnetic wave be $\boldsymbol{k}$ and that of the scattered wave $\boldsymbol{k}'$. Consider *elastic scattering*, where $|\boldsymbol{k}| = |\boldsymbol{k}'|$. The amplitude of the wave scattered by identical particles may be expressed as

$$\boldsymbol{E} = \boldsymbol{E}_1 \sum_{n=1}^N e^{i\phi_n}$$

with the phase factor of the individual scattered plane wave

$$\phi_n = (\boldsymbol{k} - \boldsymbol{k}') \cdot \boldsymbol{r}_n \equiv -\boldsymbol{q} \cdot \boldsymbol{r}_n$$

when the observation distance is much larger that the typical length of the specimen causing the scattering. Intensity of the scattered wave

$$I \propto \boldsymbol{E} \cdot \boldsymbol{E}^* = |E_1|^2 \left[N + \sum_{m \neq n} e^{i(\phi_m - \phi_n)} \right]$$

may then be expressed as

$$I = I_0 \left[1 + \frac{1}{N} \sum_{m \neq n} e^{i(\phi_m - \phi_n)} \right],$$

where I_0 is the intensity due to incoherent scattering.

The speed of light is much larger than the typical velocity of the molecules, so that the scattering events on different molecules may be considered simultaneous. Then the phase difference is brought about by the path-length difference of partial waves:

$$\phi_m - \phi_n = -\boldsymbol{q} \cdot (\boldsymbol{r}_m - \boldsymbol{r}_n),$$

where $\boldsymbol{q}$ is the change of the wave vector of the wave in scattering. Thus

$$I = I_0 \left[1 + \frac{1}{N} \int d^3\boldsymbol{r} \int d^3\boldsymbol{r}' \sum_{m \neq n} \delta(\boldsymbol{r} - \boldsymbol{r}_m) \, \delta(\boldsymbol{r}' - \boldsymbol{r}_n) \, e^{-i\boldsymbol{q}\cdot(\boldsymbol{r}-\boldsymbol{r}')} \right].$$

In the expectation value of the intensity of the scattered wave the pair correlation function appears

$$\begin{aligned} \langle I \rangle &= I_0 \left[1 + \frac{n^2}{N} \int d^3\boldsymbol{r} \int d^3\boldsymbol{r}' \, e^{-i\boldsymbol{q}\cdot(\boldsymbol{r}-\boldsymbol{r}')} g(\boldsymbol{r} - \boldsymbol{r}') \right] \\ &= I_0 \left[1 + n \int d^3\boldsymbol{r} \, e^{-i\boldsymbol{q}\cdot\boldsymbol{r}} g(\boldsymbol{r}) \right]. \end{aligned}$$

When $\boldsymbol{q} \neq 0$, the intensity of the elastically scattered wave is proportional to the structure factor (2.7):

$$\begin{aligned} \langle I(\boldsymbol{k}, \boldsymbol{q}) \rangle &= I_0 \left\{ 1 + n \int d^3\boldsymbol{r} \, e^{-i\boldsymbol{q}\cdot\boldsymbol{r}} \left[g(\boldsymbol{r}) - 1 \right] \right\} \\ &= I_0(\boldsymbol{k}) S(\boldsymbol{q}) = \frac{I_0(\boldsymbol{k})}{N} \langle \Delta\widehat{n}(\boldsymbol{q}) \Delta\widehat{n}(-\boldsymbol{q}) \rangle. \end{aligned}$$

The structure factor allows to calculate the pair correlation function.

In scattering of light the wave length is much larger than distances between particles. Scattered intensity is then sensitive to long-wave-length fluctuations of the medium. In the approach leading to the Ornstein–Zernicke form discussed above the scattered intensity is

$$I(\theta) \ \propto \ \frac{1}{f_1 + f_2 q^2} \ \propto \ \frac{1}{\sin^2\frac{\theta}{2} + \left(\frac{\lambda}{4\pi\xi}\right)^2}, \tag{2.29}$$

where λ the wave length of light and θ the scattering angle, i.e. $q = 2k \sin\frac{\theta}{2}$.

Normally, the correlation length ξ is much less than the wave length λ. Since the compressibility diverges at the critical point of fluid: $\kappa_T \to \infty$ the constant f_1 vanishes. There is no reason to expect vanishing of f_2, however. This means that the correlation length ξ diverges. Relation (2.29) shows

that there is strong peak in the forward scattering and the total scattering cross section diverges. Therefore, the otherwise transparent fluid becomes opaque near the critical point. This is the *critical opalescense*. It is caused by strong density fluctuations whose typical size ξ grows from the usual microscopic length beyond the wave length of light.

■ **Dynamic correlation functions.** Consider operators in the Heisenberg picture of the form

$$\widehat{A}(t) \equiv \exp\left(\frac{i}{\hbar}\widehat{H}t\right)\widehat{A}\exp\left(-\frac{i}{\hbar}\widehat{H}t\right),\qquad(2.30)$$

where $\widehat{H}$ is the Hamilton operator of the interacting system. In the thermodynamic equilibrium the dynamic correlation function of two such operators is

$$\boxed{C_{AB}(t-t') \equiv \frac{1}{2}\left\langle \Delta\widehat{A}(t)\Delta\widehat{B}(t') + \Delta\widehat{B}(t')\Delta\widehat{A}(t)\right\rangle.}\qquad(2.31)$$

The expectation values $\langle A\rangle = \operatorname{Tr}\widehat{\varrho}A$ are evaluated with the use of the canonical or grand canonical density operator

$$\widehat{\varrho} = \frac{1}{Z}\mathrm{e}^{-\beta\widehat{H}}.\qquad(2.32)$$

Substituting in between and outside the operators the resolution of identity $\widehat{I} = \sum_n |n\rangle\langle n|$ with the energy eigenstates we arrive at the relation

$$C_{AB}(t-t') = \frac{1}{2Z}\sum_{nn'}\left(\mathrm{e}^{-\beta E_n} + \mathrm{e}^{-\beta E_{n'}}\right)\mathrm{e}^{i(t-t')(E_n-E_{n'})/\hbar}\langle n|\Delta A|n'\rangle\langle n'|\Delta B|n\rangle.$$

Define the temporal Fourier transform by

$$\begin{aligned}
f(\omega) &= \int_{-\infty}^{\infty} dt\,\mathrm{e}^{i\omega t}f(t)\\
f(t) &= \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\mathrm{e}^{-i\omega t}f(\omega)\,.
\end{aligned}\qquad(2.33)$$

The Fourier transform of the correlation function then leads to the *spectral representation*

$$\begin{aligned}
&C_{AB}(\omega)\\
&= \frac{h}{2Z}\sum_{nn'}\delta\left(E_n - E_{n'} + \hbar\omega\right)\left(\mathrm{e}^{-\beta E_n} + \mathrm{e}^{-\beta E_{n'}}\right)\langle n|\Delta A|n'\rangle\langle n'|\Delta B|n\rangle.\qquad(2.34)
\end{aligned}$$

An important particular case is the *dynamic structure factor*

$$\begin{aligned}
S(\boldsymbol{q},\omega) &\equiv \frac{1}{N}\int_{-\infty}^{\infty} dt\,\mathrm{e}^{i\omega t}\langle\Delta\widehat{n}(\boldsymbol{q},t)\Delta\widehat{n}(-\boldsymbol{q},0)\rangle\\
&= \frac{h}{NZ}\sum_{nn'}\delta\left(E_n - E_{n'} + \hbar\omega\right)\mathrm{e}^{-\beta E_n}\left|\langle n'|\Delta\widehat{n}(-\boldsymbol{q})|n\rangle\right|^2;\qquad(2.35)
\end{aligned}$$

The static structure factor (2.7) may be obtained as the integral

$$S(\boldsymbol{q}) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, S(\boldsymbol{q}, \omega).$$

■ **Dynamic correlation function near equilibrium.** Consider the deviation φ from the equilibrium value of some quantity characterizing alone a state of incomplete equilibrium. Let the relaxation time to the state of incomplete equilibrium be much shorter than the relaxation time to complete equilibrium state. In this case the fluctuation φ is *quasistationary*. Let φ be much larger than the average fluctuation, so that the system is significantly out of equilibrium. In the course of time it will tend to equilibrium and φ will thus decrease. Since φ is the sole parameter characterizing equilibrium, its rate of change must be a function of φ only. Assume that the deviation from equilibrium is such that this function may be expanded in powers of φ. At the leading order it then follows that

$$\frac{\mathrm{d}\varphi}{\mathrm{d}t} = -\lambda\varphi\,, \tag{2.36}$$

where λ is a positive constant. Equation (2.36) is the evolution equation of the relaxation of the system towards equilibrium. The parameter $1/\lambda$ is the *relaxation time* for the system to arrive at the equilibrium. The constant term in the expansion of the right side of (2.36) is absent, because the rate of change of φ must vanish at equilibrium.

For description of smaller values of φ (closer to equilibrium) relation (2.36) is replaced by

$$\frac{\mathrm{d}\varphi(t)}{\mathrm{d}t} = -\lambda\varphi(t) + f(t)\,, \tag{2.37}$$

where $f(t)$ is a *random force* generating fluctuations of $\varphi(t)$. For the random force a white-noise probability distribution is assumed with zero mean (to maintain zero expectation value of φ) and correlation function chosen to yield the correct equilibrium correlation function for φ (the latter is assumed to be known), i.e.

$$\langle f(t)\rangle = 0\,, \qquad \langle f(t)f(t')\rangle = 2\lambda\langle\varphi^2\rangle\delta(t - t')\,. \tag{2.38}$$

For solution of the Langevin equation (2.37) it is convenient to use the equilibrium system as the initial condition in infinitely distant past. The explicit solutio

$$\varphi(t) = \int_{-\infty}^{t} e^{-\lambda(t-u)} f(u)\, du\,. \tag{2.39}$$

gives rise to the correlation function of fluctuations

$$C_{\varphi\varphi}(t - t') = \langle\varphi(t)\varphi(t')\rangle = \langle\varphi^2\rangle e^{-|t-t'|}\,. \tag{2.40}$$

This expression is has different left and right derivatives at the origin. This irregular behaviour is due the assumption of quasistationary fluctuations that the relaxation time to the incomplete equilibrium is negligibly small.

2.2 Linear response function

■ **Linear response function.** Perturbations of an equilibrium system are divided into two classes: the cause of a *mechanical perturbation* may be expressed by an additional term to the Hamiltonian of the system. If this is not possible, then the perturbation is *thermal*. In the linear response theory the response of the system to a mechanical perturbation may be calculated by expanding the density operator generated by the full Hamilton operator

$$\widehat{H} \to \widehat{H} - \sum_m \widehat{A}_m a_m$$

in (small) parameters a_m describing the intensity of the perturbation. Here, $\widehat{H}$ is the Hamilton operator of the equilibrium system and $\widehat{A}_m$ the Hermitian operators causing the perturbation (these or parts thereof are often present in $\widehat{H}$),

Let us ask the question, how much does the expectation value of an observable $\widehat{A}$ change due to a small perturbation. The answer is given by the response function (susceptibility).

To this end, consider a time-dependent small perturbation coupled with the system through the observable $\widehat{B}$

$$\widehat{H}(t) = \widehat{H} - \widehat{B}b(t). \tag{2.41}$$

Linearize the evolution equation of the density operator

$$i\hbar \frac{d\widehat{\varrho}}{dt} = \left[\widehat{H}, \widehat{\varrho}\right]$$

with respect to the factor $b(t)$ by searching the solution in the form $\widehat{\varrho}_t = \widehat{\varrho} + \delta\widehat{\varrho}$, where $\widehat{\varrho}$ is the density operator of the unperturbed equilibrium state. We obtain the equation

$$i\hbar \frac{d\delta\widehat{\varrho}}{dt} = \left[\widehat{H}, \delta\widehat{\varrho}_t\right] - b(t)\left[\widehat{B}, \widehat{\varrho}\right]. \tag{2.42}$$

Use the method of variation of constants. The trial solution is then $\delta\widehat{\varrho}_t(t) = \mathrm{e}^{-it\widehat{H}/\hbar}\widehat{u}(t)\mathrm{e}^{it\widehat{H}/\hbar}$. Substituting in equation (2.42) and integrating over time the equation obtained for the operator $\widehat{u}$ we obtain the variation of the density operator in the linear approximation

$$\delta\widehat{\varrho}_t(t) = \frac{i}{\hbar} \int_{-\infty}^t \mathrm{e}^{-i\widehat{H}t/\hbar}\left[\widehat{B}(t'), \widehat{\varrho}\right]\mathrm{e}^{i\widehat{H}t/\hbar}\, b(t')dt'\,,$$

where the operator $\widehat{B}(t')$ has been expressed in the Heisenberg picture. It has also been assumed that in far away in the past ($t \to -\infty$) the system has been in an unperturbed equilibrium state.

The change of the expectation value $\langle \widehat{A} \rangle$ due to the time-dependent perturbation in (2.41) at the time instant t in the linear approximation assumes the form

$$\delta A(t) \equiv \langle \widehat{A} \rangle_t - \langle \widehat{A} \rangle \approx \mathrm{Tr}\, \widehat{A}\, \delta\widehat{\varrho}(t)$$

$$= \frac{i}{\hbar} \int_{-\infty}^{t} \mathrm{Tr}\, \left\{ \widehat{A} \mathrm{e}^{-i\widehat{H}t/\hbar} \left[\widehat{B}(t'), \widehat{\varrho} \right] \mathrm{e}^{i\widehat{H}t/\hbar} \right\} b(t') dt'$$

$$= \frac{i}{\hbar} \int_{-\infty}^{t} \left\langle \left[\widehat{A}(t), \widehat{B}(t') \right] \right\rangle b(t') dt' = \int_{-\infty}^{\infty} \chi_{AB}(t - t') b(t') dt', \quad (2.43)$$

where the cyclic invariance of the trace has been used and the *dynamic linear response function* (or the dynamic susceptibility) defined

$$\boxed{\chi_{AB}(t - t') \equiv \frac{i}{\hbar} \theta(t - t') \left\langle \left[\widehat{A}(t), \widehat{B}(t') \right] \right\rangle .} \qquad (2.44)$$

The notation $\langle \cdots \rangle = \mathrm{Tr}\, \widehat{\varrho} \cdots$ denotes the expectation value in the unperturbed state. Note that due to the commutator the response function depends only on the fluctuating parts of the operators $\Delta\widehat{A} = \widehat{A} - \langle \widehat{A} \rangle$, $\Delta\widehat{B} = \widehat{B} - \langle \widehat{B} \rangle$.

The linear response function is nonvanishing only at a positive time argument. This is a natural consequence of *causality*: the change can only occur after its cause.

For spectral representation if is convenient to introduce a cutoff parameter $\epsilon \to 0+$, which allows to carry out the time integral under the sums over energy eigenstates:

$$\chi_{AB}(\omega) = \frac{i}{\hbar} \int_{0}^{\infty} dt\, \mathrm{e}^{(i\omega - \epsilon)t} \left\langle \left[\widehat{A}(t), \widehat{B}(t') \right] \right\rangle$$

$$= \frac{1}{Z} \sum_{nn'} \frac{\left(\mathrm{e}^{-\beta E_{n'}} - \mathrm{e}^{-\beta E_n} \right)}{\hbar\omega + E_n - E_{n'} + i\epsilon} \langle n|\Delta A|n' \rangle \langle n'|\Delta B|n \rangle$$

$$:= \chi'_{AB}(\omega) + i\chi''_{AB}(\omega), \quad (2.45)$$

where $\chi'_{AB}(\omega)$ and $\chi''_{AB}(\omega)$ are, respectively, the real and imaginary parts of the spectral response function $\chi_{AB}(\omega)$. The Fourier transform of the expectation value of the commutator is

$$\int_{-\infty}^{\infty} dt\, \mathrm{e}^{i\omega t - \epsilon|t|} \left\langle \left[\widehat{A}(t), \widehat{B}(t') \right] \right\rangle$$

$$= \frac{i\hbar}{Z} \sum_{nn'} \left(\mathrm{e}^{-\beta E_n} - \mathrm{e}^{-\beta E_{n'}} \right) \langle n|\Delta A|n' \rangle \langle n'|\Delta B|n \rangle$$

$$\times \left(\frac{1}{\hbar\omega + E_n - E_{n'} + i\epsilon} - \frac{1}{\hbar\omega + E_n - E_{n'} - i\epsilon} \right)$$

$$= \frac{2\hbar}{Z} \sum_{nn'} \delta\left(E_n - E_{n'} + \hbar\omega \right) \left(\mathrm{e}^{-\beta E_n} - \mathrm{e}^{-\beta E_{n'}} \right) \langle n|\Delta A|n' \rangle \langle n'|\Delta B|n \rangle, \quad (2.46)$$

where the Sokhotsky identity

$$\frac{1}{x \mp i\epsilon} = \pm i\pi\delta(x) + \mathcal{P}\frac{1}{x} \tag{2.47}$$

has been used. In (2.47) $\mathcal{P}$ means the principal value of the integral over x and the limit $\epsilon \to 0+$ is implied.

With the use of the Sokhotsky identity from (2.45) and (2.46) it follows that the absorptive part of the linear response function – as a function of time – is given by the expectation value of the commutator

$$\chi''_{AB}(t - t') \equiv \frac{1}{2\hbar}\left\langle \left[\widehat{A}(t), \widehat{B}(t')\right]\right\rangle . \tag{2.48}$$

The response function may thus be expressed as

$$\chi_{AB}(t - t') = 2i\theta(t - t')\chi''_{AB}(t - t'). \tag{2.49}$$

In general the system may be perturbed by several external forces or fields $h_a(t)$ coupled to the observables $\widehat{A}_a$ as

$$\widehat{H}(t) = \widehat{H} - \sum_a \widehat{A}_a\, h_a(t). \tag{2.50}$$

In this case it is necessary to define the response (susceptibility) matrix

$$\chi_{ab}(t - t') \equiv \frac{i}{\hbar}\theta(t - t')\left\langle \left[\widehat{A}_a(t), \widehat{A}_b(t')\right]\right\rangle ,$$

so that relation (2.43) is generalized for the deviations from the expectation values in the form

$$\delta A_a(t) = \sum_b \int_{-\infty}^{\infty} dt'\, \chi_{ab}(t - t')h_b(t'). \tag{2.51}$$

Since the integrals here are convolutions, it is convenient to Fourier transform them with respect to time to obtain algebraic relations:

$$\boxed{\delta A_a(\omega) = \sum_b \chi_{ab}(\omega)h_b(\omega).} \tag{2.52}$$

Example 2.3. Show that the spectral representation of the expectation value $\left\langle \left[\widehat{A}(t), \widehat{B}\right]\right\rangle$ does not contain diagonal matrix elements of the operators $\widehat{A}$ and $\widehat{B}$. Conclude from this result that

$$\left\langle \left[\widehat{A}(t), \widehat{B}\right]\right\rangle \to 0\,,\ t \to \infty\,.$$

Solution. By cyclic permutation under the trace we obtain

$$\left\langle \left[\widehat{A}(t), \widehat{B}\right]\right\rangle = \mathrm{Tr}\left\{\widehat{\rho}\left[\widehat{A}(t), \widehat{B}\right]\right\} = \mathrm{Tr}\left\{\widehat{B}\left[\widehat{\rho}, \widehat{A}(t)\right]\right\}\,.$$

Expressing the trace in the basis of eigenfunctions of the density operator $\widehat{\rho}$ and inserting a resolution of unity we arrive at relations

$$\mathrm{Tr}\left\{\widehat{B}\left[\widehat{\rho},\widehat{A}(t)\right]\right\} = \sum_{m,n}\left\langle m\left|\widehat{B}\right|n\right\rangle\left\langle n\left|\left[\widehat{\rho},\widehat{A}(t)\right]\right|m\right\rangle$$

$$= \sum_{m,n}\left\langle m\left|\widehat{B}\right|n\right\rangle\left\langle n\left|\widehat{A}\right|m\right\rangle e^{-it(E_m - E_n)/\hbar}\left(p_n - p_m\right),\quad (2.53)$$

where p_n is the eigenvalue of the density operator: $\widehat{\rho}|n\rangle = p_n|n\rangle$ and E_n the energy eigenvalue in the state $|n\rangle$, so that

$$\left\langle n\left|\widehat{A}(t)\right|m\right\rangle = e^{-it(E_m - E_n)/\hbar}\left\langle n\left|\widehat{A}\right|m\right\rangle.$$

From the explicit spectral representation (2.53) it is evident that the contribution of the diagonal matrix elements $\left\langle n\left|\widehat{A}\right|m\right\rangle$ and $\left\langle n\left|\widehat{B}\right|m\right\rangle$ to the twofold sum vanishes.

In a large system the energy levels are very close to each other, therefore the sum in (2.53) is, in practice, a high-precision integral sum. Since there are no obvious singularities in the summand, the whole expression vanishes in the limit $t \to \infty$ due to wild oscillations of the exponential (Riemann-Lebesgue theorem).

■ **Dispersion relations.** The response function $\chi_{AB}(t) = 0$, when $t < 0$ (causality). Therefore, its Fourier transform $\chi_{AB}(\omega)$ as a function of complex ω is an analytic function in the upper half plane ($\mathrm{Im}\,\omega > 0$). This is evident from the very definition for complex ω

$$\chi_{AB}(\omega) = \int_0^\infty e^{it(\mathrm{Re}\,\omega + i\mathrm{Im}\,\omega)}\chi_{AB}(t)\,dt,\qquad (2.54)$$

in which the integral converges uniformly with respect to complex ω, when $\mathrm{Im}\,\omega > \delta$ for any fixed $\delta > 0$. From representation (2.54) it also immediately follows that

$$\chi_{AB}(\omega) \to 0,\ \mathrm{Im}\,\omega \to \infty,$$
$$\chi_{AB}(\omega) \to 0,\ \mathrm{Re}\,\omega \to \pm\infty.$$

The latter limit is due the Riemann-Lebesgue lemma. Starting from the Cauchy formula on a closed half-circle contour in the upper half of the complex ω plane and sending the radius of the arc to infinity and the letting the diagonal approach the real axis we infer the representation

$$\chi_{AB}(\omega) = \frac{1}{2\pi i}\int_{-\infty}^\infty \frac{\chi_{AB}(w)}{w - \omega}\,dw,\quad \mathrm{Im}\,\omega > 0.$$

Let the variable ω now approach the real axis and use for calculation of the integral the Sokhotsky formula (2.47).

For real ω we obtain

$$\chi_{AB}(\omega) = \frac{1}{2\pi i}\, i\pi \chi_{AB}(\omega) + \frac{1}{2\pi i}\mathcal{P}\int\limits_{-\infty}^{\infty} \frac{\chi_{AB}(w)}{w-\omega}\, dw$$

so that

$$\chi_{AB}(\omega) = \frac{1}{\pi i}\mathcal{P}\int\limits_{-\infty}^{\infty} \frac{\chi_{AB}(w)}{w-\omega}\, dw\,, \tag{2.55}$$

wherefrom we immediately infer the *dispersion relations* (Kramers-Kronig relations)

$$\operatorname{Re}\chi_{AB}(\omega) = \chi'_{AB}(\omega) = \frac{1}{\pi}\mathcal{P}\int\limits_{-\infty}^{\infty} \frac{\chi''_{AB}(w)}{w-\omega}\, dw \tag{2.56}$$

$$\operatorname{Im}\chi_{AB}(\omega) = \chi''_{AB}(\omega) = -\frac{1}{\pi}\mathcal{P}\int\limits_{-\infty}^{\infty} \frac{\chi'_{AB}(w)}{w-\omega}\, dw\,. \tag{2.57}$$

All three relations (2.55), (2.56) and (2.57) are equivalent.

Physically, the function $\chi''_{AB}(\omega)$ is related to dissipation in the system of energy absorbed from some external source. It can be shown that an external field varying at the angular frequency ω loses energy to the system at power proportional to $\omega\chi''_{AB}(\omega)$.

■ **Fluctuation-dissipation theorem.** From the spectral representation of the correlation function (2.34) with the use of the δ function it follows that

$$C_{AB}(\omega)$$
$$= \left(1 + e^{-\beta\hbar\omega}\right)\frac{h}{2Z}\sum_{nn'}\delta(E_n - E_{n'} + \hbar\omega)\, e^{-\beta E_n}\, \langle n|\Delta A|n'\rangle\langle n'|\Delta B|n\rangle\,. \tag{2.58}$$

On the other hand, the spectral representation of χ''_{AB} may be cast in the form

$$\chi''_{AB}(\omega) = \frac{\pi}{Z}\left(1 - e^{-\beta\hbar\omega}\right)\sum_{nn'}\delta(E_n - E_{n'} + \hbar\omega)\, e^{-\beta E_n}\, \langle n|\Delta A|n'\rangle\langle n'|\Delta B|n\rangle.$$

Comparison with (2.58) leads to the *fluctuation-dissipation theorem* of Callen and Welton:

$$\chi''_{AB}(\omega) = \frac{1}{\hbar}\tanh\left(\frac{\beta\hbar\omega}{2}\right)C_{AB}(\omega)\,. \tag{2.59}$$

In the classical limit ($\hbar \to 0$)

$$\chi''_{AB}(\omega) = \frac{\omega}{2T}C_{AB}(\omega)\,. \tag{2.60}$$

The fluctuation-dissipation theorem establishes the mutual connection between two phenomena of rather different kind. On the right side there is a function describing spontaneous fluctuations in the system, whereas on the left side the absorptive part of the response function is related to energy dissipation.

2.3 Problems

Problem 2.1. Consider a Maxwell-Boltzmann gas in a homogeneous gravitational field as an example of an inhomogeneous system. Let the potential energy of a particle $U(z) = mgz$. Show that with the use of a natural generalization of the definition of the pair correlation function $g(\boldsymbol{r} - \boldsymbol{r}')$

$$\langle \widehat{n}(\boldsymbol{r})\widehat{n}(\boldsymbol{r}')\rangle = n\delta(\boldsymbol{r} - \boldsymbol{r}') + n^2 g(\boldsymbol{r} - \boldsymbol{r}')$$

in a homogeneous system the function $g(\boldsymbol{r} - \boldsymbol{r}') = 1$ in this case as well.

Problem 2.2. Show that the pair correlation function of the ideal quantum gas $h(\boldsymbol{r}) = o(\hbar^2)$ in the limit $\hbar \to 0$. Try to conclude that $h(\boldsymbol{r})$ actually vanishes faster than any power of $\hbar$ (this is optional).

Problem 2.3.

$$P[\delta n] \propto \mathrm{e}^{-\beta \widetilde{F}} \propto \exp\left[-\frac{1}{2TV} \sum_{\boldsymbol{q}}{}' \left(f_1 + f_2 \boldsymbol{q}^2 \right) |\delta n(\boldsymbol{q})|^2 \right], \qquad (2.61)$$

where

$$\delta n(\boldsymbol{q}) = \int d\boldsymbol{x}\, e^{-i\boldsymbol{q}\cdot\boldsymbol{x}} \delta n(\boldsymbol{x})\,.$$

The prime in the wave-vector sum means that the term with $\boldsymbol{q} = 0$ is omitted. Note that due to $\delta n^*(\boldsymbol{q}) = \delta n(-\boldsymbol{q})$ each term in the sum is actually calculated twice.

Calculate the Fourier transform of the density correlation function

$$C_{nn}(\boldsymbol{q}, \boldsymbol{q}') = \int d\boldsymbol{x}\, e^{-i\boldsymbol{q}\cdot\boldsymbol{x}} \int d\boldsymbol{x}'\, e^{-i\boldsymbol{q}'\cdot\boldsymbol{x}} \langle \delta n(\boldsymbol{x})\delta n(\boldsymbol{x}')\rangle$$

in this system.

Problem 2.4. For ideal Fermi gas, calculate two leading correction terms to the (vanishing) pair correlation function of the Maxwell-Boltzmann gas.

Problem 2.5. Evaluate the pair correlation function of the photon gas

Problem 2.6. Calculate the Fourier transform $\chi_{nn}(k, \omega)$ of the density-density response function of one-dimensional electron gas at zero temperature. Note that in one dimension electrons are spinless fermions. Here, it is safest to use the commutator representation

$$\chi_{nn}(x - x', t - t') = \frac{i}{\hbar}\theta(t - t')\big\langle \big[\widehat{n}(x, t), \widehat{n}(x', t')\big]\big\rangle\,.$$

To change the order of integration a cutoff factor $e^{-\varepsilon t}$, $\varepsilon \to 0+$ is needed in the Fourier transform, wherefrom $\varepsilon \to 0$ remains in the result.

3. Phase transitions and critical phenomena

3.1 Classification of phase transitions

■ **Classification of phase transitions.** The basic thermodynamic potential in the description of phase transitions is the Gibbs potential $G = \mu N$, because one of the equilibrium conditions – in addition to that the temperature and the pressure are uniform – is that the chemical potential coincides in all coexisting phases.

Phase transitions are traditionally classified by the singular behaviour of the derivatives of the Gibbs potential. If some of these derivatives are discontinuous, the phase transition is of *first order*. If all the first derivatives are continuous, but discontinuities (or worse singularities) appear in the second order derivatives, then we are dealing with a *second order* phase transition. These names suggest generalization according to the behaviour of higher derivatives, but this line of classification could not be consistently extended.

■ **Order parameter.** Another popular classification scheme emphasizes the behaviour of the central quantity in the modern theory of phase transition, viz. the *order parameter*. This is a quantity, which by definition is zero in one phase and assumes finite values in the other. In spite of the loose definition, in most cases there is a natural choice for the order parameter. In the gas-liquid transition, for instance, such a natural choice is the difference between the densities of liquid and gas, whereas in the paradigmatic ferromagnetic transition the order parameter is the magnetization. If the change of the order parameter in the phase transition is finite, then we are dealing with a *discontinuous phase transition*. If the order parameter tends to the zero value or departs from it in a continuous fashion, then a *continuous phase transition* takes place.

It is typical of the continuous phase transitions that the order parameter, various response functions and correlation functions exhibit non-analytic behaviour as functions of thermodynamic variables in the vicinity of the *critical point*, i.e. the point of the continuous phase transition in the space spanned by the thermodynamic variables. This non-analytic behaviour is usually a powerlike dependence in deviations from the critical-point values of variables such as the temperature and some "external field" like the pressure in the gas-liquid transition or the magnetic field strength

in the ferromagnetic transition. The exponents appearing in such asymptotic relations are the *critical exponents* (or critical indices) of the transition. The most common critical exponents will be defined and calculated below within the Landau theory of phase transitions.

In many cases phase transitions involve changes in symmetries of the system, which are called *symmetry breaking*. In the ferromagnetic transition, for instance, in the paramagnetic phase the material is often macroscopically isotropic and thus possesses the three-dimensional rotational symmetry. In the ferromagnetic phase the direction of the macroscopic magnetization establishes a preferred direction and the rotational symmetry remains at most in the plane perpendicular to the direction of the magnetization.

■ **Symmetry breaking and order parameter.** It is typical of a second order (or continuous) phase transition that some symmetry of the (usually) high-temperature phase is spontaneously broken in the low-temperature phase. The degree of symmetry breaking may be described by an order parameter vanishing in the *symmetric* (usually) high-temperature phase, but finite in the *ordered* phase with the broken symmetry. Examples:

- Structural transformation of a crystal lattice. In barium titanate (Fig. 3–1) electric polarization is brought about, this is ferroelectricity. The polarization P is the natural order parameter.
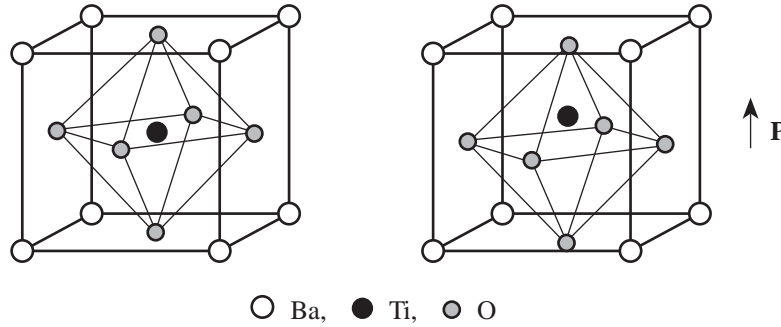

○ Ba, ● Ti, ◉ O

Figure 3–1: Structural transformation of $BaTiO_3$. The polarization P is the order parameter.

- Ferromagnetic phase transition. The broken symmetry is the spin rotation symmetry. Below the critical temperature magnetization $M \neq 0$ appears; this is the order parameter of the system.

- Superconducting transition of electron system and superfluidity transition of ^4He. Here, a *gauge symmetry* related with the particle number conservation is broken.

- Symmetry breaking of the electroweak interaction in particle physics. A gauge symmetry is broken here as well.
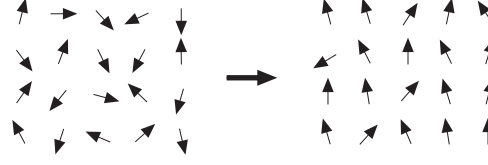
Figure 3–2: Magnetic ordering.

■ **Universality.** It is a remarkable feature of the continuous phase transitions that they are largely insensitive to material properties of the system apart from such global features like rotational or other symmetries. Physically different phase transitions may be described in a unified fashion as soon as important global properties such as the number of components and the tensor character of the order parameter, symmetries of the system and the space dimension are found to be the same. This is the *universality* of continuous phase transitions, and identification of the *universality class* of the particular phase transition is one of the important tasks of its analysis. Most importantly, the values of critical exponents turn out to coincide fairly accurately in physically different systems belonging to the same universality class.

■ **Singularities in the thermodynamic limit.** Mathematical description of continuous phase transitions is much more difficult than that of the discontinuous transitions. In the latter case different phases have chemical potentials of their own and at the phase transition the coexistence condition $\mu_1 = \mu_2$ holds. On the other hand, by definition of the first-order transition, e.g.,

$$\frac{\partial \mu_1}{\partial T} \neq \frac{\partial \mu_2}{\partial T}$$

so that rising or lowering the temperature across the transition temperature necessarily involves a reversal in the ordering of the chemical potentials and in equilibrium the phase corresponding to the minimum of the chemical potential prevails. Chemical potentials of different phases are smooth functions of the state variables.

In case of continuous phase transition, on the contrary, the number of state of equilibria changes: a single chemical potential corresponds to the symmetric phase, whereas several (even infinitely many in case of breaking of a continuous symmetry) chemical potentials of equal value but different values of the order parameter are available for the ordered phase. This is a singularity which is hard to find in the statistical ensembles, whose partition functions, say $Z = \text{Tr} \, e^{-\beta \widehat{H}}$ are smooth functions of parameters, at least in a finite system with the physically prevailing effectively short-range interactions (Coulomb force is screened is electrically neutral systems, and gravity is small).

In the thermodynamic limit, however, singular behaviour may follow

for suitable values of parameters, as in the case of Bose condensation. Other possible sources of singularity are long-range interactions and zero-temperature limit, on which, however, we shall not dwell here. Exact results for physically interesting interacting systems are rare, including the celebrated solution of the two-dimensional Ising model. There are the paramount examples of the Bose condensation and superconductivity of the variational approach to the solution of anomalous Green functions. Nevertheless, more or less phenomenological approaches are popular in description of continuous phase transitions. The most general approach among them, based on a variational principle, is that of the Landau theory.

3.2   Landau theory of phase transitions

■ **Effective thermodynamic potential.** At the critical point (point of the continuous phase transition in the parameter space) the order parameter vanishes in a continuous manner, when the symmetric phase is approached. In the Landau theory the order parameter φ is considered a macroscopic variable describing an incomplete equilibrium, whose equilibrium value is found by minimizing the proper thermodynamic potential.

The system is considered to be so close to the critical point that the order parameter is already small but still so far from the critical point that the system may be assumed to homogeneous and the thermodynamic potential a smooth function of the order parameter and state variables. The thermodynamic potential is then expanded in powers of the order parameter and the leading terms retained. Thus

$$G(p, T, \varphi) = G_0(p, T) + \alpha\varphi + A\varphi^2 + C\varphi^3 + B\varphi^4 + \dots \qquad (3.1)$$

The linear term must vanish in case of vector order parameter for a rotation-invariant Gibbs potential. The third-order term gives rise to a discontinuous transition, so that in case of continuous transition only the second and fourth order terms remain. To guarantee existence of equilibrium, the coefficient $B >$, and, although a function of p and T may usually be considered constant. For $A > 0$ the only minimum of (3.1) is $\varphi = 0$, whereas in case $A < 0$ a twofold degenerate nonvanishing solution for the minimum exists. The borderline value $A = 0$ then corresponds to the point of phase transition. The simplest smooth temperature dependence is $A = a(T - T_c)$.

■ **Ferromagnetic ordering.** Here, the basic idea of Landau theory is demonstrated in the example of the prototypical ferromagnetic transition. Denote magnetization by $\boldsymbol{m}$ to emphasize that it is an order parameter assuming values different from the equilibrium magnetization. In relations

$$dU_{\text{sys}} = TdS + \mu_0 V \boldsymbol{h} \cdot d\boldsymbol{m} \,, \qquad (3.2a)$$

$$dF_{\text{sys}} = -SdT + \mu_0 V \boldsymbol{h} \cdot d\boldsymbol{m} \,, \qquad (3.2b)$$

the quantity $\boldsymbol{h} \equiv \boldsymbol{h}(T, \boldsymbol{m})$ is the derivative of the thermodynamic potential with respect to the order parameter. In equilibrium, however, it must be

equal to the magnetic field strength $\boldsymbol{H}$. The natural parameters of the free energy are T and $\boldsymbol{m}$, i.e. $F_{\mathrm{sys}} = F_{\mathrm{sys}}(T, \boldsymbol{m})$. If the system is coupled to a magnetic field with the fixed field strength $\boldsymbol{H}$, then the equilibrium value of the magnetization $\boldsymbol{m}$ is determined by the condition that the Gibbs function has a minimum. The magnetic Gibbs potential now becomes an order-parameter dependent function

$$G_{\mathrm{sys}}(T, \boldsymbol{H}; \boldsymbol{m}) = F_{\mathrm{sys}}(T, \boldsymbol{m}) - \mu_0 V \boldsymbol{H} \cdot \boldsymbol{m}. \tag{3.3}$$

Choose $\boldsymbol{m}$ to minimize G: $\delta G/\delta \boldsymbol{m} = \delta F_{\mathrm{sys}}/\delta \boldsymbol{m} - \mu_0 V \boldsymbol{H} = \mu_0 V \boldsymbol{h} - \mu_0 V \boldsymbol{H} \to 0$. In equilibrium we must have $\boldsymbol{h}(T, \boldsymbol{m}) = \boldsymbol{H}$. In other words, $\boldsymbol{m} = \boldsymbol{m}(T, \boldsymbol{H}) \equiv \boldsymbol{M}$ is the equilibrium magnetization and the familiar result holds

$$dG_{\mathrm{sys}} = -SdT - \mu_0 V \boldsymbol{M} \cdot d\boldsymbol{H}. \tag{3.4}$$

In an isotropic system the free energy F depends on the magnitude of the order parameter $m = |\boldsymbol{m}|$. Expand F as power series

$$\boxed{F(T, m) = F_0(T) + \alpha_2(T)m^2 + \frac{1}{2}\alpha_4(T)m^4 + \cdots.} \tag{3.5}$$

Assume simplest possible smooth dependencies to provide stable minima in the vicinity of T_c:

$$\alpha_2(T) = a \cdot (T - T_c); \quad a > 0$$
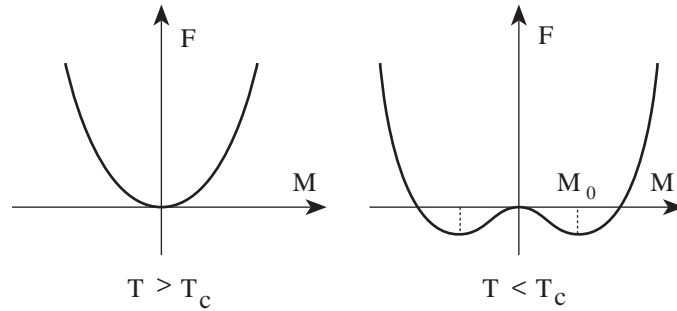$$\alpha_4(T) = b = \ \mathbf{const} \ > 0 \tag{3.6}$$

Figure 3–3: Free energy as a function of the order parameter in Landau theory.

Let first $H = 0$. Then the minimum of G is also the minimum of F. From the condition

$$\frac{\partial F}{\partial m} = 2a(T - T_c)m + 2bm^3 = 0$$

the equilibrium magnetization is found as (cf. Fig. 3–3)

$$M_0(T) = 0, \qquad\qquad T > T_c$$

$$M_0(T) = \pm\sqrt{\frac{a}{b}(T_c - T)}. \qquad T < T_c$$

(3.7)

The latter relation determines the value of the *critical exponent* β, which describes the non-analytic behaviour of the order parameter φ as a function of the temperature near the critical point as

$$\varphi(T) \sim (T_c - T)^\beta , \qquad T < T_c, \quad H = 0 .$$

(3.8)

Thus, in the Landau theory $\beta = \frac{1}{2}$.

The spontaneous magnetization $M_0(T)$ is depicted in Fig. 3–4. The minimum value of the zero-field free energy is thus

$$F(T, M_0) = F_0(T) ; \qquad\qquad T > T_c$$

$$F(T, M_0) = F_0(T) - \frac{a^2}{2b}(T_c - T)^2 ; \qquad T < T_c$$

(3.9)
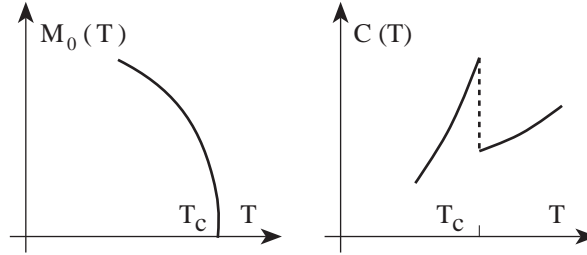
Figure 3–4: Magnetization and heat capacity.

■ **Heat capacity.** According to the definition

$$C_H = T\left(\frac{\partial S}{\partial T}\right)_H = -T\left(\frac{\partial^2 G}{\partial T^2}\right)_H .$$

In zero field $G = F$, more accurately $G(T, H = 0) = F(T, M_0(T))$, yielding $C_H(H = 0) = -T(d^2F/dT^2)$. From relations (3.9) we obtain

$$T > T_c : \qquad C_H(T) = C_0(T) \equiv -T\frac{d^2F_0}{dT^2}$$

$$T < T_c : \qquad C_H(T) = C_0(T) + \frac{a^2}{b}T$$

(3.10)

The specific heat has a jump

$$C_H(T_c^-) - C_H(T_c^+) = \frac{a^2}{b}T_c$$

at the critical temperature (Fig. 3–4).

In general, however, the singular behaviour of the heat capacity in a continuous transition is characterized by the critical exponents α and α' with the definition

$$C_H(T) \sim \begin{cases} (T - T_c)^{-\alpha}, & T > T_c, \\ (T_c - T)^{-\alpha'}, & T < T_c, \end{cases} \qquad H = 0, \tag{3.11}$$

where usually both α and α' are numerically small. The finite discontinuity in the Landau theory in these terms is described by putting $\alpha = \alpha' = 0$.

■ **Susceptibility.** If the external field $\boldsymbol{H} \neq 0$, we arrive at the equilibrium condition
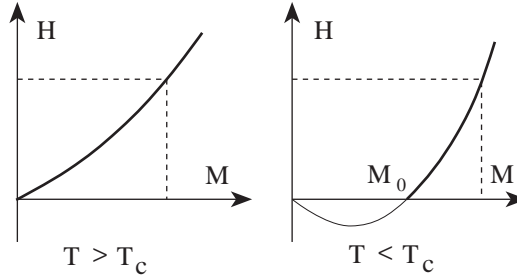
Figure 3–5: Determination of the equilibrium magnetization, relation (3.13)

$$\frac{\partial G}{\partial \boldsymbol{m}} = 0 \; \Leftrightarrow \; \frac{\partial F}{\partial \boldsymbol{m}} = \mu_0 V \boldsymbol{H}, \tag{3.12}$$

i.e., according to relations (3.5) and (3.6),

$$2a(T - T_c)M + 2bM^3 = \mu_0 V H. \tag{3.13}$$

In case $T > T_c$ (Fig. 3–5) in the limit of small field H the magnetization $M = \chi H + \mathcal{O}(H^3)$, with the susceptibility χ

$$\chi = \frac{\mu_0 V}{2a(T - T_c)}. \tag{3.14}$$

In case $T < T_c$ in the limit of small H obviously (cf. Fig. 3–5) $M = M_0 + \delta M$, where $\delta M \propto \delta H$ is small. The following relations hold,

$$\begin{aligned} \mu_0 V \delta H &= 2a(T - T_c)\delta M + 6bM_0{}^2 \delta M \\ &= 2a(T - T_c)\delta M + 6b\frac{a}{b}(T_c - T)\delta M \\ &= 4a(T_c - T)\delta M. \end{aligned}$$

This yields for the susceptibility the result

$$\chi = \frac{\delta M}{\delta H} = \frac{\mu_0 V}{4a(T_c - T)} \, .$$ (3.15)

From relations (3.14) and (3.15) it is seen that the critical exponents γ and γ' of the susceptibility, defined as

$$\chi(T) \sim \begin{cases} (T - T_c)^{-\gamma} \, , & T > T_c \, , \\ (T_c - T)^{-\gamma'} \, , & T < T_c \, , \end{cases} \quad H = 0 \, ,$$ (3.16)

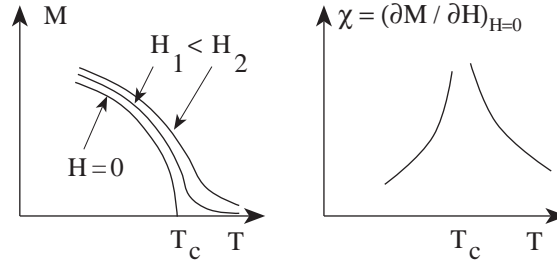in the Landau theory assume the value $\gamma = \gamma' = 1$.

Figure 3–6: Magnetization and susceptibility.

The susceptibility is depicted in Fig. 3–6. In the same plot dependence of the magnetization M on the temperature and field strength H has been sketched. In particular, at the critical temperature $T = T_c$, from the condition $\mu_0 V H = 2bM^3$ it follows

$$M(T_c , H) = \text{ const } \times H^{1/3} \, .$$ (3.17)

From this relation it follows that the critical exponent δ, which describes the non-analytic dependence of the order parameter φ of the external field h at the critical temperature as

$$\varphi(h) \sim h^{1/\delta} \, , \qquad T = T_c \, ,$$ (3.18)

in the Landau theory assumes the values $\delta = 3$.

3.3 Ginzburg-Landau theory of superconductivity

In a large system it is possible that the order parameter is not constant throughout the whole volume, especially, when the broken symmetry is continuous. Deviations from homogeneous order parameter are also necessary to describe fluctuations near the critical point. If local variability is allowed,

then a field theory is obtained with the order parameter $m(\boldsymbol{r})$ as a function of position. Such a generalization was put forward in V. Ginzburg in application to superconductivity and turned out to be very successful explanation of this phenomenon discovered already in 1911 by H. Kamerlingh–Onnes. The Ginzburg-Landau theory has proved a fruitful starting point for description of several other ordering phenomena as well.

■ **Free energy.** The order parameter is assumed to be a complex-valued function $\Psi(\boldsymbol{r})$ called *macroscopic wave function* in this context. Physically, this is quantity describing the correlated electron pairs (Cooper pairs), whose motion gives rise to the phenomenon of superconductivity in metals. The "genuine" wave function of such a pair of electrons depends on variables of both electrons, of course. The macroscopic wave function here is related to the motion of the center of mass of the Cooper pair, which is thus considered a pointlike object in the Ginzburg-Landau theory. The typical length scale up to which the electrons of the pair remain correlated, the *coherence length* ξ_0 (usually $\xi_0 \gtrsim 1000$ Å), must therefore be much less than the typical spatial scale of the macroscopic wave function for the Ginzburg-Landau theory to be consistent.

The free energy is written as local functional functional of the macroscopic wave function, where the spatial dependence is taken into account by the leading term of the gradient expansion:

$$F_{\mathrm{sys}}(T, [\Psi]) = \int d^3\boldsymbol{r} \left[f_0 + \frac{\hbar^2}{2m^*} |\nabla\Psi|^2 + a(T - T_c) |\Psi|^2 + \frac{b}{2} |\Psi|^4 \right]. \quad (3.19)$$

Here, m^* is a parameter of dimension of mass. In a system with charged particles in an magnetic field gauge invariance is imposed by replacing the gradient in the canonical momentum operator $-i\hbar\nabla$ by the covariant derivative to obtain $-i\hbar\nabla - e^*\boldsymbol{A}(\boldsymbol{r})$, where $\boldsymbol{A}$ is the vector potential and e^* the charge. With this substitution the Ginzburg-Landau free energy (3.19) remains invariant under the transformation $\Psi(\boldsymbol{r}) \to \Psi(\boldsymbol{r})\mathrm{e}^{i\alpha(\boldsymbol{r})}$ even in case of position-dependent $\alpha(\boldsymbol{r})$, when it is accompanied by the proper change of the vector potential. When the energy of the magnetic field is added, the total Ginzburg-Landau free energy is obtained in the form

$$\boxed{F = \int d^3\boldsymbol{r} \left\{ f_0 + \frac{\hbar^2}{2m^*} \left| \left(\nabla - \frac{ie^*}{\hbar} \boldsymbol{A} \right)\Psi \right|^2 + a\tau |\Psi|^2 + \frac{b}{2} |\Psi|^4 + \frac{\boldsymbol{B}^2}{2\mu_0} \right\},} \quad (3.20)$$

where for brevity the notation $\tau = T - T_c$ has been introduced. Thus, we are dealing with a 4-parameter (m^*, e^*, a, b) phenomenological theory.

■ **Variational conditions.** It is convenient to write down the stationarity equations for the functional (3.20) with the aid of the *functional derivative*, whose definition for an arbitrary functional $F[f]$ of the function $f(\boldsymbol{r})$ is

$$\delta F[f] \equiv \int d^3\boldsymbol{r} \, \delta f(\boldsymbol{r}) \frac{\delta F}{\delta f(\boldsymbol{r})} .$$

In practice, the usual chain rule together with partial integration is sufficient to arrive at expressions containing

$$\frac{\delta f(\boldsymbol{r}')}{\delta f(\boldsymbol{r})} = \delta(\boldsymbol{r}' - \boldsymbol{r})$$

which allows to resolve one spatial integral.

Since the electromagnetic field interacts with charged matter, the vector potential $\boldsymbol{A}$ is a variable quantity as well. Consider first variation of the magnetic field energy with fixed boundary conditions for the fields varied. Then

$$\delta \int_V \boldsymbol{B}^2 = \delta \int_V (\nabla \times \boldsymbol{A}) \cdot (\nabla \times \boldsymbol{A}) = 2 \int_V \boldsymbol{B} \cdot (\nabla \times \delta \boldsymbol{A})$$
$$= -2 \int_V \nabla \cdot (\boldsymbol{B} \times \delta \boldsymbol{A}) + 2 \int_V \nabla \cdot (\boldsymbol{B} \times \delta \boldsymbol{A}_c)$$
$$= -2 \int_{\partial V} \boldsymbol{n} \cdot (\boldsymbol{B} \times \delta \boldsymbol{A}) + 2 \int_V \delta \boldsymbol{A} \cdot (\nabla \times \boldsymbol{B}), \qquad (3.21)$$

where the notation $\delta \boldsymbol{A}_c$ means, that the derivatives in the nabla do not act on this factor. Taking into account the fixed boundary condition, we arrive at the result

$$\frac{\delta}{\delta \boldsymbol{A}(\boldsymbol{r})} \frac{1}{2\mu_0} \int_V \boldsymbol{B}^2 = \frac{1}{\mu_0} \nabla \times \boldsymbol{B} = \nabla \times \boldsymbol{H} \,.$$

This example illustrates construction of variations and functional derivatives. Evaluation of variations with respect to the order parameter Ψ is left as an exercise. Here, we quote only the final stationarity equations.

■ **Supercurrent density.** From the requirement of stationarity with respect to variations of $\Psi(\boldsymbol{r})^*$ and $\delta \boldsymbol{A}(\boldsymbol{r})$ the Ginzburg–Landau equations for superconductivity follow

$$-\frac{\hbar^2}{2m^*} \left(\nabla - \frac{ie^*}{\hbar} \boldsymbol{A} \right)^2 \Psi + \left(a\tau + b \, |\Psi|^2 \right) \Psi = 0 \,, \qquad (3.22a)$$

$$\boldsymbol{J} \equiv \frac{e^* \hbar}{2im^*} \left[\Psi^* (\nabla \Psi) - (\nabla \Psi^*) \Psi \right] - \frac{(e^*)^2}{m^*} \boldsymbol{A} \, |\Psi|^2 = \nabla \times \boldsymbol{H} \,. \qquad (3.22b)$$

The former is a nonlinear Schrödinger equation for superconducting particles with the mass m^* and charge e^*. The latter equation, which determines the supercurrent density $\boldsymbol{J}$, is Ampère's law $\nabla \times \boldsymbol{H} = \boldsymbol{J}$ for static fields. The first term of the current density $\boldsymbol{J}$ is the canonical current, which is not gauge invariant. Only the account of the second term gives rise to a gauge-invariant current density.

■ **Temperature-dependent coherence length.** The Ginzburg–Landau equations are nonlinear, therefore an exact solution is possible only in special cases. If there is no magnetic field, it is consistent to put $\boldsymbol{A} = 0$ everywhere. Relation (3.22b) is then automatically fulfilled, if Ψ is real.

Consider a superconductor filling the half-space $x > 0$. Then Ψ is a function of x only and the equation (3.22a) assumes the form

$$-\frac{\hbar^2}{2m^*}\frac{d^2\Psi(x)}{dx^2} + a\tau\Psi(x) + b\Psi(x)^3 = 0\,. \tag{3.23}$$

As a boundary condition, impose $\Psi(0) = 0$. The equation may be solved by multiplying by the factor $\Psi'(x)$ and constructing a first integral. The first-order differential equation obtained is also solvable. It turns out that a meaningful solution may only be found for temperatures $\tau < 0$, i.e. $T < T_c$. For the order parameter the expression

$$\Psi(x) = \sqrt{n_s}\tanh\frac{x}{2\xi}\,;\quad (x > 0), \tag{3.24}$$

follows, where

$$n_s = -\frac{a\tau}{b} \tag{3.25}$$

and

$$\xi = \frac{\hbar}{\sqrt{2am^*(T_c - T)}}\,. \tag{3.26}$$

The constant $n_s = |\Psi(\infty)|^2$ is the density of superconducting particles. The quantity ξ, which describes the thickness of the surface layer, is the *temperature-dependent coherence length.*. This is the typical length scale of the Ginzburg-Landau model. It is approximately equal to the coherence length ξ_0 of the correlated electron pairs far from T_c, but since it diverges as $\sqrt{T_c - T}$ near T_c, it is bound to become much larger than ξ_0 (which is independent of the temperature) close enough to the critical point.

■ **Meissner effect.** In a weak magnetic field the vector potential $\boldsymbol{A}$ and the field strength $\boldsymbol{H}$ are small and the wave function may be formally expanded as

$$\Psi = \Psi_0 + \Psi_1 + \Psi_2 + \dots\,,$$

where Ψ_0 is the zero-field solution obtained above, and $\Psi_n \propto |\boldsymbol{A}|^n$.

Let the region $x > 0$ be superconducting, and the magnetic field directed along the y axis. Then

$$\boldsymbol{A} = A(x)\boldsymbol{e}_z\,;\quad \boldsymbol{B} = \nabla \times \boldsymbol{A} = -A'(x)\boldsymbol{e}_y\,.$$

Rewrite equation (3.22a) in more detail,

$$-\frac{\hbar^2}{2m^*}\nabla^2\Psi + \frac{ie^*}{m^*}\boldsymbol{A}\cdot\nabla\Psi + \frac{(e^*)^2}{2m^*}\boldsymbol{A}^2\Psi + \left(a\tau + b|\Psi|^2\right)\Psi = 0.$$

The zeroth order yields the previous equation (3.23). In the first order the vector potential is absent, because the vectors $\boldsymbol{A}$ and $\nabla\Psi_0$ are orthogonal. Thus, $\Psi_1 = 0$, and the change of the wave function is of second order in $\boldsymbol{A}$. Equation (3.22b) then implies that in the first-order accuracy

$$-\frac{(e^*)^2}{m^*}\boldsymbol{A}|\Psi_0|^2 = \nabla \times \boldsymbol{H} = \frac{1}{\mu_0}\nabla \times (\nabla \times \boldsymbol{A}) = -\frac{1}{\mu_0}\nabla^2\boldsymbol{A}\,, \tag{3.27}$$

where the last form is a consequence of the relation $\nabla \cdot \boldsymbol{A} = 0$.

Equation (3.27) is readily solved deep in the superconductor, where $\Psi_0 =$ cons. For the function $A(x)$ with the account of relations (3.24) and (3.26) the following equation is obtained

$$\frac{d^2 A(x)}{dx^2} = -\frac{\mu_0 (e^*)^2 a\tau}{m^* b} A(x).$$

(3.28)

The physically meaningful solution is the exponentially falling off function

$$A(x) \xrightarrow[x \to \infty]{} \text{const} \times \exp\left(-\frac{x}{\lambda}\right),$$

(3.29)

where the parameter λ is the *penetration depth*

$$\lambda = \sqrt{\frac{bm^*}{a\mu_0 (e^*)^2 (T_c - T)}}.$$

(3.30)

Usually, $\lambda \gg 100$ Å. Since deep in the superconductor $\boldsymbol{A} = 0$, the magnetic field does not penetrate the matter. The superconductor is thus a perfect *diamagnet*. This is the *Meissner effect*.

In the Ginzburg-Landau theory both the temperature-dependent coherence length (3.26)and the penetration depth (3.30) diverge in the same way, when the critical temperature is approached. Their temperature-independent ratio

$$\kappa = \frac{\lambda}{\xi} = \frac{m^*}{\hbar e^*} \sqrt{\frac{2b}{\mu_0}},$$

(3.31)

the *Ginzburg-Landau parameter* is an important parameter of the theory, since its value determines the sign of the surface tension between the superconducting and normal phases and thus the character of the phase transition between them in strong magnetic fields.

■ **Critical field.** Superconductors thus expel magnetic field. A strong enough magnetic field, however, destroys the superconducting state. The borderline value, the *critical field* H_c may be determined thermodynamically as follows. A superconducting body possesses a magnetic moment $\boldsymbol{m} = V\boldsymbol{M} = -V\boldsymbol{H}$. The potential energy of this magnetic moment in the external field $W = -\mu_0 \int_0^H \boldsymbol{m} \cdot d\boldsymbol{H} = -\mu_0 \frac{1}{2}\boldsymbol{m} \cdot \boldsymbol{H} = \frac{1}{2} V\mu_0 H^2$ is the energy in excess to the free energy of the superconductor and the energy of the magnetic field in the absence of the superconductor (which occupies the volume of the superconductor as well). The corresponding interaction energy between the magnetic moment of the same body in the normal state and the external field is negligible due to the small numerical value of the dia- and paramagnetic susceptibilities. Therefore, the difference between the energies of the body in the magnetic field in the homogeneous superconducting state and in the normal state is – up to surface effects –

$$F_s - F_n = -V \frac{a^2 (T_c - T)^2}{2b} + \frac{1}{2} V\mu_0 H^2.$$

(3.32)

Just at the the critical field this difference vanishes, and near the critical temperature the thermodynamic critical field is

$$H_c = \frac{a(T_c - T)}{\sqrt{\mu_0 b}} \, .$$ (3.33)

Surface effects, however, turn out to be of paramount significance in many practical superconductors. The point is that the transition from, say, the superconducting to the normal state requires initial nucleation of small normal state formations, and the appearance of these is hindered by the energy cost to build up the surface, when the surface tension between the normal and superconducting states is positive. In such a case of a *superconductor of the I type* the phase transition takes place in fields larger than the thermodynamic critical field so that the magnetic field penetrates a large volume at once (the surface area between the ordinary and superconducting phases is minimized). In a *superconductor of the II type* the surface tension of the interface between the superconducting and normal states is negative, which leads to the nucleation of the normal phase in a superconducting bulk at field strengths less than the thermodynamic critical field (the borderline value is the lower critical field H_{c1}) and to the nucleation of superconducting phase at field strength larger than the thermodynamic critical field (the borderline value is the upper critical field H_{c2}). In these materials nothing remarkable happens at H_c.

In superconductors of the II type the magnetic flux penetrates the superconducting bulk as thin filaments (*vortices*) forming a vortex lattice (Abrikosov lattice). The flux in the filaments is quantized with the flux quantum h/e^*. Observations on this phenomenon as well as on quantization of magnetic flux through a superconducting ring have shown that the charge of the superconducting particle $e^* = -2e$, where $-e$ is the electron charge. The supercurrent is carried by bound pairs of electrons. These Cooper pairs are loose formations with the diameter of the of the coherence length ξ_0 and thus much larger than the distances between the conduction electrons.

The quantization of the magnetic flux may be readily demonstrated in geometries of a superconducting ring in a magnetic field and for a normal-state filament aligned with an external magnetic field in the superconducting bulk. Imagine a closed contour around the filament or along the ring deep in the bulk superconductor so that on the loop the magnetic induction vanishes and the modulus of the order parameter is constant. From relation (3.22b) and the representation $\Psi = |\Psi| \mathrm{e}^{i\phi}$ it then follows that on the contour

$$\nabla\phi = \frac{e^*}{\hbar} \, \boldsymbol{A} \, .$$ (3.34)

Integrating over the closed contour we obtain, by virtue of the Stokes theorem,

$$\Delta\phi = \oint \nabla\phi \cdot d\boldsymbol{l} = \frac{e^*}{\hbar} \oint \boldsymbol{A} \cdot d\boldsymbol{l} = \frac{e^*}{\hbar} \int \boldsymbol{n} \cdot \nabla \times \boldsymbol{A} \, dS = \frac{e^*}{\hbar} \, \Phi_B \, ,$$ (3.35)

where $\Delta\phi$ is the change of the phase of the wave function after traversing over the contour and Φ_B is the magnetic flux through a surface, whose boundary is the closed contour at hand. The wave function must, however, be a single-valued function of the position, which imposes the condition $\Delta\phi = 2\pi n$ with an integer n. Thus, the magnetic flux through a superconducting ring or normal-state filament is quantized as

$$\Phi_B = \int \boldsymbol{n} \cdot \boldsymbol{B} \, dS = \frac{h}{e^*} \, n \, . \tag{3.36}$$

In particular, this condition imposes restrictions on the appearance of normal-state vortices in the phase transition to the normal state in a type II superconductor in magnetic field.

3.4   Fluctuations in Landau theory

Landau theory is based on an effective thermodynamic potential describing the system in incomplete equilibrium described by the order parameter φ. The probability of such a state may be estimated in a manner similar to that used in the Einstein theory of fluctuations. Consider the classical canonical ensemble (for simplicity of notation).

The partition function is the measure of the phase state with the weight $\mathrm{e}^{-\beta H}$:

$$Z = \int{}' d\Gamma \, \mathrm{e}^{-\beta H(p,q)} \, . \tag{3.37}$$

The measure of the part of the phase state corresponding to the incomplete equilibrium may be written in a similar form by imposing the condition $\varphi = \varphi(p,q)$, where $\varphi(p,q)$ is the order parameter expressed as function of the variables of the phase space. Formally this is effected as

$$Z(\varphi) = \int{}' d\Gamma \, \delta\left(\varphi - \varphi(p,q)\right) \mathrm{e}^{-\beta H(p,q)} \, . \tag{3.38}$$

Obviously $Z = \int d\varphi \, Z(\varphi)$ and the relative frequency at which the incomplete equilibrium occurs in the phase space is

$$\Pr(\varphi) = \frac{Z(\varphi)}{Z} = \mathrm{e}^{\beta[F - F(\varphi)]} \, , \tag{3.39}$$

where the effective free energy is

$$F(\varphi) = -T \ln Z(\varphi) \, . \tag{3.40}$$

Substituting the expression for $F(\varphi)$ in the Landau theory (inhomogeneous system)

$$F(\varphi) = F_0 + \int d^3\boldsymbol{r} \, \left[g(\nabla\varphi)^2 + a(T - T_c)\varphi^2 + B\varphi^4 \right] \tag{3.41}$$

we arrive at the probability density for the order parameter in the form

$$\Pr(\varphi) \propto e^{-\beta \int d^3r \left[g(\nabla\varphi)^2 + a(T-T_c)\varphi^2 + B\varphi^4 \right]}. \tag{3.42}$$

Calculations with such a weight are only possible in the form of an expansion in B. The leading order is given by the Gaussian distribution corresponding to $B = 0$. Already in this approximation problems in definition of the mathematical quantities involved appear. For instance, the correlation function of the order parameter is

$$\langle \varphi(\boldsymbol{r})\varphi(\boldsymbol{r}') \rangle = \frac{\displaystyle\int \prod_{\boldsymbol{r}} d\varphi(\boldsymbol{r})\, \varphi(\boldsymbol{r})\varphi(\boldsymbol{r}')\, e^{-\beta \int d^3r \left[g(\nabla\varphi)^2 + a(T-T_c)\varphi^2 \right]}}{\displaystyle\int \prod_{\boldsymbol{r}} d\varphi(\boldsymbol{r})\, e^{-\beta \int d^3r \left[g(\nabla\varphi)^2 + a(T-T_c)\varphi^2 \right]}}. \tag{3.43}$$

In continuum space both the denominator and the numerator consist of a formally infinite-fold integral, to which some meaning should be prescribed.

The simplest thing to do is to put the system on a lattice in a finite box, which restricts the integrals over values of the order parameter at different positions to a finite number. In case of a Gaussian integral corresponding to the probability density function of the form

$$p(\boldsymbol{x}) = \sqrt{\det \frac{\boldsymbol{s}}{2\pi}}\, e^{-\frac{1}{2}\boldsymbol{x}\boldsymbol{s}\boldsymbol{x}} \tag{3.44}$$

it is also possible to use for the correlation function the expression

$$\boxed{\langle x_i x_j \rangle = (\boldsymbol{s}^{-1})_{ij}\,,} \tag{3.45}$$

in which the dimension of the space of integration does not appear explicitly. This means that

$$\langle \varphi(\boldsymbol{r})\varphi(\boldsymbol{r}') \rangle = \frac{T}{2} \left[-g\nabla^2 + a(T-T_c) \right]^{-1}(\boldsymbol{r},\boldsymbol{r}') = \frac{T}{2} G(\boldsymbol{r}-\boldsymbol{r}')\,, \tag{3.46}$$

where $G(\boldsymbol{r}-\boldsymbol{r}')$ is the Green function of the operator $-g\nabla^2 + a(T-T_c)$, i.e. the solution of the equation

$$\left[-g\nabla^2 + a(T-T_c) \right] G(\boldsymbol{r}) = \delta(\boldsymbol{r}) \tag{3.47}$$

with vanishing boundary condition at infinity.

More constructively calculation of the correlation function is convenient to carry out in the wave-vector space. Put the system in a, say, cubic box and define the coefficients of the Fourier series as

$$\varphi(\boldsymbol{k}) = \frac{1}{V} \int d^3r\, e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} \varphi(\boldsymbol{r})\,, \tag{3.48}$$

and calculate the Fourier coefficients of the correlation function

$$\frac{1}{V^2} \int d^3r \int d^3r'\, e^{-i\boldsymbol{k}\cdot\boldsymbol{r} - i\boldsymbol{k}'\cdot\boldsymbol{r}'} \langle \varphi(\boldsymbol{r})\varphi(\boldsymbol{r}') \rangle = \langle \varphi(\boldsymbol{k})\varphi(\boldsymbol{k}') \rangle\,. \tag{3.49}$$

On the other hand, assuming the usual translation invariance we may write

$$\langle \varphi(\boldsymbol{r})\varphi(\boldsymbol{r}')\rangle = C(\boldsymbol{r} - \boldsymbol{r}') \tag{3.50}$$

and

$$\frac{1}{V^2} \int d^3\boldsymbol{r} \int d^3\boldsymbol{r}'\, \mathrm{e}^{-i\boldsymbol{k}\cdot\boldsymbol{r}-i\boldsymbol{k}'\cdot\boldsymbol{r}'} C(\boldsymbol{r} - \boldsymbol{r}')$$
$$= \frac{1}{V} \int d^3\boldsymbol{r}'\, \mathrm{e}^{-i(\boldsymbol{k}+\boldsymbol{k}')\cdot\boldsymbol{r}'} \frac{1}{V} \int d^3\boldsymbol{r}\, \mathrm{e}^{-i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}')} C(\boldsymbol{r} - \boldsymbol{r}') = \delta_{\boldsymbol{k}',-\boldsymbol{k}} C(\boldsymbol{k})\,. \tag{3.51}$$

Comparison of relations (3.49) and (3.51) yields

$$\langle \varphi(\boldsymbol{k})\varphi(\boldsymbol{k}')\rangle = \delta_{\boldsymbol{k}',-\boldsymbol{k}} \langle \varphi(\boldsymbol{k})\varphi(-\boldsymbol{k})\rangle = \delta_{\boldsymbol{k}',-\boldsymbol{k}} \langle |\varphi(\boldsymbol{k})|^2\rangle\,, \tag{3.52}$$

since for a real $\varphi(\boldsymbol{r})$ from (3.48) it follows that $\varphi^*(\boldsymbol{k}) = \varphi(-\boldsymbol{k})$. Express now the Gaussian weight in terms of $\varphi(\boldsymbol{k})$. Substitution of the Fourier series of $\varphi(\boldsymbol{r})$ yields

$$\int d^3\boldsymbol{r}\, \left[g(\nabla\varphi)^2 + a(T - T_c)\varphi^2\right]$$
$$= \int d^3\boldsymbol{r} \sum_{\boldsymbol{k}} \sum_{\boldsymbol{k}'} \left[-g\boldsymbol{k}\cdot\boldsymbol{k}' + a(T - T_c)\right] \varphi(\boldsymbol{k})\varphi(\boldsymbol{k}')\, \mathrm{e}^{i\boldsymbol{k}\cdot\boldsymbol{r}+i\boldsymbol{k}'\cdot\boldsymbol{r}}$$
$$= V \sum_{\boldsymbol{k}} \left[gk^2 + a(T - T_c)\right] |\varphi(\boldsymbol{k})|^2\,. \tag{3.53}$$

In view of expressions (3.52) and (3.53) it appears convenient to carry out the integration over the real and imaginary parts of $\varphi(\boldsymbol{k})$. These are not all independent variables, since

$$\varphi(\boldsymbol{k}) = \varphi_R(\boldsymbol{k}) + i\varphi_I(\boldsymbol{k}) = \varphi^*(-\boldsymbol{k}) = \varphi_R(-\boldsymbol{k}) - i\varphi_I(-\boldsymbol{k})\,. \tag{3.54}$$

Therefore, it is sufficient to integrate over values of $\varphi_R(\boldsymbol{k})$ and $\varphi_I(\boldsymbol{k})$ in a "half space" of wave vectors, chosen, for instance, by the condition $k_1 \geq 0$. In calculation of the correlation function $\langle|\varphi(\boldsymbol{k})|^2\rangle$ this feature is unimportant, however, because all integrals over values of $\varphi_R(\boldsymbol{k}')$ and $\varphi_I(\boldsymbol{k}')$ with $\boldsymbol{k}' \neq \boldsymbol{k}$ cancel in the expression

$$\langle|\varphi(\boldsymbol{k})|^2\rangle = \frac{\displaystyle\int \prod_{\boldsymbol{k},k_1\geq 0} d\varphi_R(\boldsymbol{k})d\varphi_I(\boldsymbol{k})\, \left[\varphi_R^2(\boldsymbol{k}) + \varphi_I^2(\boldsymbol{k})\right]\, \mathrm{e}^{-\beta V \sum_{\boldsymbol{k}}\left[gk^2+a(T-T_c)\right]|\varphi(\boldsymbol{k})|^2}}{\displaystyle\int \prod_{\boldsymbol{k},k_1\geq 0} d\varphi_R(\boldsymbol{k})d\varphi_I(\boldsymbol{k})\, \mathrm{e}^{-\beta V \sum_{\boldsymbol{k}}\left[gk^2+a(T-T_c)\right]|\varphi(\boldsymbol{k})|^2}}\,. \tag{3.55}$$

Thus, we are left with the following ratio of twofold Gaussian integrals

$$\langle|\varphi(\boldsymbol{k})|^2\rangle = \frac{\int\limits_{-\infty}^{\infty} d\varphi_R(\boldsymbol{k}) \int\limits_{-\infty}^{\infty} d\varphi_I(\boldsymbol{k}) \left[\varphi_R^2(\boldsymbol{k}) + \varphi_I^2(\boldsymbol{k})\right] \mathrm{e}^{-\beta V\left[gk^2 + a(T-T_c)\right]|\varphi(\boldsymbol{k})|^2}}{\int\limits_{-\infty}^{\infty} d\varphi_R(\boldsymbol{k}) \int\limits_{-\infty}^{\infty} d\varphi_I(\boldsymbol{k}) \,\mathrm{e}^{-\beta V\left[gk^2 + a(T-T_c)\right]|\varphi(\boldsymbol{k})|^2}} \,.$$

(3.56)

Calculation yields

$$\langle|\varphi(\boldsymbol{k})|^2\rangle = \frac{T}{V}\frac{1}{gk^2 + a(T-T_c)}\,,$$

(3.57)

therefore

$$\langle\varphi(\boldsymbol{k})\varphi(\boldsymbol{k}')\rangle = \frac{T}{V}\delta_{\boldsymbol{k}',-\boldsymbol{k}}\frac{1}{gk^2 + a(T-T_c)}\,.$$

(3.58)

We see that the length scale of the correlation function, the *correlation length*, is

$$\xi = \sqrt{\frac{g}{a(T-T_c)}}\,, \qquad T > T_c\,.$$

(3.59)

Below T_c a similar relation follows:

$$\xi = \sqrt{\frac{g}{2a(T_c-T)}}\,, \qquad T < T_c\,.$$

(3.60)

Therefore, in Landau theory values of the critical exponents of the correlation length

$$\xi(T) \sim \begin{cases} (T-T_c)^{-\nu}\,, & T > T_c\,, \\ (T_c-T)^{-\nu'}\,, & T < T_c\,, \end{cases} \qquad H = 0\,,$$

(3.61)

are equal and $\nu = \nu' = \frac{1}{2}$.

   Expression for the correlation function as a function of the position vector may now be calculated as the Fourier series

$$\langle\varphi(\boldsymbol{r})\varphi(\boldsymbol{r}')\rangle = \sum_{\boldsymbol{k}}\sum_{\boldsymbol{k}'}\langle\varphi(\boldsymbol{k})\varphi(\boldsymbol{k}')\rangle\,\mathrm{e}^{i\boldsymbol{k}\cdot\boldsymbol{r}+i\boldsymbol{k}'\cdot\boldsymbol{r}'} = \frac{T}{V}\sum_{\boldsymbol{k}}\frac{\mathrm{e}^{i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}')}}{gk^2 + a(T-T_c)}\,.$$

(3.62)

Further, it is customary to pass to the thermodynamic limit, which produces the familiar integral sum and the correlation function may be calculated as the inverse Fourier transform

$$\langle\varphi(\boldsymbol{r})\varphi(\boldsymbol{r}')\rangle = T\int\frac{d^3\boldsymbol{k}}{(2\pi)^3}\frac{\mathrm{e}^{i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}')}}{gk^2 + a(T-T_c)} = \frac{T}{4\pi g}\frac{\mathrm{e}^{-|\boldsymbol{r}-\boldsymbol{r}'|/\xi}}{|\boldsymbol{r}-\boldsymbol{r}'|}\,.$$

(3.63)

At the critical temperature $\xi \to \infty$ and

$$\langle\varphi(\boldsymbol{r})\varphi(\boldsymbol{r}')\rangle = \frac{T}{4\pi g|\boldsymbol{r}-\boldsymbol{r}'|}\,, \qquad T = T_c\,,$$

(3.64)

which fixes the value of the critical exponent η of the correlation function

$$\langle \varphi(\boldsymbol{r})\varphi(\boldsymbol{r}')\rangle \sim \frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|^{1+\eta}}\,, \qquad T=T_c \qquad (3.65)$$

in the Landau theory as $\eta = 0$.

3.5 Perturbation theory for correlation functions

The value of the functional integral described above depends on the method of approximation in the from of an iterated ordinary integral. Perturbation expansion brought about by the expansion in the fourth-order term of the effective free energy is unambiguous, however.

Most conveniently the rules of the perturbation expansion – including the *Feynman rules* for construction of a graphical representation of the terms of the perturbation expansion – may be obtained by the following trick.

■ **Generating function.** Consider the *generating function* of correlation functions of the order parameter

$$G(A) = \int \mathcal{D}\varphi \, e^{-\beta F(\varphi)+\varphi A}\,, \qquad (3.66)$$

where the shorthand notation

$$\varphi A := \int d\boldsymbol{x}\,\varphi(\boldsymbol{x})A(\boldsymbol{x}) \qquad (3.67)$$

has been introduced and will be frequently used henceforth. Correlation functions are obviously coefficients of the normalized functional Taylor expansion of $G(A)$, e.g.

$$\langle \varphi(\boldsymbol{x})\varphi(\boldsymbol{x}')\rangle = \frac{1}{G(A)}\frac{\delta^2 G(A)}{\delta A(\boldsymbol{x})\delta A(\boldsymbol{x}')}\bigg|_{A=0} \qquad (3.68)$$

■ **S-matrix functional.** The starting point for the construction of perturbation expansion of various quantities is the *S-matrix functional*

$$H(\varphi) = \exp\left(\frac{1}{2}\frac{\delta}{\delta\varphi}\Delta\frac{\delta}{\delta\varphi}\right)\exp\left[V(\varphi)\right]\,. \qquad (3.69)$$

In the present case the *propagator* Δ is the correlation function of the order parameter

$$\Delta(\boldsymbol{x},\boldsymbol{x}') = \langle \varphi(\boldsymbol{x})\varphi(\boldsymbol{x}')\rangle = \frac{T}{2}\left[-g\nabla^2 + a(T-T_c)\right]^{-1}(\boldsymbol{x},\boldsymbol{x}')\,,$$

and the interaction functional $V(\varphi)$ in the generating function is

$$V(\varphi) = \varphi A - \beta B \varphi^4 \,.$$

Assuming that basic rules of integration apply to functional integral (which is rigorously so for Gaussian integrals), the S-matrix functional (3.69) may be cast into a functional integral with the aid of the (formal) identity

$$\exp\left(\frac{1}{2}\frac{\delta}{\delta\varphi}\Delta\frac{\delta}{\delta\varphi}\right) = \left(\det\frac{K}{2\pi}\right)^{\frac{1}{2}}\int\mathcal{D}\phi\,\exp\left(-\frac{1}{2}\phi K\phi + \phi\frac{\delta}{\delta\varphi}\right)\,, \qquad (3.70)$$

where K is the differential operator, whose Green function is the propagator Δ, i.e. $K\Delta = 1$. The operator exponential here gives rise to the shift of the functional argument $\varphi \to \varphi + \phi$ through the Taylor expansion. Therefore

$$H(\varphi) = \left(\det\frac{K}{2\pi}\right)^{\frac{1}{2}}\int\mathcal{D}\phi\,\exp\left[-\frac{1}{2}\phi K\phi + V(\varphi + \phi)\right]\,. \qquad (3.71)$$

For the generating function of correlation functions $G(A)$ we obtain the representation

$$G(A) = \exp\left(-\beta F_0\right)\exp\left(\frac{1}{2}\frac{\delta}{\delta\varphi}\Delta\frac{\delta}{\delta\varphi}\right)\exp\left(-\beta B\varphi^4 + \varphi A\right)\bigg|_{\varphi=0}\,, \qquad (3.72)$$

which is the most convenient starting point for construction of the perturbation expansion in powers of the coupling constant B. It should be noted that there are no ambiguities in the meaning of the quantities on the right side of relation (3.72), contrary to the functional-integral representation (3.66).

3.6 Problems

Problem 3.1. Consider the following expansion in the order parameter ϕ of the Gibbs free energy

$$G(p, T, \phi) = G_0(p, T) + a(T - T_0)\phi^2 - C\phi^3 + B\phi^4 \,,$$

where a, B and C are positive constants. Find the equilibrium value of the order parameter, show that there is a first order phase transition in this system and find the transition temperature.

Problem 3.2. There are systems in which (on the p,T plane) a line of second-order transitions changes into a line of first-order transitions at the *tricritical* point. Near the tricritical point the Landau expansion of the Gibbs free energy may be written as

$$G(\phi, p, T) = G_0(p, T) + A\phi^2 + B\phi^4 + D\phi^6 \,,$$

where $D > 0$. The line of second-order transitions is determined by the conditions $A(T_C(p)) = 0$, $B > 0$. On the line of first-order transitions $B < 0$ so that at the tricritical point $A = B = 0$. Find the value of the order parameter on the line of first-order transitions in the ordered phase and establish a connection between A, B and D (which is the equation of the line of first-order transitions).

Problem 3.3. Using a constant modulus trial function $|\Psi|e^{i\phi}$ for the solution of the Ginzburg-Landau equations for a superconductor show that the phase of the superconducting wave function satisfies

$$\phi(\boldsymbol{r}_2) = \exp\left(\frac{ie^*}{\hbar}\int_{\boldsymbol{r}_1}^{\boldsymbol{r}_2}\boldsymbol{A}\cdot d\boldsymbol{r}\right)\phi(\boldsymbol{r}_1)\,.$$

Problem 3.4. Calculate the thermodynamic potential Ω for the case, when the effective-potential functional has the Gaussian form

$$\Omega[\phi] = \int d\boldsymbol{r}\left[g(\nabla\phi(\boldsymbol{r}))^2 + a(T - T_C)\phi^2(\boldsymbol{r})\right]\,,$$

and integration in the wave-vector space is restricted in a ball of radius Λ: $k \leq \Lambda$. The result should be something like

$$\Omega = \frac{T_C V}{12\pi^2}\left\{\Lambda^3\ln\frac{Vg}{\pi T_C} + \left[\Lambda^3\ln\left(\frac{a}{g}(T - T_C) + \Lambda^2\right)\right.\right.$$

$$\left.\left. -\frac{2}{3}\Lambda^3 + \frac{2a(T - T_C)\Lambda}{g} - \left[\frac{a(T - T_C)}{g}\right]^{3/2}\arctan\left(\Lambda\sqrt{\frac{g}{a(T - T_C)}}\right)\right]\right\}\,.$$

Problem 3.5. Using the thermodynamic potential Ω from the preceding problem calculate the contribution of order-parameter fluctuations to the heat capacity near the critical point and compare it with the jump in the heat capacity given by the Landau theory. Infer a condition for applicability of the Landau theory (the Ginzburg criterion).

4. Perturbation theory

4.1 Generating functionals

In this chapter a convenient graphical representation will be described for the correlation functions in the classical fluctuation theory. In fact this representation is fairly generic and may be applied for construction of the perturbation expansion of Green functions of particle physics, i.e. for vacuum expectation values of products of fields, Green functions of many-particle quantum systems at finite temperature and second-quantized representations of stochastic problems. The main differences are in the particular form of the propagators and other coefficient functions, which have to be calculated separately in each case. This also implies recapitulation of the Feynman rules for different problems. The graphical representation and its consequences are generic and hold in all cases.

■ **Generating functionals.** In the construction of perturbation theory, it is convenient to use the *full Green functions*. Full Green functions are coefficient functions of the Maclaurin expansion of the *generating function(al) of Green functions*

$$G_n(x_1, \ldots, x_n) = \left. \frac{\delta^n G(A)}{\delta A(x_1) \ldots \delta A(x_n)} \right|_{A=0}. \tag{4.1}$$

The generic functional form of the functional $G(A)$ is

$$G(A) = \exp\left(\frac{1}{2} \frac{\delta}{\delta\varphi} \Delta \frac{\delta}{\delta\varphi} \right) \exp\left[\overline{V}(\varphi) + \varphi A \right] \Big|_{\varphi=0}. \tag{4.2}$$

Here, the *vertex functional* $V = \overline{V} + \varphi A$ is usually of the form

$$V(\varphi) = \varphi A + \overline{V} = \varphi A + \sum_{n=3}^{\infty} \frac{1}{n!} v_n \varphi^n. \tag{4.3}$$

The coefficient functions v_n (called *potentials* henceforth) are symmetric functions of their arguments as are the *vertex factors*

$$V_n(x_1, \ldots, x_n) = \frac{\delta^n V(\varphi)}{\delta\varphi(x_1) \ldots \delta\varphi(x_n)}. \tag{4.4}$$

An important related functional is the generating functional of *connected Green functions*

$$W(A) = \ln G(A), \tag{4.5}$$

whose derivatives with respect to the *source field* A are the *connected Green functions*

$$W_n(x_1, \ldots, x_n) = \left. \frac{\delta^n W(A)}{\delta A(x_1) \ldots \delta A(x_n)} \right|_{A=0}. \tag{4.6}$$

These names are related to the topological structure of the diagrammatic representation of these quantities, which will be explained in the following section.

It is worth noting that the connected Green functions are properly normalized in the sense of the relation (3.68). For instance, the connected two-point Green function assumes the form

$$W_2(x_1, x_2) = \frac{G_2(x_1, x_2)}{G(0)} - \frac{G_1(x_1)}{G(0)} \frac{G_1(x_2)}{G(0)}.$$

Although the generating functional $G(A)$ is the quantity of primary interest, for purposes of further generalizations we shall construct the graphical perturbation expansion for a slightly more general *S-matrix functional*

$$H(\varphi) = \exp\left(\frac{1}{2} \frac{\delta}{\delta\varphi} \Delta \frac{\delta}{\delta\varphi} \right) \exp\left[V(\varphi)\right]. \tag{4.7}$$

It should be noted that the form of the S-matrix functional (4.7), (4.3) is completely generic and applicable in all problems of quantum field theory and stochastic field theory to be discussed in subsequent chapters. It is also readily seen that in generating functionals $G(A)$ vertex factors coincide with the potentials $V_n = v_n$, since $\varphi = 0$ in this case.

Usually, the functional $V(\varphi)$ is polynomial and the vertex factors local in space and time, e.g.

$$V_n(x_1, \ldots, x_n) = \delta(x_1 - x_2) \cdots \delta(x_{n-1} - x_n) v_n(x_1), \tag{4.8}$$

although this is not required for the construction of the subsequent graphical expansion of (4.7).

■ **Graph representation of generating functionals.** Expanding the exponential of the vertex functional as well as the *reduction operator*

$$P = \exp\left(\frac{1}{2} \frac{\delta}{\delta\varphi} \Delta \frac{\delta}{\delta\varphi} \right). \tag{4.9}$$

in the definition (4.7) we arrive at the representation

$$H(\varphi) = \sum_{n,m=0}^{\infty} \frac{1}{n!m!} \left(\frac{1}{2} \frac{\delta}{\delta\varphi} \Delta \frac{\delta}{\delta\varphi} \right)^m V^n \tag{4.10}$$

for the S-matrix functional. For each term of this expansion a convenient graphical representation may be constructed as follows.

Depict each functional V by a dot (vertex). Depict the kernel function of the reduction operator Δ by a line. A *graph* is a set of vertices and lines

(*edges*) connecting them. A product of n functionals V corresponds to n vertices in a graph. The functional derivative $\dfrac{\delta}{\delta\varphi}$ attaches one end of the Δ line to the vertex, describing the functional V on which the derivative is acting. Thus, a vertex (dot) with n lines attached corresponds to the vertex factor V_n (4.4). In analytical expressions, to each end of a Δ line a space-time variable x (one of the arguments of the propagator) is assigned, over which a subsequent integration (from the reduction operator) is carried out.

Figure 4–1: Simple graphs of the S-matrix functional

For instance, the action of the operator $\dfrac{1}{2}\dfrac{\delta}{\delta\varphi}\Delta\dfrac{\delta}{\delta\varphi}$ on V^2 gives rise to graphs of fig. 4–1, which analytically correspond to the expression

$$\frac{1}{2}\frac{\delta}{\delta\varphi}\Delta\frac{\delta}{\delta\varphi}V^2 = V\int d\boldsymbol{x}\int d\boldsymbol{x}'\Delta(\boldsymbol{x},\boldsymbol{x}')\frac{\delta^2 V}{\delta\varphi(\boldsymbol{x})\delta\varphi(\boldsymbol{x}')}$$
$$+ \int d\boldsymbol{x}\int d\boldsymbol{x}'\frac{\delta V}{\delta\varphi(\boldsymbol{x})}\Delta(\boldsymbol{x},\boldsymbol{x}')\frac{\delta V}{\delta\varphi(\boldsymbol{x}')}. \quad (4.11)$$

The reduction operator P contains all powers of the differential operator $\dfrac{1}{2}\dfrac{\delta}{\delta\varphi}\Delta\dfrac{\delta}{\delta\varphi}$ thus giving rise to any number of lines, whereas the exponential $e^{V(\varphi)}$ generates all powers of V, therefore the graphical expression for the S-matrix functional may be stated as

$$H(\varphi) = 1 + \{\text{all graphs with vertex factors } V_n \text{ and lines } \Delta\} = 1 + \sum_i C_i\gamma_i. \quad (4.12)$$

Here, C_i is the *symmetry coefficient* of the graph γ_i. The analytic expression corresponding to any graph may readily be established by the simple rules (called *Feynman rules* in particle physics) described above.

■ **Feynman rules for Green functions.** The source field A of the generating functional $G(A)$ appears in the interaction functional $V(\varphi)$ only in the combination φA. Apart from itself, this quantity generates only one vertex factor $A(x)$ to which just one line is attached. In the graphs of $G(A)$ the field variable $\varphi = 0$, so that $\varphi A = 0$, and only the vertex factor with the source field A is present. Green functions are functional derivatives with respect to A. In a graph the derivative $\dfrac{\delta}{\delta A(x)}$ removes one source field and assigns

the value x to the coordinate and time (and possible tensor) argument to the end of the propagator line attached. Thus, a graph from the representation of the n-point Green function $G_n(t_1, \boldsymbol{x}_1, \ldots, t_n, \boldsymbol{x}_n)$ contains lines with arguments of the Green function at one or both ends and contains only vertex factors independent of the field variable φ.

In applications the physical systems considered are in most cases translation invariant (or periodic) with local in space and time interaction functional. In this case it is much more convenient to carry out the calculation of integrals corresponding to various graphs of the model for Fourier-transformed Green functions. In the evaluation of the Green functions the following normalization of the wave-vector representation is used

$$G_n(t_1, \boldsymbol{x}_1, \ldots, t_n, \boldsymbol{x}_n) = \int \frac{d\omega_1}{2\pi} \cdots \int \frac{d\omega_n}{2\pi} \int \frac{d\boldsymbol{k}_1}{(2\pi)^d} \cdots \int \frac{d\boldsymbol{k}_n}{(2\pi)^d}$$

$$\times \; e^{\sum_{l=1}^{n} [-i\omega_l t_l + i\boldsymbol{k}_l \cdot \boldsymbol{x}_l]} 2\pi\delta\left(\sum_{l=1}^{n} \omega_l\right)(2\pi)^d\delta\left(\sum_{l=1}^{n} \boldsymbol{k}_l\right) G_n(\omega_1, \boldsymbol{k}_1, \ldots, \omega_n, \boldsymbol{k}_n)\,.$$

$$(4.13)$$

The δ functions, which automatically factorize in translation invariant models, are singled out explicitly from the definition of Green functions in the Fourier space and the corresponding "conservation laws" of wavevectors and frequencies implied in the Fourier-transformed Green functions. In particular, for the connected two-point function we obtain

$$W_2(t_1, \boldsymbol{x}_1, t_2, \boldsymbol{x}_2) = \int \frac{d\omega}{2\pi} \int \frac{d\boldsymbol{k}}{(2\pi)^d} \, e^{-i\omega(t_l - t_2) + i\boldsymbol{k}\cdot(\boldsymbol{x}_1 - \boldsymbol{x}_2)} W_2(\omega, \boldsymbol{k}, -\omega, -\boldsymbol{k})$$

$$\equiv \int \frac{d\omega}{2\pi} \int \frac{d\boldsymbol{k}}{(2\pi)^d} \, e^{-i\omega(t_l - t_2) + i\boldsymbol{k}\cdot(\boldsymbol{x}_1 - \boldsymbol{x}_2)} D(\omega, \boldsymbol{k})\,. \quad (4.14)$$

Here, the *full propagator* $D(\omega, \boldsymbol{k}) = W_2(\omega, \boldsymbol{k}, -\omega, -\boldsymbol{k})$ has been introduced, which is obviously the Fourier transform of $W_2(t, \boldsymbol{x}, 0, 0)$. From the representation (4.2) it immediately follows that in a free system

$$D(\omega, \boldsymbol{k}) = \Delta(\omega, \boldsymbol{k})\,, \qquad S_I = 0\,,$$

hence the name. In view this the function Δ is often called the *free* (or *bare*) propagator. The inverse Fourier transform (4.14) has been quoted here for the connected two-point function W_2, because the Fourier transform of the full two-point function

$$G_2 = W_2 + W_1^2$$

may not exist in a translation-invariant system in which $W_1 = G_1$ is necessarily a constant (it may, of course, be equal to zero, in which case this problem does not arise).

Representation (4.14) is also valid for the propagator Δ corresponding to a line in a graph. Thus, in the Fourier space to each line a wave vector (and frequency) argument is prescribed with the subsequent integration over it.

In the vertex factors we still have integrals over all coordinate (and time) variables of the vertex factor. However, if the interaction functional is local, then the vertex factor is of the structure (4.8) and all but one coordinate integrals are removed by the δ functions. Thus, for models with local interaction functionals to each vertex of a graph a single coordinate (and time) variable is prescribed with the subsequent integration over it. Moreover, in a translation invariant system the potential $v_n(x)$ must be a constant or a derivative acting on a δ function. Therefore, after passing to the Fourier representation (4.14) this remaining integral over the coordinate of the vertex gives rise to the δ function for wave vectors

$$V_n(x_1, \ldots, x_n) = v_n \delta(x_1 - x_2) \cdots \delta(x_{n-1} - x_n)$$

$$\rightarrow V_n(k_1, \ldots, k_n) = v_n(\boldsymbol{k}_1, \ldots, \boldsymbol{k}_n) \delta\left(\sum_{l=1}^{n} k_l\right), \quad (4.15)$$

where the Fourier transform of the potential $v_n(\boldsymbol{k}_1, \ldots, \boldsymbol{k}_n)$ is a polynomial function of wave vectors (interaction functionals with time derivatives are practically nonexistent). In a graph the Fourier-space integrals are those corresponding to the inverse Fourier transforms of propagators, i.e. to each line corresponds an integral in the Fourier space. The number of these integrals is reduced by the vertex δ functions leaving Fourier integrals over closed loops of lines and vertices in the graph.

Thus, for the most important case of a translation invariant system with a local interaction functional the Feynman rules for graphs in the Fourier space are

- To each line corresponds a propagator $\Delta(\omega, \boldsymbol{k})$.

- To each vertex corresponds the potential in the Fourier space $v_n(\boldsymbol{k}_1, \ldots, \boldsymbol{k}_n)$. In each vertex conservation laws of wave-vector and frequency hold.

- Integrations over all loop wave-vectors and frequencies are carried out.

■ **Recursion formula for symmetry coefficients.** The Feynman rules give the prescription for writing analytic expressions corresponding to graphs. The problem then is to determine the symmetry coefficient C_i. At low orders the symmetry coefficients may be found by inspection of the expansion (4.10). For instance, the term in (4.10) corresponding to graphs of fig. 4–1 has the coefficient $\frac{1}{2}$, by which its analytical expression (4.11) should be multiplied. Both terms in (4.11 have coefficients equal to 1 (these, of course, are nontrivial for higher powers of V and the differential operator) and both correspond to one of the graphs of fig. 4–1, therefore the symmetry coefficients of these graphs are equal to $\frac{1}{2}$.

At high orders methods of graph theory are the most adequate to this end, but for low-order graphs coefficients may be calculated with the use of

a recursive formula taking as the starting point, e.g., the coefficient of the graph corresponding to V^n (i.e. n vertices without lines) which is $1/n!$.

The recursion relation is based on the Vasil'ev identity (the variable notation x includes coordinates, time and possible indices)

$$\frac{\delta H(\varphi)}{\delta \Delta(x, x')} = \frac{1}{2} \frac{\delta}{\delta \varphi(x)} \frac{\delta}{\delta \varphi(x')} H(\varphi) \,. \tag{4.16}$$

Graphically, the operator on the left-hand side removes a line from a graph in all possible ways leaving open ends with arguments x and x', while the operator on the right-hand opens two arguments – again in all possible ways – between which a line might be attached. Consider now two graphs γ and γ' such that γ' is obtained from γ by removing a line. Then on the lhs of relation (4.16) γ' is produced multiplied by the number of ways to generate it by removing a line from γ. Denote this number $N(\gamma \to \gamma')$. On the rhs the same graph appears as many times as two ends can be opened to produce γ by attaching a line to γ'. This is the number of ways to construct γ from γ' by adding a line $N(\gamma' \to \gamma)$, if the functional derivatives act on different vertices (so that two equal terms are produced). If the derivatives act on the same vertex, then the coefficient $\frac{1}{2}$ remains intact. Putting coefficients of the graphs on both sides equal gives rise to the recursion relation

$$C_\gamma = \epsilon \frac{N(\gamma' \to \gamma)}{N(\gamma \to \gamma')} C_{\gamma'} \,, \tag{4.17}$$

where $\epsilon = \frac{1}{2}$, if the line is attached to a single vertex, otherwise $\epsilon = 1$.

As an example, consider the graphs in fig. 4–1. Both can be produced from a graph consisting of two isolated vertices with the coefficient $\frac{1}{2}$. The closed loop may be attached to either vertex, i.e. twice, and removed, obviously, only one way. With the account of the factor $\epsilon = \frac{1}{2}$ the symmetry coefficient of the graph becomes $\frac{1}{2}$. The line between the vertices may be attached and removed one way only, thus the coefficient remains equal to $\frac{1}{2}$ as well.

> **Example 4.1.** Evaluate the symmetry coefficient of the graph in fig. 4–2.
>
> **Solution.** To three isolated vertices with the coefficient $\frac{1}{6}$ a line may be attached in three ways and removed in one way. To this graph a line between the remaining isolated and any other vertex may be attached in two ways and removed in two ways as well. The last line to obtain the graph in fig. 4–2 may be attached in only one way, but removing any of the three lines returns us to the open chain. Thus, the coefficient of the three-vertex closed loop in fig. 4–2 is $\frac{1}{6}$, i.e. the same as for three isolated vertices. However, the coefficient of an n-vertex closed loop is $\frac{1}{2n}$.
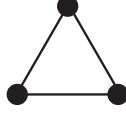
Figure 4–2: Three-vertex simple loop

■ **Connected graphs.** In a *connected graph* there is a continuous path of lines and vertices between any pair of vertices. *Mayer's first theorem* states that

$$\ln H(\varphi) = \sum_{\text{conn,i}} C_i \gamma_i \,, \tag{4.18}$$

where the sum is taken over the connected graphs of the representation (4.12) of the S-matrix functional. In particular, it follows from this theorem that the graphical representation of the functional $W(A)$ consists of just the connected graphs of the representation of $G(A)$, hence the name of connected Green functions for W_n.

The combinatorial proof of Mayer's first theorem requires acquaintance with some notions of the graph theory, which are not presented here. Another simple proof if this statement is based on the identity (4.16), from which it follows that

$$\Delta \frac{\delta H(\varphi)}{\delta \Delta} = \frac{1}{2} \frac{\delta}{\delta \varphi} \Delta \frac{\delta}{\delta \varphi} H(\varphi) \,. \tag{4.19}$$

The analytic operations on both sides of this identity have transparent graphical interpretations. On the left side a line is removed from a graph and then attached again exactly in the same place in all possible ways. This operation does not change the structure of the graph, although it may change the symmetry coefficient. In particular, the number of lines in a graph remains the same. The operation on the right side, on the contrary, adds a line to a graph in all possible ways.

Substitute now the representation

$$H(\varphi) = e^{W(\varphi)}$$

in the identity (4.19) to obtain

$$\Delta \frac{\delta W(\varphi)}{\delta \Delta} = \frac{1}{2} \left[\frac{\delta}{\delta \varphi} \Delta \frac{\delta}{\delta \varphi} W + \frac{\delta W}{\delta \varphi} \Delta \frac{\delta W}{\delta \varphi} \right] \,. \tag{4.20}$$

Since the operation on the right side increases the number of lines by one, whereas the operation on the left side does not change the number of lines, with the aid of this identity all graphs of W may be reproduced starting from the graphs without lines, which is a single vertex corresponding to the interaction functional V. Since the derivative with respect to the field φ

does not affect the connectedness of a graph, the relation (4.20) conserves connectedness of a graph in an obvious way: If the n-line input on the right side consists of a sum of connected graphs, then the result of the right-side operation is also a sum of connected graphs with $n + 1$ lines. The starting point of this construction is the single vertex V, which is connected, and Mayer's first theorem follows by induction.

4.2   Calculation of graphs

In this section a few basic tricks for calculation of integrals represented in the form of Feynman graphs are reviewed. This handicraft yields relatively simple results, when the wave-vector integrals may be carried out over the whole wave vector space with "massless" propagators of the simple form $\Delta(\boldsymbol{k}) = k^{-2}$. Physically, this is the case in the Ginzburg-Landau theory directly at critical temperature, when the temperature ("mass") term in the propagator

$$\Delta_{GL}(\boldsymbol{k}) = \langle |\varphi(\boldsymbol{k})|^2 \rangle = \frac{T}{2} \frac{1}{gk^2 + a(T - T_c)} \tag{4.21}$$

vanishes: $T = T_c$. In (4.21) the thermodynamic limit is implied, in which the volume factor of relation (3.58) goes into the definition of the δ function in the wave-vector space: $V\delta_{\boldsymbol{k}, -\boldsymbol{k}'} \to \delta(\boldsymbol{k} + \boldsymbol{k}')$. It should be noted that calculation of loop integrals with massless propagators may give rise to expressions nonintegrable at the origin in the wave-vector space. These are the *infra-red* divergences (IR divergences) of the model. At low orders of perturbation theory the IR divergences may usually be detected by inspection of the analytic expressions for the graphs with the use of the standard convergence rules. If there is any suspicion, however, that IR divergences might be present, then the wave-vector integrals must be calculated with the use of "massive" propagators (or with the use of some other IR cutoff), which in the Ginzburg-Landau theory means that $T \neq T_c$.

Moreover, in Ginzburg-Landau theory – as in any coarse-grained effective model – there is a minimum length scale ℓ (in solid state this would be the lattice spacing), below which the large-scale model does not work any more. In the wave vector space this gives rise to a large wave-number cutoff (*ultra-violet* cutoff, *UV cutoff*) $\Lambda \sim \ell^{-1}$ in the wave-vector integrals of perturbation theory. The UV cutoff is often introduced with the use of a step function in the expression for the propagator, i.e.

$$\Delta_{GL}(\boldsymbol{k}, \Lambda) = \frac{T}{2} \frac{\theta(\Lambda - k)}{gk^2 + a(T - T_c)}. \tag{4.22}$$

Calculation of wave-vector integrals with this propagator is rather tedious and the results most often cannot be expressed even in terms of widely known special functions, let alone elementary functions. Nevertheless, calculation with the UV cutoff is necessary, when the wave-vector integrals are divergent in the limit $\Lambda \to \infty$. These singularities are the *UV divergences* of the model. Later it will be shown that there are ingenious ways

to circumvent the use of an explicit UV cutoff in case of UV divergent integrals.

However, in the theory of critical phenomena in particular, but also in many other cases, there are physically interesting quantities which do not depend on the microscopic details of the physical model (*universal* quantities). In those cases wave-vector integrals of perturbation expansion may be calculated in the limit $\Lambda \to \infty$, i.e. over the whole wave-vector space. This leads to tremendous simplification of both calculation and the appearance of the results. In fact, the convergence of the wave-vector integrals in the limit $\Lambda \to \infty$ may be regarded as an indication of the independence of the effective model on the microscale physics.

■ **Massless propagator.** Therefore, we will start from the technically simplest case of the massless propagator without the UV cutoff and will put, for simplicity, all irrelevant constants equal to the unity:

$$\Delta(\boldsymbol{k}) = \frac{1}{k^2} \,. \tag{4.23}$$

The simplest one-loop graph (or subgraph) depending on external wave vector in a model with the propagator (4.23) corresponds to the wave-vector integral (calculations will be carried out for a generic space dimension d, which eventually will be regarded as a complex number):

$$\gamma_D(\boldsymbol{k}) = \int \frac{d\boldsymbol{q}}{(2\pi)^d} \frac{1}{q^2(\boldsymbol{k}-\boldsymbol{q})^2} \,. \tag{4.24}$$

Inspection reveals that there are no IR divergences in (4.24) above two dimensions, provided the external wave vector $\boldsymbol{k} \neq 0$. The wave-integral in (4.24) is UV convergent as well below four dimensions. Thus, the convergence conditions of the integral in (4.24) are $2 < d < 4$.

When integrals are carried out over the whole wave-vector space, it is customary to parametrize the integrand in such a way that all wave-vector integrals become Gaussian. To this end the first step is the *Feynman parametrization* based on the identity

$$\frac{1}{a^\alpha b^\beta} = \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} \int\limits_0^1 dt \, \frac{t^{\alpha-1}(1-t)^{\beta-1}}{[at+(1-t)b]^{\alpha+\beta}} \,. \tag{4.25}$$

Proof of this identity is a useful exercise in the methods of calculus of complex variable. For (4.24) we obtain

$$\gamma_D(\boldsymbol{k}) = \int\limits_0^1 dt \int \frac{d\boldsymbol{q}}{(2\pi)^d} \frac{1}{[q^2t+(1-t)(\boldsymbol{k}-\boldsymbol{q})^2]^2} \,.$$

With the aid of the α (Schwinger) representation

$$\frac{1}{A^z} = \frac{1}{\Gamma(z)} \int\limits_0^\infty d\alpha \, \alpha^{z-1} e^{-A}$$

I arrive at a Gaussian integral over $d\boldsymbol{q}$, which results in the expression with a twofold parametric integral

$$\gamma_D(\boldsymbol{k}) = \frac{\pi^{d/2}}{(2\pi)^d} \int\limits_0^1 dt \int\limits_0^\infty d\alpha \, \alpha^{1-d/2} e^{-\alpha k^2 t(1-t)} \,.$$

The parametric integral over $d\alpha$ is an integral representation of Euler's Γ function, whereas the resulting integral over dt is an integral representation of Euler's B function. Thus

$$\gamma_D(\boldsymbol{k}) = \frac{\Gamma(2-d/2)\Gamma^2(d/2-1)}{(4\pi)^{d/2}\Gamma(d-2)k^{4-d}} \,. \tag{4.26}$$

Although this expression corresponds to physical space dimension $d = 3$ only, it is customary to use the right-side expression in (4.26) as the definition of the original loop integral for any value of d in the region of formal convergence, i.e. $2 < \operatorname{Re} d < 4$, where d is regarded as a complex number. Additional words should be said for complex values of d beyond this belt, because the original loop integral does not converge for $\operatorname{Re} d \leq 2$ or $4 \leq \operatorname{Re} d$. I will return to this point in the discussion of the renormalization group.

From the explicit expression (4.26) it is seen that the basic one-loop integral (4.24) gives rise to a power-law propagator in the wave-vector space, but with a non-integer power of $1/k^2$. Feynman parametrization (4.25) allows to calculate one-loop integrals with rather arbitrary powers of the wave vector in the way demonstrated above. For the generic one-loop integral the result is

$$\int d\boldsymbol{q} \, \frac{1}{q^{2\alpha}(\boldsymbol{k}+\boldsymbol{q})^{2\beta}} = \frac{\pi^\mu}{k^{2(\alpha+\beta-\mu)}} \, \Gamma \left[\begin{array}{c} \mu-\alpha, \, \mu-\beta, \, \alpha+\beta-\mu \\ \alpha, \, \beta, \, 2\mu-\alpha-\beta \end{array} \right] , \tag{4.27}$$

where the following shorthand notation has been used:

$$\Gamma \left[\begin{array}{c} \mu-\alpha, \, \mu-\beta, \, \alpha+\beta-\mu \\ \alpha, \, \beta, \, 2\mu-\alpha-\beta \end{array} \right] = \frac{\Gamma(\mu-\alpha)\Gamma(\mu-\beta)\Gamma(\alpha+\beta-\mu)}{\Gamma(\alpha)\Gamma(\beta)\Gamma(2\mu-\alpha-\beta)} \,. \tag{4.28}$$

With the repeated use of this relation it is possible to calculate several multi-loop integrals with massless propagators and integrations over the whole wave-vector space.

■ **Massive propagator.** From the explicit expression (4.26) it is seen that the massless one-loop integral diverges in the limit $k \to 0$, when $d < 4$. Therefore, in a graph of high enough order containing a product of several one-loop integrals (4.24) a non-integrable term of the form $k^{n(d-4)}$ will appear rendering the corresponding loop integral divergent. This is one of the most direct manifestations of the IR singularities at the critical point. To analyze consequences of these singularities the starting point should be a finite expression. The most natural way to regularize the IR behaviour of loop integrals is to calculate them slightly above the critical temperature,

so that the temperature parameter (or mass in the particle-field theory parlance) in (4.21) is positive: $A = a(T - T_c) > 0$.

In this case the basic one-loop integral is

$$\gamma_D(\boldsymbol{k}, A) = \int \frac{d\boldsymbol{q}}{(2\pi)^d} \frac{1}{(q^2 + A)\left[(\boldsymbol{k} - \boldsymbol{q})^2 + A\right]} \,. \qquad (4.29)$$

With the use of Feynman parametrization and Schwinger representation the wave-vector integral is transformed into a Gaussian integral as before and gives rise to the parametric integral

$$\gamma_D(\boldsymbol{k}, A) = \frac{1}{(4\pi)^{d/2}} \int\limits_0^1 dt \int\limits_0^\infty d\alpha \, \alpha^{1-d/2} e^{-\alpha[A+k^2 t(1-t)]} \,. \qquad (4.30)$$

Now direct calculation over $d\alpha$ would give rise to a rather inconvenient parametric integral over dt. Therefore, use the following Mellin representation (inverse Mellin transform) of the exponential function

$$e^{-x} = \frac{1}{2\pi i} \int\limits_{s_0-i\infty}^{s_0+i\infty} ds \, \Gamma(s) x^{-s} \,, \qquad s_0 > 0 \,, \qquad (4.31)$$

where the integral goes over a contour along the imaginary axis in the complex s plane such that the poles of $\Gamma(s)$ lie to the left of the contour. With the aid of (4.31) the parametric integral (4.30) gives rise to the integral

$$\gamma_D(\boldsymbol{k}, A) = \frac{1}{(4\pi)^{d/2}} \int\limits_0^1 dt \int\limits_0^\infty d\alpha \, \frac{1}{2\pi i} \int\limits_{s_0-i\infty}^{s_0+i\infty} ds \, \Gamma(s) \alpha^{1-d/2-s} k^{-2s} t^{-s} (1-t)^{-s} e^{-\alpha A} \,.$$
$$(4.32)$$

The point is that now the integrals over $d\alpha$ and dt give rise to Euler's Γ and B functions, respectively, and the remaining parametric integral may often be identified with the Mellin representation of a known special function. It is, however, necessary to take care that the contour in the s plane is such that the integrals over $d\alpha$ and dt converge for all values of s on that contour. In this approach, it may be necessary to deform the contour to meet these criteria, which produces additional terms corresponding to residues at the poles of $\Gamma(s)$. In (4.32) the convergence conditions require Re $s = s_0 < 2-d/2$ and $s_0 < 1$. These conditions may be without additional terms simply by moving the contour close to the imaginary axis. If it were necessary to consider the limit $d \to 4-$, however, it would advisable to move the contour to the left from the origin of the s plane, which would then produce an additional term due to the pole of $\Gamma(s)$ at the origin. For the time being, require $d < 4$ to obtain

$$\gamma_D(\boldsymbol{k}, A) = \frac{1}{(4\pi)^{d/2} 2\pi i} \int\limits_{s_0-i\infty}^{s_0+i\infty} ds \, \frac{\Gamma(s)\Gamma^2(1-s)\Gamma(2-d/2-s)}{\Gamma(2-2s)k^{2s} A^{2-d/2-s}} \,. \qquad (4.33)$$

With the use of the duplication formula

$$\Gamma(2z) = \frac{1}{\sqrt{2\pi}} 2^{2z-1/2}\Gamma(z)\Gamma\left(z + \frac{1}{2}\right) \tag{4.34}$$

I obtain

$$\gamma_D(\boldsymbol{k}, A) = \frac{\sqrt{\pi}}{(4\pi)^{d/2}A^{2-d/2}4\pi i} \int\limits_{s_0-i\infty}^{s_0+i\infty} ds \left(\frac{4A}{k^2}\right)^s \frac{\Gamma(s)\Gamma(1-s)\Gamma(2-d/2-s)}{\Gamma(3/2-s)} . \tag{4.35}$$

Comparison with the Mellin-Barnes representation of the hypergeometric function

$$\frac{\Gamma(c)}{2\pi i\Gamma(a)\Gamma(b)} \int\limits_{\substack{s_0-i\infty \\ \max\{-\operatorname{Re}a, -\operatorname{Re}b\}<s_0<0}}^{s_0+i\infty} ds \frac{\Gamma(a+s)\Gamma(b+s)\Gamma(-s)}{\Gamma(c+s)} (-z)^s = {}_2F_1(a,b;c;z) \tag{4.36}$$

yields the result

$$\gamma_D(\boldsymbol{k}, A) = \frac{\Gamma(2-d/2)}{(4\pi)^{d/2}A^{2-d/2}} {}_2F_1\left(1, 2 - \frac{d}{2}; \frac{3}{2}; -\frac{k^2}{4A}\right) . \tag{4.37}$$

Calculation with the sharp UV cutoff (4.22) and mass $[A = a(T - T_c) > 0]$ gives rise to more complicated parametric integrals and will not be discussed here.

4.3 Schwinger and Dyson equations

■ **Schwinger equation.** Representation (4.7) for the S-matrix functional gives rise to the graphical expansion with fairly transparent construction rules independent of the particular structure of the interaction functional V. For generating functions, however, it is convenient to single out the linear in the source field term explicitly

$$V(\varphi) = \varphi A + \sum_{n=3}^{\infty} \frac{1}{n!} v_n \varphi^n \equiv \varphi A + \overline{V}(\varphi) . \tag{4.38}$$

In this case an alternative functional representation becomes evident

$$H(\varphi) = \exp\left[\overline{V}\left(\frac{\delta}{\delta A}\right)\right] \exp\left(\frac{1}{2}A\Delta A + \varphi A\right) , \tag{4.39}$$

since for any functional $F(\varphi)$ we may write

$$F\left(\frac{\delta}{\delta A}\right) e^{\varphi A} = F(\varphi)e^{\varphi A} . \tag{4.40}$$

Thus, we see that

$$\exp\left[\frac{1}{2}\frac{\delta}{\delta\varphi}\Delta\frac{\delta}{\delta\varphi}\right]\exp\left[\varphi A + \overline{V}(\varphi)\right]$$
$$= \exp\left[\overline{V}\left(\frac{\delta}{\delta A}\right)\right]\exp\left(\frac{1}{2}A\Delta A + \varphi A\right). \quad (4.41)$$

Taking now the derivative with respect to φ of both sides of this equality and using again the identity (4.40) we obtain

$$\left[A + \overline{V}'\left(\frac{\delta}{\delta A}\right)\right]H(\varphi) = \exp\left[\overline{V}\left(\frac{\delta}{\delta A}\right)\right]A\exp\left(\frac{1}{2}A\Delta A + \varphi A\right), \quad (4.42)$$

where

$$\overline{V}'(x) = \frac{\delta\overline{V}}{\delta\varphi(x)}.$$

The right side of (4.42) may be cast in the form

$$\exp\left[\overline{V}\left(\frac{\delta}{\delta A}\right)\right]A\exp\left(\frac{1}{2}A\Delta A + \varphi A\right)$$
$$= \Delta^{-1}\left(\frac{\delta}{\delta A} - \varphi\right)\exp\left[\overline{V}\left(\frac{\delta}{\delta A}\right)\right]\exp\left(\frac{1}{2}A\Delta A + \varphi A\right). \quad (4.43)$$

From here we infer an important relation between derivatives of the functional H:

$$\frac{\delta H}{\delta\varphi} + \Delta^{-1}\varphi H = \Delta^{-1}\frac{\delta H}{\delta A}. \quad (4.44)$$

Combining these results we arrive at the *Schwinger equation* for the functional H

$$\left[A + \Delta^{-1}\varphi - \Delta^{-1}\frac{\delta}{\delta A} + \overline{V}'\left(\frac{\delta}{\delta A}\right)\right]H(\varphi) = 0. \quad (4.45)$$

In addition to these two functional differential equations, a set of equations may obtained by differentiating either of the functional representations (4.7) or (4.39) with respect to potentials v_n $(n \geq 3)$:

$$\frac{\delta H}{\delta v_n} = \frac{1}{n!}\frac{\delta^n H}{\delta A^n}, \qquad n = 3, 4, \ldots \quad (4.46)$$

The *connection equations* (4.46) together with the relations (4.19), (4.44) and the Schwinger equation (4.45) form a closed system of functional differential equations for the S-matrix functional H as a functional of the functions φ, A, Δ and v_n. These equations do not contain any explicit reference to the perturbation theory, which was used to derive them, therefore they may be used as the basis for the construction of nonperturbative functionals H. The most important equation in this respect is the Schwinger equation (4.45). When expanded in powers of A, it gives rise to an infinite set of coupled integro-differential equations for Green functions of all orders.

From the structure and symmetries of these equations important physical conclusions about the behaviour of the system may be extracted.

■ **Generating functional of one-irreducible Green functions.** It is customary to proceed one step further in the topological classification of the graphs of perturbation theory. A graph is *one-irreducible* (one-particle irreducible in particle physics), if it remains connected after the elimination of one line (edge). This property characterizes graphs in the expression for the (first) *Legendre transform* Γ of the generating functional $W(A)$. Here, $W(A)$ is the original generating functional of connected Green functions, i.e. the field $\varphi = 0$ in the S-matrix functional $H(\varphi)$. This functional is the result of the change of variables, in which first define the new field variable α by

$$\alpha(x) = \frac{\delta W}{\delta A(x)}\,. \tag{4.47}$$

The source field A is then solved as a function of α, Δ and v_n from this definition. The Legendre transform itself is defined as the functional

$$\Gamma(\alpha) = W(A) - \alpha A\,, \tag{4.48}$$

where it assumed that $A(\alpha)$ is substituted in the right side. *One-irreducible Green functions* are obtained from the Legendre transform in the same fashion as full and connected Green functions (4.1 and (4.6) from their respective generating functionals

$$\Gamma_n(x_1,\ldots,x_n) = \left.\frac{\delta^n\Gamma(\alpha)}{\delta\alpha(x_1)\ldots\delta\alpha(x_n)}\right|_{\alpha=0}\,. \tag{4.49}$$

Directly from the definitions it follows that

$$\Gamma_1 = \frac{\delta\Gamma}{\delta\alpha} = -A\,, \quad \frac{\delta^2\Gamma}{\delta\alpha\delta\alpha}\frac{\delta^2 W}{\delta A\delta A} = -1\,, \quad \frac{\delta\Gamma}{\delta v_n} = \frac{\delta W}{\delta v_n}\,, \; n = 3, 4, \ldots \tag{4.50}$$

The functional differential equations for H may be cast into equations for the functional Γ with the aid of these relations. To this end it is also necessary to change the variables in the derivative with respect to A:

$$\frac{\delta}{\delta A} = \frac{\delta\alpha}{\delta A}\frac{\delta}{\delta\alpha} = W_2\frac{\delta}{\delta\alpha} = -\Gamma_2^{-1}\frac{\delta}{\delta\alpha}\,. \tag{4.51}$$

According to these prescriptions, e.g.

$$W_3 = \frac{\delta W_2}{\delta A} = \Gamma_2^{-1}\frac{\delta}{\delta\alpha}\Gamma_2^{-1} = -(\Gamma_2^{-1})^3\Gamma_3\,.$$

This is symbolic notation. A bit more expanded form is

$$W_3(123) = \frac{\delta W_2(23)}{\delta A(1)} = -\Gamma_2^{-1}(11')\Gamma_2^{-1}(22')\Gamma_2^{-1}(33')\Gamma_3(1'2'3')$$

$$= W_2(11')W_2(22')W_2(33')\Gamma_3(1'2'3')\,.$$

The Schwinger equation (4.45) has a simple generic form only for the functional H. To demonstrate equations for W and Γ brought about by the Schwinger equation for H, consider the simplest interaction functional $\overline{V}(\varphi) = v_3\varphi^3/6$.

For the present choice of $\overline{V}$ the Schwinger equation assumes the form [here, the Schwinger equation is written for $G(A) = H(0)$]

$$\left[A - \Delta^{-1}\frac{\delta}{\delta A} + \frac{1}{2}v_3\frac{\delta^2}{\delta A^2} \right] G(A) = 0\,. \tag{4.52}$$

For the functional $W(A) = \ln G(A)$ this yields

$$A - \Delta^{-1}\frac{\delta W}{\delta A} + \frac{1}{2}v_3\left(\frac{\delta^2 W}{\delta A^2} + \frac{\delta W}{\delta A}\frac{\delta W}{\delta A} \right) = 0\,. \tag{4.53}$$

This equation is readily cast in the form of an equation for the functional Γ

$$-\Gamma_1 - \Delta^{-1}\alpha + \frac{1}{2}v_3\left[-\left(\frac{\delta^2\Gamma}{\delta\alpha^2} \right)^{-1} + \alpha\alpha \right] = 0\,. \tag{4.54}$$

Derivative of this equation with respect to α yields the *Dyson equation*

$$-\Gamma_2 - \Delta^{-1} + \frac{1}{2}v_3\left[\left(\Gamma_2^{-1} \right)^2\Gamma_3 + 2\alpha \right] = 0\,. \tag{4.55}$$

It is customary to write the Dyson equation in the form, in which the left argument of Γ_2 coincides with the left argument of v_3 and the right argument of Γ_2 coincides with the right argument of both v_3 and Γ_3.

The Dyson equation is often written for the full (or *dressed*) propagator $D = W_2$. In the expanded form it is

$$D^{-1}(12) = \Delta^{-1}(12) - \frac{1}{2}v_3(134)\left[D(35)D(46)\Gamma_3(652) + 2\alpha(3)\delta(42) \right]$$
$$= \Delta^{-1}(12) - \Sigma(12)\,, \quad \text{(4.56)}$$

where the *self energy* $\Sigma(12)$ has been introduced. In the graphical form

where the wavy line depicts α, the thick line W_2, the dot v_3 and the shaded circle with dots Γ_3.

The Dyson equation is an exact integro-differential equation for the full propagator D, therefore it can be used to extract nonperturbative properties and to construct nonperturbative solutions for D. To this end, however, approximations for the three-point function Γ_3 are needed, whose accuracy may be difficult to control.

■ **Graphs of the generating functional** Γ. To analyze the graphical representation of the functional Γ it is convenient to extract the term which does not correspond to a graph. To this end, write

$$W(A) = \frac{1}{2} A \Delta A + \overline{W}(A). \tag{4.57}$$

Here, $W(A)$ consists of connected graphs of the functional $G(A)$. For the new variable α the equation

$$\alpha = \Delta A + \frac{\delta \overline{W}(A)}{\delta A}$$

follows. Thus, the leading-order approximation for $A(\alpha) = \Delta^{-1}\alpha + \dots$. Substitution in the definition (4.48) of Γ allows to extract the term which cannot be represented as a graph

$$\Gamma(\alpha, \Delta, \{v_n\}) = -\frac{1}{2}\,\alpha\Delta^{-1}\alpha + \overline{\Gamma}(\alpha, \Delta, \{v_n\}). \tag{4.58}$$

With the use of the identity

$$\exp\left(-\varphi A\right) F\left(\frac{\delta}{\delta\varphi}\right) \exp\left(\varphi A\right) = F\left(A + \frac{\delta}{\delta\varphi}\right) \tag{4.59}$$

the substitution of (4.58) in the connection equations (4.46) yields

$$\frac{\delta\overline{\Gamma}}{\delta v_n} = \frac{1}{n!}\left(\frac{\delta W}{\delta A} + \frac{\delta}{\delta A}\right)^n 1 = \frac{1}{n!}\left(\alpha - \Gamma_2^{-1}\frac{\delta}{\delta\alpha}\right)^n 1, \qquad n = 3, 4, \dots \tag{4.60}$$

Multiplying by v_n and contracting all arguments (integrating over continuous variables and summing over indices in v_n) we arrive at the identities

$$v_n \frac{\delta\overline{\Gamma}}{\delta v_n} = \frac{1}{n!} v_n \left(\alpha - \Gamma_2^{-1}\frac{\delta}{\delta\alpha}\right)^n 1$$

$$= \frac{1}{n!} v_n \left(\alpha - \Gamma_2^{-1}\frac{\delta}{\delta\alpha}\right)^{n-2} \left(\alpha^2 - \Gamma_2^{-1}\right), \qquad n = 3, 4, \dots \tag{4.61}$$

which, in particular, allow to construct all graphs of $\overline{\Gamma}$ by iterations. The reason is that the operation on the left side of (4.61) does not change the number of n-point vertices, while the operation on the right side increases it by one. Thus, in the simplest case $n = 3$ substitution of $\Gamma^{(0)} = -\frac{1}{2}\,\alpha\Delta^{-1}\alpha$ in the right side of (4.61) leads to the equation

$$v_3 \frac{\delta\overline{\Gamma}^{(1)}}{\delta v_3} = \frac{1}{6} v_3 \alpha^3 + \frac{1}{2}\alpha v_3\Delta$$

with the obvious solution

$$\overline{\Gamma}^{(1)} = \frac{1}{6} v_3 \alpha^3 + \frac{1}{2}\alpha v_3\Delta = \frac{1}{6}\ \text{}\ + \frac{1}{2}\ \text{} \tag{4.62}$$

with one-irreducible graphs only. Here, the wavy line depicts the field α, the dot the vertex factor v_3 and the plain line the propagator Δ.

Moreover, relation (4.61) conserves the property of one-irreducibility: if the input of Γ on the right side contains only one-irreducible graphs, then the output on the left side contains only one-irreducible graphs as well.

This conclusion is readily seen in the first equation ($n = 3$) of the set (4.61). In the symbolic notation we obtain

$$v_3 \frac{\delta \overline{\Gamma}}{\delta v_3} = \frac{1}{6} v_3 \left(\alpha - \Gamma_2^{-1} \frac{\delta}{\delta \alpha} \right) \left(\alpha^2 - \Gamma_2^{-1} \right)$$

$$= \frac{1}{6} v_3 \left(\alpha^3 + 3\alpha W_2 + W_2^3 \Gamma_3 \right) , \quad (4.63)$$

where we have replaced $\Gamma_2^{-1} = -W_2$. Relation (4.63) reveals the topological properties in the notation with explicit contractions

$$v_3(123) \frac{\delta \overline{\Gamma}}{\delta v_3(123)} = \frac{1}{6} v_3(123) \Big[(\alpha(1)\alpha(2)\alpha(3)$$

$$+ 3\alpha(1) W_2(23) + W_2(11') W_2(22') W_2(33') \Gamma_3(1'2'3') \Big]. \quad (4.64)$$

This relation is topologically even more transparent in the graphical form

$$v_3 \frac{\delta \overline{\Gamma}}{\delta v_3} = \frac{1}{6} \quad \text{} \quad + \frac{1}{2} \quad \text{} \quad + \frac{1}{6} \quad \text{} \quad . \quad (4.65)$$

Consider now a graph with lines on the right side of relation (4.65). It is obvious from the structure of the right-side expression that removal of any line from the subgraphs corresponding to W_2 or Γ_3 on the right side yields a one-irreducible graph, provided W_2 is connected and Γ_3 one-irreducible. The operation of elimination and restoration of the vertex factor v_3 in all possible ways on the left side does not change any topological properties, but only the symmetry coefficient of the graph. Therefore, the graphs produced to $\overline{\Gamma}$ at the next order in v_3 are one-irreducible as well. The same conclusion is readily obtained for any vertex factor in a similar manner.

Thus, the graphs of $\overline{\Gamma}$ may be constructed directly by iterations of the connection equations (4.61). This, however, is not necessary, because these graphs turn out to be a subclass of the graphs of $\overline{W}$. To see this, analyze the change of variables

$$A = -\Gamma_1 = \Delta^{-1}\alpha - \overline{\Gamma}_1$$

in the right side of the definition (4.48) of the functional Γ. With the use of the representation (4.57) we obtain

$$\Gamma = -\frac{1}{2} \alpha \Delta^{-1} \alpha + \frac{1}{2} \overline{\Gamma}_1 \Delta \overline{\Gamma}_1 + \overline{W} \left(\Delta^{-1}\alpha - \overline{\Gamma}_1 \right) . \quad (4.66)$$

The second term on the right side is represented by a sum of one-reducible graphs due to Δ in between one-irreducible graphs of $\overline{\Gamma}_1$. In the third term recall that every source field A is connected by the propagator Δ to the rest of any graph of $\overline{W}$. Therefore, in the substitution $A \to \Delta^{-1}\alpha - \overline{\Gamma}_1$ the second term inevitably produces a one-reducible graph. Since there are no such graphs in the representation, the one-reducible graphs from the second and third terms in (4.66) mutually cancel. Thus, we are left with the one-irreducible graphs brought about by the substitution $\Delta A \to \alpha$ in $\overline{W}(A)$. In other words

$$\Gamma(\alpha) = -\frac{1}{2}\,\alpha\Delta^{-1}\alpha + \sum_{\mathrm{one-irr,i}} C_i\gamma_i\,(\Delta A \to \alpha)\;. \tag{4.67}$$

From relation (4.62) and its generalizations to arbitrary n we conclude that the *tree graphs* (i.e. graphs without closed loops of propagator lines) sum up to the interaction functional $\overline{V}$ with the field α instead of φ:

$$\Gamma(\alpha) = -\frac{1}{2}\,\alpha\Delta^{-1}\alpha + \overline{V}(\alpha) + \sideset{}{'}\sum_{\mathrm{one-irr,i}} C_i\gamma_i\,(\Delta A \to \alpha)\;, \tag{4.68}$$

where the prime means that the sum goes over graphs with closed loops of propagators. Due to this, the functional Γ is sometimes called the *effective action* or *effective potential*.

4.4 Problems

Problem 4.1. Construct vertex factors brought about by the non-local density-density interaction functional

$$\int d\boldsymbol{x} \int d\boldsymbol{x}\, \frac{g|\psi(\boldsymbol{x})|^2|\psi(\boldsymbol{x}')|^2}{2|\boldsymbol{x} - \boldsymbol{x}'|}\;.$$

Calculate also the Fourier transforms of these vertex factors with respect to all coordinate and time variables.

Problem 4.2. Evaluate the symmetry coefficient of a closed loop consisting of n two-point vertices and n lines connecting them.

Problem 4.3. Write the Schwinger equation for generating functionals W and Γ, when the interaction functional is $\overline{V} = \frac{1}{24}v_4\varphi^4$. With the aid of these equations, write the Dyson equation.

Problem 4.4. Solve the functional equations of motion for the functionals $W(A)$ and $\Gamma(\alpha)$ by iterations to the fourth order in the number of lines for the interaction functional $\overline{V} = \frac{1}{24}v_4\varphi^4$.

Problem 4.5. Show that

$$\exp\left(-\varphi A\right) F\left(\frac{\delta}{\delta\varphi}\right) \exp\left(\varphi A\right) = F\left(A + \frac{\delta}{\delta\varphi}\right)$$

for any functional

$$F(\varphi) = \sum_{n=0}^{\infty} \frac{1}{n!} \int dx_1 \cdots \int dx_1 F_n(x_1, \ldots, x_n) \varphi(x_1) \cdots \varphi(x_n) \,.$$