

Lectures on Selected Topics in Statistical Mechanics

D. ter Haar

LECTURES ON SELECTED TOPICS IN STATISTICAL MECHANICS

by

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Preface

The present lecture notes were prepared for a set of lectures which were given at the 1971 Simla Summer School of Statistical Mechanics, organized by the Centre of Advanced Study in Theoretical Physics and Astrophysics of the University of Delhi and the Centre for Postgraduate Studies of the University of Himachal Pradesh. Because of lack of time not all the material presented here was covered in my lectures. I want to stress that some parts lean very heavily on the original papers given in the list of references at the end of the notes.

Because these are lecture notes, the choice of material is highly subjective and I have, for obvious reasons, covered those subjects in which I myself have been or am interested. All the same, I hope that this personal selection may prove to be of interest to other people, especially as it contains some unpublished material as well as some material which is not easily available.

I should like to express my thanks to the organizers of the Summer School, and especially to Professor F.C. Auluck for inviting me to give these lectures and for their generous hospitality.

Simla, Himachal Pradesh,
June 1971

D. ter Haar

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CHAPTER 1

The Occupation Number Representation

Let us first of all note that although statistical mechanics deals with 'large' systems of interacting particles, whereas field theory deals with particles and quantized fields or with interacting fields, in the second quantization formalism these problems become very similar. This has led to the introduction of diagram techniques in statistical mechanics both at zero and at non-zero temperatures.

Let us also note the need to use representative ensembles because of our restricted knowledge about the actual physical systems we are dealing with. Bearing in mind that the total number of particles in the system is also not known accurately, we are led to the use of grand ensembles. We shall start the introduction with a recapitulation of some relevant formulae from ensemble theory.

1.1 Classical Petit Ensembles

If we consider an ensemble of n systems consisting of N identical atoms (or molecules), if $p_1^{(i)}, \dots, p_s^{(i)}, q_1^{(i)}, \dots, q_s^{(i)}$ are the generalized momenta and coordinates of the i th atom, if $D(q_1^{(1)}, \dots, q_s^{(N)}, p_1^{(1)}, \dots, p_s^{(N)})$; $t) d\Omega$ is the number of systems in the ensemble with a representative point, $q_1^{(1)}, \dots, q_s^{(N)}, p_1^{(1)}, \dots, p_s^{(N)}$, within a volume element $d\Omega$ of phase space or Γ -space, where

$$d\Omega = \prod_{i=1}^N \prod_{j=1}^s dp_j^{(i)} dq_j^{(i)},$$

and if we introduce the ensemble density $\rho = D/n$, one can show that when we consider an ensemble representing a system in thermodynamic equilibrium at an absolute temperature T , ρ is given by the equation

$$\rho = e^{\beta(\psi - \epsilon)}, \quad (1.1)$$

where ψ is a function of β , where

$$\beta = \frac{1}{k_B T} \quad (1.2)$$

(k_B : Boltzmann's constant), and where ϵ is the energy of the system as function of the p 's and q 's, that is, the Hamiltonian:

$$\epsilon = H(p, q). \quad (1.3)$$

From the definition of ρ it follows that it must be normalized

$$\int \rho d\Omega = 1, \quad (1.4)$$

where the integration is over the whole of Γ -space. From (1.1) and (1.4) it follows that ψ must satisfy the equation

$$e^{-\beta\psi} = \int e^{-\beta\epsilon} d\Omega, \quad (1.5)$$

and one shows by standard methods that ψ is the Helmholtz free energy F , apart possibly from an additive multiple of β^{-1} . To fix this constant and ensure the proper transition from quantal formulae we can write

$$e^{-\beta F} = \frac{1}{N!} \int e^{-\beta\epsilon} \frac{d\Omega}{h^{3N}} \equiv Z_{\Gamma}^{(N)}, \quad (1.6)$$

where h is Planck's constant. The function $Z_{\Gamma}^{(N)}$ is called the partition function.

Once we know ψ (or $Z_{\Gamma}^{(N)}$) we can by differentiation find the average values of various phase functions, for which we have the general formula

$$\overline{g(p,q)} = \int g \rho d\Omega. \quad (1.7)$$

For instance, we have

$$\bar{\epsilon} = \frac{\partial \beta \psi}{\partial \beta}, \quad (1.8)$$

which is the Gibbs-Helmholtz equation, and for the pressure P

$$P = - \frac{\partial \psi}{\partial V}, \quad (1.9)$$

where V is the volume.

If we are dealing with point particles, so that $s=3$, the kinetic energy part of ϵ is simply $\sum_i p_i^2/2m$, and the integration over the momenta is straightforward and leads to

$$Z_{\Gamma}^{(N)} = Q_N / v_0^N, \quad (1.10)$$

where

$$v_0 = \left(\frac{\beta h^2}{2\pi m} \right)^{\frac{3}{2}}, \quad (1.11)$$

which is essentially the cube of the thermal de Broglie wavelength, that is, the de Broglie wavelength of a particle moving with a kinetic energy equal to $k_B T$, and where Q_N is the so-called configurational partition function,

$$Q_N = \frac{1}{N!} \int e^{-U(r_i)} \prod_i d^3 r_i \quad (1.12)$$

where $U(r_i)$ is the total potential energy of the system.

1.2 Classical Grand Ensembles

We now consider an ensemble, the systems of which do not necessarily all contain N particles. If $D(p_1^{(1)}, \dots, p_s^{(N)}, q_1^{(1)}, \dots, q_s^{(N)}; t) d\Omega$ is the number of systems in the ensemble containing N particles and with their representative points within $d\Omega_N$, and if again $\rho = D/n$, we now find that for an ensemble representing a system in thermodynamic equilibrium and able to exchange particles with its surroundings, ρ is given by

$$\rho = \frac{1}{N!} e^{-q + \alpha N - \beta \epsilon}, \quad (1.13)$$

where β and ϵ have the same meaning as in (1.1), where α can be shown to be the partial Helmholtz free energy multiplied by β , and where the grand potential - or q -potential -, which because of the normalization of ρ satisfies the equation

$$e^q = \sum_N \frac{1}{N!} e^{\alpha N} \int e^{-\beta \epsilon} d\Omega_N, \quad (1.14)$$

can be shown to be equal to βPV in the case of a homogeneous system. We note in passing that we can write (1.14) in the form

$$e^q = \sum_N h^{sN} e^{\alpha N} Z_I^{(N)}. \quad (1.15)$$

The grand-ensemble averages $\langle g \rangle$ of phase functions are now given by the formula

$$\langle g \rangle = \sum_N \int g \rho d\Omega_N, \quad (1.16)$$

and many of them follow from q through differentiation. For example, we have

$$\langle N \rangle = \frac{\partial q}{\partial \alpha}, \quad (1.17)$$

$$\langle \epsilon \rangle = - \frac{\partial q}{\partial \beta}, \quad (1.18)$$

$$P = \frac{1}{\beta} \frac{\partial q}{\partial V}. \quad (1.19)$$

If we are not dealing with stationary ensembles, such as the ones described by (1.1) and (1.13), the ensemble density ρ satisfies the following equation of motion:

$$\dot{\rho} = \{H, \rho\}, \quad (1.20)$$

where the dot indicates a time derivative and the curly brackets a Poisson bracket:

$$\{A, B\} = \sum_{i,j} \left[\frac{\partial A}{\partial q_j^{(i)}} \frac{\partial B}{\partial p_j^{(i)}} - \frac{\partial A}{\partial p_j^{(i)}} \frac{\partial B}{\partial q_j^{(i)}} \right] \quad (1.21)$$

1.3 Quantal Petit Ensembles

In quantum statistical mechanics the density matrix takes over the rôle of the ensemble density. Its equation of motion is the quantal counterpart of (1.20):

$$i\hbar \dot{\rho}_{op} = [H_{op}, \rho_{op}]_- , \quad (1.22)$$

where

$$[A_{op}, B_{op}]_- = A_{op} B_{op} - B_{op} A_{op} \quad (1.23)$$

is a commutator, and where we indicate operators by the subscript 'op' or by a caret '^'.

Averages of phase functions are double averages in the quantal case: once over all the systems in an ensemble, and once for each system over the state of the system. The density matrix, or statistical operator, is defined in such a way that the average \bar{g} of a phase function g is now given by the equation

$$\bar{g} = \text{Tr } \rho_{op} g_{op} . \quad (1.24)$$

A special example of (1.24) is the normalization condition

$$\text{Tr } \rho_{op} = 1 . \quad (1.25)$$

For an ensemble representing a system in thermodynamic equilibrium, (1.1) is replaced by

$$\rho_{op} = \exp \left[\beta (\Psi - H_{op}) \right] , \quad (1.26)$$

where H_{op} is the energy (Hamiltonian) operator, and where β and Ψ have the same physical meaning as in (1.1). Equations (1.8) and (1.9) are again valid, but (1.5) must be replaced by

$$e^{-\beta \Psi} = \text{Tr } \exp(-\beta H_{op}) . \quad (1.27)$$

1.4 Quantal Grand Ensembles

Instead of (1.13), we now have

$$\rho_{op} = \exp(-q + \alpha N_{op} - \beta H_{op}) , \quad (1.28)$$

where q , α , and β have the same meaning as before, and where N_{op} is the number operator. Equation (1.25) again holds, and also (1.24):

$$\langle g \rangle = \text{Tr } \rho_{op} g_{op} , \quad (1.29)$$

but the trace involves summation over N - if we work in a representation in which N is diagonal. Equations (1.17) to (1.19) remains the same, while (1.14) is replaced by

$$e^q = \text{Tr } \exp(\alpha N_{op} - \beta H_{op}) . \quad (1.30)$$

We must bear in mind that, if we work with systems of bosons (or fermions) the complete orthonormal systems which we use to choose for our representation must be properly symmetrised (or antisymmetrised).

1.5 Occupation-number Representation

It is often convenient to use a formalism which employs creation and annihilation operators. This formalism we shall call the occupation-number representation, although it is widely known as the second-quantisation representation. This term, however, is a misnomer, as nowhere is there a further introduction of the quantum of action; it derives from the fact that in this formalism the wavefunctions become operators. We shall use Dirac's bra and ket notation as it is particularly suitable for our discussion.

For a system of N identical particles one can use as a complete orthonormal set of basic functions the set

$$|i_1, i_2, \dots, i_N\rangle = \frac{1}{N!} \sum_P \epsilon_P \varphi_{i_1}(P_1) \varphi_{i_2}(P_2) \dots \varphi_{i_N}(P_N), \quad (1.31)$$

where the φ_{i_1} form a complete orthonormal set of single-particle kets (we do not need to and shall not specify the representation in which we are working), where P_1, P_2, \dots, P_N is a permutation of the N numbers $1, \dots, N$, where ϵ_P is 1 for bosons, while for fermions $\epsilon_P = +1$ or -1 according as to whether P is an even or odd permutation. The complete orthonormal ket set $|i_1, \dots, i_N\rangle$ is a set with the proper symmetry features. The bra set corresponding to the ket set (1.31) is

$$\langle i_1, i_2, \dots, i_N| = \frac{1}{N!} \sum_P \epsilon_P \varphi_{i_1}^*(P_1) \varphi_{i_2}^*(P_2) \dots \varphi_{i_N}^*(P_N), \quad (1.32)$$

where φ_i^* is the conjugate complex of φ_i - or the Hermitean conjugate, if we are dealing with particles described by spinors. The sets (1.31) and (1.32) satisfy the orthonormality relation

$$\langle i'_1, i'_2, \dots, i'_N | i_1, i_2, \dots, i_N \rangle = \frac{1}{N!} \sum_P \epsilon_P \delta(i_1 - i'_{P_1}) \dots \delta(i_N - i'_{P_N}) \quad (1.33)$$

as well as a completeness or closure relation. We have assumed here that i is a continuous parameter. If it is a discrete one, the Dirac δ -function must be replaced by a Kronecker δ -function.

If $|\Psi\rangle$ is a wavefunction of the N -particle system with the correct symmetry properties, we have

$$|\Psi\rangle = \int \dots \int di_1, \dots, di_N |i_1, \dots, i_N\rangle \langle i_1, \dots, i_N | \Psi \rangle \quad (1.34)$$

Similarly, an operator Ω_{op} operating on N-particle functions in the Hilbert space spanned by the set (1.31) will have the form

$$\Omega_{op} = \int, \dots, \int d i_1, \dots, d i_N d i_1', \dots, d i_N' | i_1, \dots, i_N \rangle \langle i_1', \dots, i_N' | \Omega_{op} | i_1', \dots, i_N' \rangle \langle i_1', \dots, i_N' | . \quad (1.35)$$

Let us now consider systems in which the numbers of particles may have any arbitrary value. That is, let us consider the Hilbert space which is the direct product space of the Hilbert spaces corresponding to $0, 1, \dots, N, \dots$ particles. These latter Hilbert spaces are spanned by the sets (1.31) with $N = 0, 1, \dots, N, \dots$, respectively, and the complete orthonormal set spanning the product space will be the set

$$|0\rangle, |i\rangle, |i_1, i_2\rangle, \dots, |i_1, i_2, \dots, i_N\rangle, \dots, \quad (1.36)$$

where $|0\rangle$ is the vacuum state in which there is no particle present.

We now introduce creation - or construction - operators which will produce a ket corresponding to N particles from one corresponding to N-1 particles in the following way

$$\hat{a}^+(i) |i_1, \dots, i_N\rangle = \sqrt{N+1} |i, i_1, \dots, i_N\rangle . \quad (1.37)$$

From (1.37) it follows that all the $|i_1, \dots, i_N\rangle$ can be obtained from the vacuum state by the repeated action of creation operators:

$$|i_1, \dots, i_N\rangle = \frac{1}{\sqrt{N!}} \hat{a}^+(i_1) \hat{a}^+(i_2) \dots \hat{a}^+(i_N) |0\rangle . \quad (1.38)$$

From the definitions (1.37) and (1.31) one can prove - and we leave the proof to the reader - that the $\hat{a}^+(i)$ satisfy the (anti)commutation relations

$$[\hat{a}^+(i), \hat{a}^+(j)]_- = 0, \quad \text{for bosons;} \quad (1.39a)$$

$$[\hat{a}^+(i), \hat{a}^+(j)]_+ = 0, \quad \text{for fermions;} \quad (1.39b)$$

where

$$[A_{op}, B_{op}]_+ = A_{op} B_{op} + B_{op} A_{op} \quad (1.40)$$

is an anticommutator.

Consider now the equations which are the adjoint of (1.37):

$$\langle i_1, \dots, i_N | \hat{a}(i) = \sqrt{N+1} \langle i, i_1, \dots, i_N | , \quad (1.41)$$

where $\hat{a}(i)$ is the adjoint of $\hat{a}^+(i)$. From (1.41) it follows that

$$[\hat{a}(i), \hat{a}(j)]_- = 0, \quad \text{for bosons;} \quad (1.42a)$$

$$[\hat{a}(i), \hat{a}(j)]_+ = 0, \quad \text{for fermions.} \quad (1.42b)$$

To find out what $\hat{a}(i)$ does to a ket vector, we consider the matrix element

$$\langle i'_1, \dots, i'_{N-1} | \hat{a}(i) | i_1, \dots, i_N \rangle.$$

We have written $N-1$ indices on the left and N indices on the right because (i) equation (1.41) tells us that $\hat{a}(i)$ operating from the right on an N -particle function produces an $(N+1)$ -particle function, and (ii) $|i_1, \dots, i_N\rangle$ is orthogonal onto $|i'_1, \dots, i'_{N'}\rangle$, if $N \neq N'$. From equations (1.41) and (1.31) or (1.33) it follows that

$$\begin{aligned} \langle i'_1, \dots, i'_{N-1} | \hat{a}(i) | i_1, \dots, i_N \rangle &= \frac{1}{\sqrt{N}} \left\{ \delta(i - i_1) \langle i'_1, \dots, i'_{N-1} | i_2, \dots, i_N \rangle \right. \\ &\quad \pm \delta(i - i_2) \langle i'_1, \dots, i'_{N-1} | i_1, i_3, \dots, i_N \rangle + \dots + \\ &\quad \left. (\pm 1)^{N-1} \delta(i - i_N) \langle i'_1, \dots, i'_{N-1} | i_1, \dots, i_{N-1} \rangle \right\} \end{aligned} \quad (1.43)$$

As equation (1.43) must hold for any bra $\langle i'_1, \dots, i'_{N-1} |$, we have

$$\begin{aligned} \hat{a}(i) | i_1, \dots, i_N \rangle &= \frac{1}{\sqrt{N}} \left\{ \delta(i - i_1) | i_2, \dots, i_N \rangle \pm \delta(i - i_2) | i_1, i_3, \dots, i_N \rangle \right. \\ &\quad + \dots + (\pm 1)^{N-2} \delta(i - i_{N-1}) | i_1, \dots, i_{N-2}, i_N \rangle \\ &\quad \left. + (\pm 1)^{N-1} \delta(i - i_N) | i_1, \dots, i_{N-1} \rangle \right\}. \end{aligned} \quad (1.44)$$

In equations (1.43) and (1.44) the upper (lower) signs correspond to the boson (fermion) case. From equation (1.44) we see that the $\hat{a}(i)$ are annihilation operators. Provided the state i is represented in the ket $|i_1, \dots, i_N\rangle$, $\hat{a}(i)$ operating upon that ket produces another ket where that state has been removed. In the case of bosons the state i may occur more than one, and there may be more than one non-vanishing term on the right-hand side of (1.44).

From equations (1.44), (1.37), and (1.41) we find the (anti)commutation relations

$$\left[\hat{a}(i), \hat{a}^+(j) \right]_- = \delta(i - j), \quad \text{for bosons;} \quad (1.45a)$$

$$\left[\hat{a}(i), \hat{a}^+(j) \right]_+ = \delta(i - j), \quad \text{for fermions.} \quad (1.45b)$$

Let us now consider (1.35) for the special case where Ω_{op} is of the form

$$\Omega_{op} = \sum_{i=1}^N \hat{\Omega}_i^{(1)} + \frac{1}{2} \sum_{i,j=1}^N \hat{\Omega}_{ij}^{(2)}, \quad (1.46)$$

where the $\hat{\Omega}_i^{(1)}$ are single-particle operators and the $\hat{\Omega}_{ij}^{(2)}$ are two-particle operators. Moreover, let us assume that the $\hat{\Omega}_i^{(1)}$ have all the same form and

differ only in the particle on which they operate and that, *mutatis mutandis*, the same is true for the $\hat{\Omega}_{ij}^{(2)}$ (compare equations (1.49) below). From equation (1.35) and equation (1.38) and its adjoint, we find, if we also use the orthonormality and symmetry properties of the kets:

$$\begin{aligned} \Omega_{op} = & \int d\mathbf{i} d\mathbf{i}' \langle \mathbf{i} | \hat{\Omega}^{(1)} | \mathbf{i}' \rangle \hat{a}^+(\mathbf{i}) \hat{a}(\mathbf{i}') \\ & + \frac{1}{2} \int d\mathbf{i} d\mathbf{j} d\mathbf{i}' d\mathbf{j}' \langle \mathbf{i} \mathbf{j} | \hat{\Omega}^{(2)} | \mathbf{i}' \mathbf{j}' \rangle \hat{a}^+(\mathbf{i}) \hat{a}^+(\mathbf{j}) \hat{a}(\mathbf{j}') \hat{a}(\mathbf{i}') . \end{aligned} \quad (1.47)$$

A case of particular interest, as it often is applicable, is the one where we choose the φ_i to be plane waves in a volume V , that is, where we use the momentum eigenfunctions in the coordinate representation:

$$\varphi_i \rightarrow V^{-\frac{1}{2}} e^{i(\underline{k} \cdot \underline{r})} , \quad (1.48)$$

where the \underline{k} form a discrete set, if the volume V is finite. In that case we write $\hat{a}_{\underline{k}}^+$ and $\hat{a}_{\underline{k}}$ rather than $\hat{a}^+(\underline{k})$ and $\hat{a}(\underline{k})$. Let in the coordinate representation the $\hat{\Omega}_i^{(1)}$ and $\hat{\Omega}_{ij}^{(2)}$ have the form

$$\hat{\Omega}_i^{(1)} = -\frac{\hbar^2}{2m} \nabla_i^2 + U(\underline{r}) , \quad \hat{\Omega}_{ij}^{(2)} = v(\underline{r}_i - \underline{r}_j) , \quad (1.49)$$

which corresponds to Ω_{op} being the Hamiltonian of a system of point particles of mass m moving in a common potential $U(\underline{r})$ and interacting solely through binary forces governed by the interaction potential $v(\underline{r}_i - \underline{r}_j)$. We now get from equation (1.47)

$$\Omega_{op} = \sum_{\underline{k}} \frac{\hbar^2 \underline{k}^2}{2m} \hat{a}_{\underline{k}}^+ \hat{a}_{\underline{k}} + \frac{1}{V} \sum_{\underline{k}, \underline{q}} U(\underline{q}) \hat{a}_{\underline{k}}^+ \hat{a}_{\underline{k}-\underline{q}} + \frac{1}{2V} \sum_{\underline{k}, \underline{k}', \underline{q}} v(\underline{q}) \hat{a}_{\underline{k}}^+ \hat{a}_{\underline{k}}^+ \hat{a}_{\underline{k}'+\underline{q}} \hat{a}_{\underline{k}-\underline{q}} \quad (1.50)$$

where

$$U(\underline{q}) = \int d^3 \underline{r} e^{-i(\underline{q} \cdot \underline{r})} U(\underline{r}) , \quad v(\underline{q}) = \int d^3 \underline{r} e^{-i(\underline{q} \cdot \underline{r})} v(\underline{r}) . \quad (1.51)$$

We note in conclusion that the operators

$$n_{op}(i) = \hat{a}^+(i) \hat{a}(i) , \quad (1.52)$$

the so-called occupation-number operators, will when operating upon a ket $|i_1, \dots, i_N\rangle$ reproduce this ket, multiplied by an integer which is equal to the number of times i occurs amongst the numbers i_1, \dots, i_N , as follows from equation (1.44). One can thus also characterize the kets $|i_1, \dots, i_N\rangle$ by the numbers of particles which are in a given single-particle state:

$$|i_1, \dots, i_N\rangle \rightarrow |n(j_1), n(j_2), \dots\rangle , \quad (1.53)$$

where now the j_1, j_2, \dots are all different. In the case of bosons the $n(j)$ can take on any integral value, but in the case of fermions they must be 0 or 1. We shall not further develop the formalism using the $n(j)$ -representation.

CHAPTER 2

The Green Function Method in Statistical Mechanics

2.1 The Double-time Temperature-dependent Green Functions

There are many cases when we want to know the thermodynamic averages of thermodynamic quantities and it is, therefore, of interest to have a formalism which enables us to evaluate such averages — either exactly, or at least in some more or less well-defined approximation. The Green function formalism, which was first introduced by Bogolyubov and Tyablikov, is such a scheme. It has turned out to be especially useful in the theory of magnetism, as we shall see in these lectures.

Let H_{op} be the Hamiltonian of the system we are considering and let N_{op} be the number operator for the particles in the system. If again

$$\beta = \frac{1}{k_B T} , \quad (1.1)$$

(k_B : Boltzmann's constant, T : absolute temperature), we have for the grand ensemble average of any thermodynamic quantity A , the equation

$$\langle A \rangle = \frac{\text{Tr } A_{op} \exp[-\beta (H_{op} - \mu N_{op})]}{\text{Tr } \exp[-\beta (H_{op} - \mu N_{op})]} , \quad (1.2)$$

where μ is the partial thermodynamic or chemical potential.

Sometimes it is just as convenient to use a canonical ensemble as a grand ensemble. In that case, we have instead of equation (1.2)

$$\langle A \rangle = \frac{\text{Tr } A_{op} \exp(-\beta H_{op})}{\text{Tr } \exp(-\beta H_{op})} . \quad (1.3)$$

We now define in the usual way time-dependent operators. If we are using a canonical ensemble, we use the normal Heisenberg representation:

$$A_{op}(t) = \exp(iH_{op} t) A_{op} \exp(-iH_{op} t) \quad (1.4)$$

(we are using units in which $\hbar = 1$). However, if we are using a grand ensemble, it is more convenient to generalize equation (1.4) and to define $A_{op}(t)$ through the equation

$$A_{op}(t) = \exp(i H'_{op} t) A_{op} \exp(-i H'_{op} t), \quad (1.5)$$

where

$$H'_{op} = H_{op} - \mu N_{op}. \quad (1.6)$$

We can now define the double-time temperature-dependent Green functions through the equation

$$\langle\langle A_{op}(t); B_{op}(t') \rangle\rangle_a = \pm i \theta(\mp t \pm t') \left\{ \langle A_{op}(t) B_{op}(t') \rangle - \eta \langle B_{op}(t') A_{op}(t) \rangle \right\} \quad (1.7)$$

where η is a parameter which we shall choose to be either +1 or -1, but which we leave undetermined for the moment. The function θ is the Heaviside function

$$\begin{aligned} \theta(t) &= 0, t < 0; \\ &= 1, t > 0; \end{aligned} \quad (1.8)$$

and the indices 'a' and 'r' indicate the advanced and retarded Green functions. We shall not introduce here the causal Green functions.

We now want the equation of motion for the Green functions. We first of all note that as the same operator H'_{op} occurs in equations (1.2) and (1.5) and the same operator H_{op} in equation (1.3) and equation (1.4), and as the trace of a product of operators is invariant under a cyclic permutation of the operators, the Green functions depend on t and t' only through the combination $t - t'$. Let us denote differentiation with respect to t by a dot. We shall use the relations

$$i \dot{A}_{op} = [A_{op}, H'_{op}]_-, \quad (1.9)$$

$$i \dot{A}_{op} = [A_{op}, H_{op}]_-, \quad (1.10)$$

according to whether we are dealing with a grand or with a canonical ensemble, and where

$$[a_{op}, b_{op}]_{\mp} = a_{op} b_{op} \mp b_{op} a_{op}. \quad (1.11)$$

Moreover, we have

$$\dot{\theta}(t - t') = -\dot{\theta}(t' - t) = \delta(t - t'), \quad (1.12)$$

where $\delta(t)$ is the Dirac delta-function. We thus find

$$\begin{aligned} i \langle\langle A_{op}(t); B_{op}(t') \rangle\rangle &= \delta(t - t') \left\{ \langle A_{op}(t) B_{op}(t') \rangle - \eta \langle B_{op}(t') A_{op}(t) \rangle \right\} \\ &+ \langle\langle [A_{op}(t), H'_{op}]_-; B_{op}(t') \rangle\rangle, \end{aligned} \quad (1.13)$$

or

$$i \langle\langle A_{op}(t); B_{op}(t') \rangle\rangle = \delta(t-t') \{ \langle A_{op}(t) B_{op}(t') \rangle - \eta \langle B_{op}(t') A_{op}(t) \rangle \} \\ + \langle\langle [A_{op}(t), H_{op}]_-; B_{op}(t') \rangle\rangle. \quad (1.14)$$

We note: (i) that the equation of motion is the same for the retarded as for the advanced Green function, and (ii) that in equations (1.13) and (1.14) more complicated Green functions appear.

We now introduce the Fourier transform of the Green functions by the equations

$$\langle\langle A_{op}(t); B_{op}(t') \rangle\rangle = \int_{-\infty}^{+\infty} \langle\langle A_{op}; B_{op} \rangle\rangle_E e^{-iE(t-t')} dE, \quad (1.15)$$

$$\langle\langle A_{op}; B_{op} \rangle\rangle_E = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \langle\langle A_{op}(t); B_{op}(t') \rangle\rangle e^{iE(t-t')} d(t-t'). \quad (1.16)$$

Dropping the index 'E' and only writing down the equations for the canonical case, knowing that the grand-canonical case can be obtained by changing H_{op} to H'_{op} , we can write equation (1.14) in the form

$$E \langle\langle A_{op}; B_{op} \rangle\rangle = \frac{1}{2\pi} \langle A_{op} B_{op} - \eta B_{op} A_{op} \rangle + \langle\langle [A_{op}, H_{op}]_-; B_{op} \rangle\rangle. \quad (1.17)$$

We must now discuss spectral representations. We define first of all the correlation functions

$$F_{BA}(t, t') = \langle B_{op}(t') A_{op}(t) \rangle, \quad F_{AB}(t, t') = \langle A_{op}(t) B_{op}(t') \rangle, \quad (1.18)$$

and note that the Green functions are linear combinations of F_{BA} and F_{AB} .

We now define a function $J(\omega)$ by the equation

$$F_{BA}(t, t') = \int_{-\infty}^{+\infty} J(\omega) e^{-i\omega(t-t')} d\omega. \quad (1.19)$$

From equations (1.18) and (1.3), and using a representation in which H_{op} is diagonal,

$$\langle \nu | H_{op} | \mu \rangle = \delta_{\nu\mu} E_{\nu}, \quad (1.20)$$

we find after some straightforward calculations

$$J(\omega) = \frac{1}{Z} \sum_{\nu, \mu} \langle \nu | B_{op} | \mu \rangle \langle \mu | A_{op} | \nu \rangle e^{-\beta E_{\nu}} \delta(\omega - E_{\nu} + E_{\mu}), \quad (1.21)$$

where

$$Z = \text{Tr} \exp(-\beta H_{op}). \quad (1.22)$$

Similarly, if we write

$$F_{AB}(t, t') = \int_{-\infty}^{+\infty} J'(\omega) e^{-i\omega(t-t')} d\omega, \quad (1.23)$$

we find

$$J'(\omega) = J(\omega) e^{\beta \omega}. \quad (1.24)$$