1 Mathematical Introduction

1-1 BASIC DEFINITIONS

The properties of a quantum mechanical system composed of many identical particles are most conveniently described in terms of the second-quantized, Heisenberg representation, particle-creation, and annihilation operators. The creation operator, $\psi\dagger(\mathbf{r},t)$, when acting to the right on a state of the system, adds a particle to the state at the space-time point $\mathbf{r},t$; the annihilation operator $\psi(\mathbf{r},t)$, the adjoint of the creation operator, acting to the right, removes a particle from the state at the point $\mathbf{r},t$.

The macroscopic operators of direct physical interest can all be expressed in terms of products of a few ψ's and $\psi\dagger$'s. For example, the density of particles at the point $\mathbf{r},t$ is

$$n(\mathbf{r},t) = \psi\dagger(\mathbf{r},t)\psi(\mathbf{r},t) \tag{1-1a}$$

Since the act of removing and then immediately replacing a particle at $\mathbf{r},t$ measures the density of particles at that point, the operator for the total number of particles is

$$N(t) = \int d\mathbf{r}\,\psi\dagger(\mathbf{r},t)\psi(\mathbf{r},t) \tag{1-1b}$$

Similarly, the total energy of a system of particles of mass m interacting through an instantaneous two-body potential $v(r)$ is given by

$$\begin{aligned} H(t) = &\int d\mathbf{r}\,\frac{\nabla\psi\dagger(\mathbf{r},t)\cdot\nabla\psi(\mathbf{r},t)}{2m} \\ &+ 1/2\int d\mathbf{r}\,d\mathbf{r}'\,\psi\dagger(\mathbf{r},t)\psi\dagger(\mathbf{r}',t)\,v(|\mathbf{r}-\mathbf{r}'|)\psi(\mathbf{r}',t)\psi(\mathbf{r},t) \end{aligned} \tag{1-2}$$

In general we shall take $\hbar = 1$.

The equation of any operator X(t) in the Heisenberg representation is

$$\frac{i\,\partial X(t)}{\partial t} = [X(t),H(t)] \tag{1-3}$$

Since $[H(t),H(t)] = 0$, we see that the Hamiltonian is independent of time. Also the Hamiltonian does not change the number of particles, $[H,N(t)] = 0$, and therefore N(t) is also independent of time. Because of the time independence of H, (1-3) may be integrated in the form

$$X(t) = e^{iHt}X(0)e^{-iHt} \tag{1-4}$$

Particles may be classified into one of two types: Fermi-Dirac particles, also called fermions, which obey the exclusion principle, and Bose-Einstein particles, or bosons, which do not. The wave function of any state of a collection of bosons must be a symmetric function of the coordinates of the particles, whereas, for fermions, the wave function must be antisymmetric. One of the main advantages of the second-quantization formalism is that these symmetry requirements are very simply represented in the equal-time commutation relations of the creation and annihilation operators. These commutation relations are

$$\begin{aligned} &\psi(\mathbf{r},t)\psi(\mathbf{r}',t) \mp \psi(\mathbf{r}',t)\psi(\mathbf{r},t) = 0 \\ &\psi\dagger(\mathbf{r},t)\psi\dagger(\mathbf{r}',t) \mp \psi\dagger(\mathbf{r}',t)\psi\dagger(\mathbf{r},t) = 0 \\ &\psi(\mathbf{r},t)\psi\dagger(\mathbf{r}',t) \mp \psi\dagger(\mathbf{r}',t)\psi(\mathbf{r},t) = \delta(\mathbf{r}-\mathbf{r}') \end{aligned} \tag{1-5}$$

where the upper sign refers to Bose-Einstein particles and the lower sign refers to Fermi-Dirac particles. We see, for fermions, that $\psi^2(\mathbf{r},t) = 0$. This is an expression of the exclusion principle in space —it is impossible to find two identical fermions at the same point in space and time.

We shall be interested in describing the behavior of many-particle systems at finite temperature. For a system in thermodynamic equilibrium the expectation value of any operator X may be computed by using the grand-canonical ensemble of statistical mechanics. Thus

$$\langle X\rangle = \frac{\sum_i \langle i|X|i\rangle\, e^{-\beta(E_i - \mu N_i)}}{\sum_i e^{-\beta(E_i - \mu N_i)}} \tag{1-6a}$$

Here $|i\rangle$ represents a state of the system, normalized to unity, with energy E_i and number of particles N_i. The sum runs over all states of the system with all possible numbers of particles. A more compact way of writing the average (1-6a) is

$$\langle X\rangle = \frac{\mathrm{tr}\left[e^{-\beta(H-\mu N)}X\right]}{\mathrm{tr}\left[e^{-\beta(H-\mu N)}\right]} \tag{1-6b}$$

where tr denotes the trace.

The thermodynamic state of the system is now defined by the parameters μ, the chemical potential, and β, the inverse temperature measured in energy units, i.e., $\beta = 1/k_BT$, where k_B is Boltzmann's constant. Zero temperature, or $\beta \to \infty$, describes the ground state of the system.

The Green's functions, which shall form the base of our discussion of many-particle systems, are thermodynamic averages of products of the operators $\psi(1)$ and $\psi(1')$. (We use the abbreviated notation 1 to mean $\mathbf{r}_1t_1$ and 1′ to mean $\mathbf{r}_{1'}t_{1'}$, etc.) The one-particle Green's function is defined by

$$G(1,1') = (1/i)\,\langle T(\psi(1)\psi\dagger(1'))\rangle \tag{1-7a}$$

while the two-particle Green's function is defined by

$$G_2(12,1'2') = (1/i^2)\,\langle T(\psi(1)\psi(2)\psi\dagger(2')\psi\dagger(1'))\rangle \tag{1-7b}$$

In these Green's functions, T represents the Wick time-ordering operation. When applied to a product of operators it arranges them in chronological order with the earliest time appearing on the right and the latest on the left. For bosons, this is the full effect of T. For fermions, however, it is convenient to define T to include an extra factor, ± 1, depending on whether the resulting time-ordered product is an even or odd permutation of the original order. Thus, for example,

$$\begin{aligned} T(\psi(1)\psi\dagger(1')) &= \psi(1)\psi\dagger(1') \qquad \text{for } t_1 > t_{1'} \\ &= \pm\psi\dagger(1')\psi(1) \qquad \text{for } t_1 < t_{1'} \end{aligned}$$

As in (1-5), the upper sign refers to bosons and the lower to fermions. We shall use this sign convention throughout these lectures.

The one-particle Green's function G(1,1′) has a direct physical interpretation. It describes the propagation of disturbances in which a single particle is either added to or removed from the many-particle equilibrium system. For example, when $t_1 > t_{1'}$ the creation

operator acts first, producing a disturbance by adding a particle at the space-time point $\mathbf{r}_{1'}t_{1'}$. This disturbance then propagates to the later time $t_{1'}$ when a particle is removed at $\mathbf{r}_{1'}$ ending the disturbance and returning the system to its equilibrium state. For $t_1 < t_{1'}$, ψ acts first. The disturbance, which is now produced by the removal of a particle at $\mathbf{r}_1 t_1$, propagates to time $t_{1'}$, when it is terminated by the addition of a particle at the point $\mathbf{r}_{1'}$.

Similarly, the two-particle Green's function describes, for the various time orders, disturbances produced by the removal or addition of two particles. For example, when t_1 and t_2 are both later than $t_{1'}$ and $t_{2'}$, $G_2(12,1'2')$ describes the addition of two particles and the subsequent removal of two particles. Yet when t_1 and $t_{1'}$ are later than t_2 and $t_{2'}$, the two-particle Green's function describes the disturbance produced by the addition of one particle and the removal of one particle, and the subsequent return to equilibrium by the removal of a particle and the addition of a particle. We shall make extensive use of this physical interpretation of the Green's functions.

In addition to the one-particle Green's function we define the correlation functions

$$G^{>}(1,1') = (1/i)\langle\psi(1)\psi\dagger(1')\rangle$$
$$G^{<}(1,1') = \pm(1/i)\langle\psi\dagger(1')\psi(1)\rangle \tag{1-8}$$

The notation $>$ and $<$ is intended as a reminder that for $t_1 > t_{1'}$, $G = G^{>}$, while for $t_1 < t_{1'}$, $G = G^{<}$.

1-2 THE BOUNDARY CONDITION

The time-development operator e^{-itH} bears a strong formal similarity to the weighting factor $e^{-\beta H}$ that occurs in the grand-canonical average. Indeed for $t = -i\beta$, the two are the same. We can exploit this mathematical similarity to discover identities obeyed by the Green's functions. In particular we shall now derive a fundamental relation between $G^{>}$ and $G^{<}$.

Our argument is based on the fact that the time dependence of ψ and $\psi\dagger$, given by (1-4), may be used to define the creation and annihilation operators and therefore $G^{>}$ and $G^{<}$, for complex values of their time arguments. In fact, the function $G^{>}$, which we may write as

$$G^{>}(1,1') = \frac{\mathrm{tr}\left[e^{-\beta(H-\mu N)}\, e^{it_1H}\,\psi(\mathbf{r}_1,0)\, e^{-i(t_1-t_{1'})H}\,\psi\dagger(\mathbf{r}_{1'},0)\, e^{-it_{1'}H}\right]}{i\,\mathrm{tr}\left[e^{-\beta(H-\mu N)}\right]}$$

is an analytic function for complex values of the time arguments in the region $0 > \mathrm{Im}(t_1 - t_{1'}) > -\beta$. This analyticity follows directly from the assumption that the $e^{-\beta(H-\mu N)}$ factor is sufficient to guarantee the absolute convergence of the trace for real time. Similarly $G^{<}(1,1')$ is an analytic function in the region $0 < \mathrm{Im}(t_1 - t_{1'}) < \beta$.

To derive the relation between $G^{>}$ and $G^{<}$ we notice that the expression

$$G^{<}(1,1')\big|_{t_1=0} = \pm\frac{1}{i}\,\frac{\mathrm{tr}\left[e^{-\beta(H-\mu N)}\,\psi\dagger(\mathbf{r}_{1'},t_{1'})\,\psi(\mathbf{r}_1,0)\right]}{\mathrm{tr}\left[e^{-\beta(H-\mu N)}\right]}$$

may be rearranged, using the cyclic invariance of the trace (tr AB = tr BA), to become

$$G^{<}(1,1')\big|_{t_1=0}$$
$$= \pm\frac{1}{i}\,\frac{\mathrm{tr}\left\{e^{-\beta(H-\mu N)}\left[e^{\beta(H-\mu N)}\,\psi(\mathbf{r}_1,0)\, e^{-\beta(H-\mu N)}\,\psi\dagger(\mathbf{r}_{1'},t_{1'})\right]\right\}}{\mathrm{tr}\left[e^{-\beta(H-\mu N)}\right]}$$
$$= \pm(1/i)\langle e^{\beta(H-\mu N)}\,\psi(\mathbf{r}_1,0)\, e^{-\beta(H-\mu N)}\,\psi\dagger(\mathbf{r}_{1'},t_{1'})\rangle$$

Because $\psi(\mathbf{r}_1,0)$ removes a particle, we have

$$\psi(\mathbf{r}_1,0)f(N) = f(N+1)\psi(\mathbf{r}_1,0)$$

where f(N) is any function of the number operator N. In particular,

$$e^{-\beta\mu N}\,\psi(\mathbf{r}_1,0)\, e^{\beta\mu N} = e^{\beta\mu}\,\psi(\mathbf{r}_1,0) \qquad e^{-\beta\mu(N+1)}\,\psi(1,0) = \psi(1,0)\,e^{-\beta\mu}$$

and from (1-7) it follows that

$$e^{\beta H}\,\psi(\mathbf{r}_1,0)\, e^{-\beta H} = \psi(\mathbf{r}_1,-i\beta)$$

Thus

$$G^{<}(1,1')\big|_{t_1=0} = \pm(1/i)\langle\psi(\mathbf{r}_1,-i\beta)\psi\dagger(1')\rangle\, e^{\beta\mu}$$
$$= \pm e^{\beta\mu}\, G^{>}(1,1')\big|_{t_1=-i\beta} \tag{1-9}$$

This relationship is crucial to all our Green's function analysis.

Notice that (1-9) follows directly from the cyclic invariance of the trace and the structure of the time dependence of $\psi(1)$. Since G_2 is also defined as a trace, we can go through an entirely similar analysis for it, splitting it into several non-time-ordered expectation

values of ψ's and $\psi\dagger$'s and proving a set of relations similar to (1-9). However, this analysis is much too complicated because G_2 is composed of too many different analytic pieces, corresponding to all the different possible time orderings of its four time variables.

We employ the following simple device to exhibit a relation like (1-9) for G_2. We consider the time variable to be restricted to the interval

$$0 \leq it \leq \beta$$

Equation (1-4) defines the field operators and therefore the Green's functions for imaginary times. To complete the definition of the Green's functions in this time domain, we extend the definition of the time-ordering symbol T to mean "$i \times t$" ordering when the times are imaginary. The further down the imaginary axis a time is, the "later" it is. Then the Green's functions are well defined in the interval $0 \leq it \leq \beta$. For example, the one-particle Green's function is

$$G(1,1') = G^{>}(1,1') \qquad \text{for } it_1 > it_{1'}$$

$$= G^{<}(1,1') \qquad \text{for } it_1 < it_{1'}$$

For $0 < it_{1'} < \beta$, we have

$$G(1,1')\,|_{t_1=0} = G^{<}(1,1')|_{t_1=0} \qquad (\text{since } 0 = it_1 < it_{1'} \text{ for all } t_{1'})$$

and

$$G(1,1')\,|_{t_1=-i\beta} = G^{>}(1,1')\,|_{t_1=-i\beta} \qquad (\text{since } \beta = it_1 > it_{1'} \text{ for all } t_{1'})$$

Therefore (1-9) can be restated as a relation between the values of $G(1,1')$ at the boundaries of the imaginary time domain:

$$G(1,1')\,|_{t_1=0} = \pm e^{\beta\mu} G(1,1')\,|_{t_1=-i\beta} \tag{1-10}$$

Moreover, we can see immediately that G_2 on the imaginary time axis obeys exactly this same boundary condition.

$$G_2(12,1'2')\,|_{t_1=0} = \pm e^{\beta\mu} G_2(12,1'2')\,|_{t_1=-i\beta} \tag{1-11a}$$

and also

$$G_2(12,1'2')\,|_{t_{1'}=0} = \pm e^{-\beta\mu} G_2(12,1'2')\,|_{t_{1'}=-i\beta} \tag{1-11b}$$

These boundary conditions on G and G_2 will be used over and over again in the subsequent analysis.

It is only at a later stage that we shall need the imaginary-time Green's functions. Now we shall restrict our attention to the one-particle function, for which (1-9) is a suitable representation of the boundary condition.

Because of the translational and rotational invariance of the Hamiltonian (1-2) in space and its translational invariance in time, $G^{>}$ and $G^{<}$ depend only on $|\mathbf{r}_1 - \mathbf{r}_{1'}|$ and $t_1 - t_{1'}$. When we want to emphasize that these functions depend only on the difference variables, we shall write them as $G^{>(<)}(1-1')$ or as $G^{>(<)}(|\mathbf{r}_1-\mathbf{r}_{1'}|, t_1-t_{1'})$. In terms of the difference variables, (1-9) is

$$G^{<}(\mathbf{r},t) = \pm e^{\beta\mu} G^{>}(\mathbf{r},\, t - i\beta)$$

We now introduce the Fourier transforms of $G^{>}$ and $G^{<}$, defined by

$$G^{>}(\mathbf{p},\omega) = i \int d\mathbf{r} \int_{-\infty}^{\infty} dt\; e^{-i\mathbf{p}\cdot\mathbf{r} + i\omega t}\, G^{>}(\mathbf{r},t)$$

$$G^{<}(\mathbf{p},\omega) = \pm i \int d\mathbf{r} \int_{-\infty}^{\infty} dt\; e^{-i\mathbf{p}\cdot\mathbf{r} + i\omega t}\, G^{<}(\mathbf{r},t) \tag{1-12}$$

Note the explicit factors of i and $\pm$ i that we have included here to make $G^{>}(\mathbf{p},\omega)$ and $G^{<}(\mathbf{p},\omega)$ real nonnegative quantities. Equation (1-9) then becomes the simple relationship

$$G^{<}(\mathbf{p},\omega) = e^{-\beta(\omega-\mu)}\, G^{>}(\mathbf{p},\omega) \tag{1-13}$$

It is useful to introduce the "spectral function" $A(\mathbf{p},\omega)$ defined by

$$A(\mathbf{p},\omega) = G^{>}(\mathbf{p},\omega) \mp G^{<}(\mathbf{p},\omega) \tag{1-14}$$

The boundary condition on G can then be represented by writing

$$G^{>}(\mathbf{p},\omega) = [1 \pm f(\omega)]\, A(\mathbf{p},\omega)$$

$$G^{<}(\mathbf{p},\omega) = f(\omega) A(\mathbf{p},\omega) \tag{1-15}$$

where

$$f(\omega) = 1/[e^{\beta(\omega-\mu)} \mp 1] \tag{1-16}$$

The term f can be recognized as the average occupation number in the grand-canonical ensemble of a mode with energy ω.

[The statement is, more precisely, that when the Hamiltonian can be diagonalized to the form $\Sigma_\lambda \epsilon_\lambda \psi_\lambda \dagger \psi_\lambda$ then $\psi_\lambda \dagger$ is a creation operator for a mode of the system with energy ϵ_λ. The average occupation number of the mode λ is $\langle \psi_\lambda \dagger \psi_\lambda \rangle = f(\epsilon_\lambda)$.]

From the definitions of $G^>$ and $G^<$ it follows that

$$A(\mathbf{p},\omega) = \int d\mathbf{r} \int_{-\infty}^{\infty} dt\, e^{-i\mathbf{p}\cdot\mathbf{r} + i\omega t} \langle [\psi(\mathbf{r},t)\psi\dagger(0,0) \mp \psi\dagger(0,0)\psi(\mathbf{r},t)] \rangle$$

Thus, as a consequence of the equal-time commutation relation (1-5), A satisfies the sum rule

$$\int \frac{d\omega}{2\pi} A(\mathbf{p},\omega) = \int d\mathbf{r}\, e^{-i\mathbf{p}\cdot\mathbf{r}} \langle [\psi(\mathbf{r},0)\psi\dagger(0,0) \mp \psi\dagger(0,0)\psi(\mathbf{r},0)] \rangle$$

$$= \int d\mathbf{r}\, \delta(\mathbf{r}) = 1 \qquad (1\text{-}17)$$

We can use the relations that we have just derived to find G for the trivial case of free particles, for which the Hamiltonian is

$$H_0 = \int d\mathbf{r} \frac{\nabla\psi\dagger(\mathbf{r},t)\cdot\nabla\psi(\mathbf{r},t)}{2m}$$

We notice that

$$G^<(\mathbf{p},\omega) = \int dt \frac{e^{i\omega t}}{\Omega} \langle \psi\dagger(\mathbf{p},0)\psi(\mathbf{p},t) \rangle$$

where Ω is the volume of the system and $\psi(\mathbf{p},t)$ is the spatial Fourier transform of $\psi(\mathbf{r},t)$. Since $\psi(\mathbf{p},0)$ removes a free particle with momentum $\mathbf{p}$, it must remove energy $p^2/2m$ from the system. Thus,

$$\psi(\mathbf{p},t) = e^{iHt}\psi(\mathbf{p},0)\, e^{-iHt} = e^{-i(p^2/2m)t}\psi(\mathbf{p},0)$$

so that

$$G^<(\mathbf{p},\omega) = (2\pi/\Omega)\,\delta(\omega - p^2/2m)\,\langle \psi\dagger(\mathbf{p},0)\psi(\mathbf{p},0) \rangle$$

Hence $A(\mathbf{p},\omega)$ is proportional to $\delta(\omega - p^2/2m)$, and the constant of proportionality is determined from the sum rule (1-17) to be 2π. Thus, for free particles,

$$A(\mathbf{p},\omega) = A_0(\mathbf{p},\omega) = 2\pi\,\delta(\omega - p^2/2m) \qquad (1\text{-}18)$$

$$G_0^>(\mathbf{r},t) = \int \frac{d\mathbf{p}}{(2\pi)^3} e^{i\mathbf{p}\cdot\mathbf{r} - i(p^2/2m)t} \frac{1 \pm f(p^2/2m)}{i}$$

$$G_0^<(\mathbf{r},t) = \int \frac{d\mathbf{p}}{(2\pi)^3} e^{i\mathbf{p}\cdot\mathbf{r} - i(p^2/2m)t} \frac{f(p^2/2m)}{i} \qquad (1\text{-}19)$$

Since $\psi\dagger(\mathbf{p},0)\psi(\mathbf{p},0)$ is the operator representing the density of particles with momentum $\mathbf{p}$, it follows that for free particles the average number of particles with momentum $\mathbf{p}$ is

$$\langle n(\mathbf{p}) \rangle = \frac{\langle \psi\dagger(\mathbf{p},0)\psi(\mathbf{p},0) \rangle}{\Omega} = f(p^2/2m)$$

$$= \frac{1}{e^{\beta(p^2/2m - \mu)} \mp 1} \qquad (1\text{-}20)$$

This is a result familiar from elementary statistical mechanics.

2 Information Contained in $G^>$ and $G^<$

2-1 DYNAMICAL INFORMATION

Now that we have set down the preliminaries, we shall try to gain some insight into $G^>$ and $G^<$.

The Fourier transform of the field operator $\psi(\mathbf{r},t)$, given by

$$\psi(\mathbf{p},\omega) = \int d\mathbf{r} \int dt\, e^{-i\mathbf{p}\cdot\mathbf{r}+i\omega t}\psi(\mathbf{r},t)$$

is an operator which annihilates a particle with momentum $\mathbf{p}$ and energy ω. Thus $G^<(\mathbf{p},\omega)$ can be identified as the average density of particles in the system with momentum p and energy ω:

$$G^<(\mathbf{p},\omega) = \langle n(\mathbf{p},\omega)\rangle = A(\mathbf{p},\omega)f(\omega) \tag{2-1}$$

The interpretation of this result is evident. As we have pointed out, $f(\omega)$ is the average occupation number of a mode with energy ω; the spectral function $A(\mathbf{p},\omega)$ is a weighting function with total weight unity, which whenever it is nonzero defines the spectrum of possible energies ω, for a particle with momentum $\mathbf{p}$ in the medium.

To check this result, we may note that the density of particles,

$$\langle n(\mathbf{r},t)\rangle = \langle\psi^\dagger(\mathbf{r},t)\psi(\mathbf{r},t)\rangle = \pm iG^<(\mathbf{r}t,\mathbf{r}t)$$

$$= \int \frac{d\omega}{2\pi}\frac{d\mathbf{p}}{(2\pi)^3}\, G^<(\mathbf{p},\omega) \tag{2-2}$$

This says that the total density of particles is equal to the integral over all $\mathbf{p}$ and ω of the density of particles with momentum $\mathbf{p}$ and energy ω. Since $\langle n(\mathbf{r},t)\rangle$ is independent of $\mathbf{r}$ and t, we shall represent it simply by the symbol n.

As an example, for a system of free particles,

$$A_0(\mathbf{p},\omega) = 2\pi\,\delta(\omega - p^2/2m)$$

Hence $A_0(\mathbf{p},\omega)$ is nonvanishing only when $\omega = p^2/2m$. This says that the only possible energy value for a free particle with momentum $\mathbf{p}$ is $p^2/2m$. The total density of particles with momentum $\mathbf{p}$ is

$$\langle n(\mathbf{p})\rangle = \int \frac{d\omega}{2\pi}\langle n(\mathbf{p},\omega)\rangle = f\left(\frac{p^2}{2m}\right) = \frac{1}{e^{\beta(p^2/2m-\mu)} \mp 1} \tag{2-3}$$

To see what happens in the classical limit, we explicitly write the factors of $\hbar$ in the expression for the density:

$$n = \int \frac{d\mathbf{p}}{(2\pi\hbar)^3}\,\frac{1}{e^{\beta(p^2/2m-\mu)} \mp 1} \tag{2-4}$$

In order that at a fixed temperature the density not diverge as $\hbar \to 0$, the factor $e^{-\beta\mu}$ must become very large. Thus the classical limit is given by $\beta\mu \to -\infty$. We may then neglect the ∓ 1 in the denominator of (2-3), so that the momentum distribution becomes the familiar Maxwell-Boltzmann distribution

$$\langle n(\mathbf{p})\rangle = (\text{const})\, e^{-\beta(p^2/2m)}$$

Equation (2-4) indicates that $\beta\mu \to -\infty$ is also the low-density limit.

On the other hand, for a highly degenerate (i.e., high-density) Fermi gas, $\beta\mu$ becomes very large and positive. Defining the Fermi momentum p_f by $\mu = p_f^2/2m$, we find

$$\langle n(\mathbf{p})\rangle \approx 0 \qquad \text{for } p > p_f$$

$$\approx 1 \qquad \text{for } p < p_f$$

All states with momentum $p < p_f$ are filled, and all states with $p > p_f$ are empty.

For a Bose system, μ cannot become positive, but instead it approaches zero as the density increases. Then the total density of particles with nonzero momentum cannot become arbitrarily large, but it is instead limited by

$$\int \frac{d\mathbf{p}}{(2\pi)^3}\,\frac{1}{e^{\beta(p^2/2m)} - 1} = \frac{1}{2\pi^2}\left(\frac{2m}{\beta}\right)^{3/2}\int_0^\infty \frac{x^2\,dx}{e^{x^2} - 1}$$

In order to reach a higher density, the system puts a macroscopic

number of particles into the mode $p = 0$. The mathematical possibility of this occurrence is the fact that at $\mu = 0$, $f(0) = \infty$. This phenomenon, called the Bose-Einstein condensation, is reflected in the physical world as the phase transition of He^4 to the superfluid state.

When there is an interaction between the particles, $A(\mathbf{p},\omega)$ will not be a single delta function. To see the detailed structure of A, let us compute $G^>(\mathbf{p},\omega)$ by explicitly introducing sums over states. Then $G^>(\mathbf{p},\omega)$ is

$$
\begin{aligned}
G^>(\mathbf{p},\omega) &= A(\mathbf{p},\omega)\,|\,1 \pm f(\omega)\,| \\
&= \int_{-\infty}^{\infty} dt\, \frac{e^{i\omega t}}{\Omega} \sum_i e^{-\beta(E_i - \mu N_i)} \frac{\langle i\,|\,\psi(\mathbf{p})\, e^{-iHt}\, \psi\dagger(\mathbf{p})\,|\,i\rangle}{\mathrm{tr}\left[e^{-\beta(H-\mu N)}\right]} \\
&= \frac{1}{\Omega} \sum_{i,j} e^{-\beta(E_i - \mu N_i)}\, |\langle i\,|\,\psi\dagger(\mathbf{p})\,|\,j\rangle|^2 \\
&\quad \times \frac{2\pi\,\delta(\omega + E_i - E_j)}{\mathrm{tr}\left[e^{-\beta(H-\mu N)}\right]}
\end{aligned}
\tag{2-5}
$$

It is clear then that the values of ω for which $A(\mathbf{p},\omega)$ is nonvanishing are just the possible energy differences which result from adding a single particle of momentum $\mathbf{p}$ to the system. Almost always the energy spectrum of the system is sufficiently complex so that $A(\mathbf{p},\omega)$ finally appears to have no delta functions in it but is instead a continuous function of ω. However, there are often sharp peaks in A. These sharp peaks represent coherent and long-lived excitations which behave in many ways like free or weakly interacting particles. These excitations are usually called quasi-particles.

We can notice from (2-5) that $G^>(\mathbf{p},\omega)$ is proportional to the averaged transition probability for processes in which an extra particle with momentum $\mathbf{p}$, when added to the system, increases the energy of the system by ω. This transition probability measures the density of states available for an added particle. Therefore, $G^>(p,\omega)$ is the density of states available for the addition of an extra particle with momentum $\mathbf{p}$ and energy ω.

Similarly $G^<(\mathbf{p},\omega)$ is proportional to the averaged transition probability for processes involving the removal of a particle with momentum $\mathbf{p}$, and leading to a decrease of the energy of the system by ω. Since the transition probability for the removal of a particle is just a measure of the density of particles, we again see that $G^<(\mathbf{p},\omega)$ is the density of particles with momentum $\mathbf{p}$ and energy ω. The interpretation of $G^>$ as a density of states and $G^<$ as a density of particles will be used many times in our further work.

In terms of these two transition probabilities, the boundary condition (1-12) is

$$
\frac{\text{T.P. (adding } \mathbf{p},\omega)}{\text{T.P. (removing } \mathbf{p},\omega)} = \frac{A(1 \pm f(\omega))}{Af(\omega)} = e^{\beta(\omega - \mu)} \tag{2-6}
$$

This statement, called the "detailed balancing condition," is a direct consequence of the use of an equilibrium ensemble.

2-2 STATISTICAL MECHANICAL INFORMATION CONTAINED IN G

In addition to the detailed dynamical information, G contains all possible information about the statistical mechanics of the system.

We have already seen how we can write the expectation value of the density of particles in terms of $G^<$. Similarly we can express the total energy, i.e., the expectation value of the Hamiltonian (1-2), in terms of $G^<$. To do this we must make use of the equations of motion for ψ and $\psi\dagger$. Using the equation of motion (1-3) and the commutation relations, (1-5), we see that

$$
\left(i\frac{\partial}{\partial t} + \frac{\nabla^2}{2m}\right)\psi(\mathbf{r},t) = \int d\bar{\mathbf{r}}\; v(\mathbf{r} - \bar{\mathbf{r}})\,\psi\dagger(\bar{\mathbf{r}},t)\,\psi(\bar{\mathbf{r}},t)\,\psi(\mathbf{r},t) \tag{2-7a}
$$

and

$$
\begin{aligned}
&\left(-i\frac{\partial}{\partial t'} + \frac{\nabla'^2}{2m}\right)\psi\dagger(\mathbf{r}',t') \\
&\quad = \psi\dagger(\mathbf{r}',t') \int d\bar{\mathbf{r}}'\; v(\mathbf{r}' - \bar{\mathbf{r}}')\,\psi\dagger(\bar{\mathbf{r}}',t')\,\psi(\bar{\mathbf{r}}',t')
\end{aligned}
\tag{2-7b}
$$

Therefore it follows that

$$
\begin{aligned}
&1/4 \int d\mathbf{r} \left[\left(i\frac{\partial}{\partial t} - i\frac{\partial}{\partial t'}\right)\psi\dagger(\mathbf{r},t')\,\psi(\mathbf{r},t)\right]_{t'=t} \\
&\quad = 1/4 \int d\mathbf{r} \left[\left(+\frac{\nabla^2}{2m} + \frac{\nabla'^2}{2m}\right)\psi\dagger(\mathbf{r}',t)\,\psi(\mathbf{r},t)\right]_{\mathbf{r}'=\mathbf{r}} \\
&\qquad + 1/2 \int d\mathbf{r}\, d\bar{\mathbf{r}}\; \psi\dagger(\mathbf{r},t)\,\psi\dagger(\bar{\mathbf{r}},t)\, v(\mathbf{r} - \bar{\mathbf{r}})\,\psi(\bar{\mathbf{r}},t)\,\psi(\mathbf{r},t)
\end{aligned}
\tag{2-8}
$$

The right side of (2-8) is half the kinetic energy plus all the potential energy. When we add the other half of the kinetic energy we find that

$$\langle H \rangle = 1/4 \int dr \left[\left(i \frac{\partial}{\partial t} - i \frac{\partial}{\partial t'} + \frac{\nabla \cdot \nabla'}{m} \right) \times \langle \psi^\dagger(r',t') \psi(r,t) \rangle \right]_{r'=r,\, t'=t}$$

$$= \pm \frac{i}{4} \int dr \left[\left(i \frac{\partial}{\partial t} - i \frac{\partial}{\partial t'} + \frac{\nabla \cdot \nabla'}{m} \right) G^<(rt, r't') \right]_{r'=r,\, t'=t}$$

$$= \Omega \int \frac{dp}{(2\pi)^3} \frac{d\omega}{2\pi} \frac{\omega + (p^2/2m)}{2} f(\omega) A(p,\omega) \tag{2-9}$$

where Ω is the volume of the system. Equation (2-9) is very useful for evaluating ground-state energies, specific heats, etc.

All statistical-mechanical information can be obtained from the grand partition function

$$Z_g = \mathrm{tr}\left[e^{-\beta(H - \mu N)} \right] \tag{2-10a}$$

We shall now show how we can find Z_g from G. Statistical mechanics tells us that in the limit of large volume the grand partition function is related to the pressure P by

$$Z_g = e^{\beta P \Omega} \tag{2-10b}$$

Differentiating the logarithm of Z_g with respect to μ at fixed β and Ω, we find

$$\beta\Omega \left. \frac{\partial P}{\partial \mu} \right|_{\beta\Omega} = \frac{\partial}{\partial \mu} \ln Z_g = \frac{\partial}{\partial \mu} \ln \mathrm{tr}\left[e^{-\beta(H - \mu N)} \right]$$

$$= \beta \frac{\mathrm{tr}\left[e^{-\beta(H - \mu N)} N \right]}{\mathrm{tr}\left[e^{-\beta(H - \mu N)} \right]}$$

$$= \beta \langle N \rangle$$

so that the density of particles is given by

$$n = \left. \frac{\partial P}{\partial \mu} \right|_{\beta\Omega} \tag{2-11}$$

This is a very commonly used thermodynamic identity. Since we know that, in the limit $\mu \to -\infty$, the density and the pressure both go to zero, we can integrate (2-11) to obtain

$$P(\beta,\mu) = \int_{-\infty}^{\mu} d\mu'\, n(\beta,\mu') \tag{2-12}$$

Consequently if, for a given β, we know the Green's function as a function of μ, we can calculate P and hence the partition function.

Unfortunately, the integral in (2-12) can rarely be performed explicitly. One of the few cases for which a moderately simple result emerges is for a free gas. Here

$$n(\beta,\mu) = \int \frac{dp}{(2\pi)^3} \frac{1}{e^{\beta[(p^2/2m) - \mu]} \mp 1} \tag{2-13a}$$

and hence

$$P(\beta,\mu) = \mp \frac{1}{\beta} \int \frac{dp}{(2\pi)^3} \ln \left\{ 1 \mp e^{-\beta[(p^2/2m) - \mu]} \right\} \tag{2-13b}$$

In the classical limit, $\beta\mu \to -\infty$. Then we see that

$$n = \int \frac{dp}{(2\pi)^3} e^{-\beta[(p^2/2m) - \mu]}$$

and

$$P = \beta^{-1} \int \frac{dp}{(2\pi)^3} e^{-\beta[(p^2/2m) - \mu]}$$

so that $P = \beta^{-1} n = n K_B T$. This is the well-known equation of state of an ideal gas.

There is, however, another method of constructing the grand partition function, which is very useful in practice. Let us write a coupling constant λ in front of the potential energy term in (1-2). Then

$$H = H_0 + \lambda V$$

where H_0 is the kinetic energy and V is the potential energy operator,

$$V = 1/2 \int dr\, d\bar{r}\, \psi^\dagger(r) \psi^\dagger(\bar{r}) v(|r - \bar{r}|) \psi(\bar{r}) \psi(r)$$

When we differentiate $\ln Z_g$ with respect to λ, at fixed β, μ, and Ω, we find

$$\frac{\partial}{\partial \lambda} \ln Z_g = \frac{1}{Z_g} \mathrm{tr}\left[\frac{\partial}{\partial \lambda} e^{-\beta(H_0 + \lambda V - \mu N)} \right] = -\beta \langle V \rangle \tag{2-14}$$

(We do not have to worry about the noncommutability of V with

$H_0 - \mu N$ because of the cyclic invariance of the trace.) Integrating both sides of (2-14) with respect to λ, from $\lambda = 0$ to $\lambda = 1$, we find

$$[\ln Z_g]_{\lambda=1} - [\ln Z_g]_{\lambda=0} = -\beta \int_0^1 \frac{d\lambda}{\lambda} \langle \lambda V \rangle_\lambda \tag{2-15}$$

Now $\langle \lambda V \rangle_\lambda$ is the expectation value of the potential energy, for coupling strength λ. It may be expressed in terms of $G^<$ by subtracting from (2-8) half the kinetic energy. Then

$$\langle \lambda V \rangle_\lambda = \Omega \int \frac{dp}{(2\pi)^3} \frac{d\omega}{2\pi} \frac{\omega - (p^2/2m)}{2} A_\lambda(p,\omega) f(\omega) \tag{2-16}$$

so that

$$\begin{aligned} \beta P\Omega &= [\ln Z_g]_{\lambda=1} \\ &= [\ln Z_g]_{\lambda=0} - \beta\Omega \int_0^1 \frac{d\lambda}{\lambda} \\ &\quad \times \int \frac{dp}{(2\pi)^3} \frac{d\omega}{2\pi} \frac{\omega - (p^2/2m)}{2} A_\lambda(p,\omega) f(\omega) \end{aligned} \tag{2-17}$$

The constant term, $[\ln Z_g]_{\lambda=0}$, is just $\beta P\Omega$ for free particles, which we have evaluated in (2-13b).

3 The Hartree and Hartree-Fock Approximations

3-1 EQUATIONS OF MOTION

We have seen that the one-particle Green's function contains very useful dynamic and thermodynamic information. However, to extract this information we must first develop techniques for determining G.

Our methods will be based on the equation of motion satisfied by the one-particle Green's function. This equation of motion is derived from the equation of motion (2-7a) for $\psi(1)$. From (2-7a) it follows that

$$\begin{aligned} (1/i) \langle T\left[\left(i\frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m}\right)\psi(1)\psi^\dagger(1')\right]\rangle &= \pm (1/i) \int dr_2\, v(r_1 - r_2) \langle T(\psi(1)\psi(2)\psi^\dagger(2^+)\psi^\dagger(1'))\rangle |_{t_2=t_1} \\ &= \pm i \int dr_2\, v(r_1 - r_2) G_2(12;1'2^+) |_{t_2=t_1} \end{aligned} \tag{3-1}$$

Here, the notation 2^+ is intended to serve as a reminder that the time argument of $\psi^\dagger(2)$ must be chosen to be infinitesimally larger than the time arguments of the ψ's in order that the time ordering in G_2 reproduce the order of factors that appears in (2-7a). [Since ψ's commute (or anticommute) at equal times, we do not have to worry about the time ordering of $\psi(1)$ and $\psi(2)$.]

To convert (3-1) into an equation for G we must take the time derivatives outside the T-ordering symbol. The spatial derivatives commute with the time-ordering operation, but the time derivative does not. Since T changes the time ordering when $t_1 = t_{1'}$, the difference

$$\frac{\partial}{\partial t_1} \langle T(\psi(1)\psi^\dagger(1'))\rangle - \langle T\left(\frac{\partial}{\partial t_1}\psi(1)\psi^\dagger(1')\right)\rangle$$

$T\,\psi(1)\psi^\dagger(1') = \delta(t_1 - t_{1'})\,\psi(1)\psi^\dagger(1') \pm [1 - \delta(t_1 - t_{1'})]\,\psi^\dagger(1')$

must be proportional to a delta function of $t_1 - t_{1'}$. The constant of proportionality is the discontinuity of $\langle T(\psi(1)\psi\dagger(1'))\rangle$ as t_1 passes through $t_{1'}$, i.e.,

$$\frac{\partial}{\partial t_1}\langle T(\psi(1)\psi\dagger(1'))\rangle - \langle T\left(\frac{\partial}{\partial t_1}\psi(1)\psi\dagger(1')\right)\rangle$$

$$= \delta(t_1 - t_{1'})\langle(\psi(1)\psi\dagger(1') \mp \psi\dagger(1')\psi(1))\rangle$$

$$= \delta(t_1 - t_{1'})\delta(\mathbf{r}_1 - \mathbf{r}_{1'}) = \delta(1 - 1')$$

In this way we find that (3-1) becomes an equation of motion for G:

$$\left(i\frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m}\right)G(1,1')$$

$$= \delta(1 - 1') \pm i\int d\mathbf{r}_2\, v(\mathbf{r}_1 - \mathbf{r}_2)G_2(12;1'2^+)|_{t_2=t_1} \qquad (3\text{-}2a)$$

In a similar fashion we can also write an equation of motion for G_2 involving G_3, one for G_3 involving G_4, and so on. As we shall have no need for these equations we shall not write them down.

Starting from the equation of motion of $\psi\dagger(1')$, we also derive the adjoint equation of motion,

$$\left(-i\frac{\partial}{\partial t_{1'}} + \frac{\nabla_{1'}^2}{2m}\right)G(1,1')$$

$$= \delta(1 - 1') \pm i\int d\mathbf{r}_2\, G_2(12^-;1'2)v(\mathbf{r}_2 - \mathbf{r}_{1'}) \qquad (3\text{-}2b)$$

Equations (3-2) are equally valid for the real-time and the imaginary-time Green's functions. The only difference between the two cases is that for imaginary times one has to interpret the delta function in time as being defined with respect to integrations along the imaginary time axis.

Equations (3-2a) and (3-2b) each determine G in terms of G_2. It is in general impossible to know G_2 exactly. We shall find G by making approximations for G_2 in the equations of motion (3-2).

However, even if G_2 were precisely known, (3-2) would not be sufficient to determine G unambiguously. These equations are first-order differential equations in time, and thus a single supplementary boundary condition is required to fix their solution precisely. The necessary boundary condition is, of course, condition (1-10):

$$G(1,1')|_{t_1=0} = \pm e^{\beta\mu}G(1,1')|_{t_1=-i\beta} \qquad (1\text{-}10)$$

A very natural representation of G which automatically takes the quasi-periodic boundary condition into account is to express G as a Fourier series, which we write in momentum space as

$$G(p, t - t') = \frac{1}{-i\beta}\sum_\nu e^{-iz_\nu(t-t')}G(p,z_\nu) \quad \text{for } \begin{matrix} 0 \le it \le \beta \\ 0 \le it' \le \beta \end{matrix} \qquad (3\text{-}3)$$

where $z_\nu = (\pi\nu/-i\beta) + \mu$. The sum is taken to run over all even integers for Bose statistics and over all odd integers for Fermi statistics in order to reproduce correctly the $\pm$ in the boundary condition.

The equation of motion directly determines the Fourier coefficient $G[(\pi\nu/-i\beta) + \mu]$. However we want to know the spectral weight function A. To relate G to A we invert the Fourier series (3-3):

$$G(p,z_\nu) = \int_0^{-i\beta} dt\, e^{i[(\pi\nu/-i\beta)+\mu](t-t')}G(p, t - t')$$

This integral must be independent of t' and is most simply evaluated by taking $t' = 0$. Then

$$G(p,t) = G^>(p,t) = \int\frac{d\omega}{2\pi i}e^{-i\omega t}\frac{A(p,\omega)}{1 \mp e^{-\beta(\omega-\mu)}}$$

and we find

$$G(p,z_\nu) = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi i}\int_0^{-i\beta}dt\left[e^{i[(\pi\nu/-i\beta)+\mu-\omega]t}\right]\frac{A(p,\omega)}{1 \mp e^{-\beta(\omega-\mu)}}$$

$$= \int\frac{d\omega}{2\pi}\frac{A(p,\omega)}{z_\nu - \omega} \qquad (3\text{-}4)$$

Thus, the Fourier coefficient is just the analytic function

$$G(p,z) = \int\frac{d\omega}{2\pi}\frac{A(p,\omega)}{z - \omega} \qquad (3\text{-}5)$$

evaluated at $z = z_\nu = (\pi\nu/-i\beta) + \mu$. The procedure for finding A from the Fourier coefficients is then very simple. One merely continues the Fourier coefficients—a function defined on the points $z = (\pi\nu/-i\beta) + \mu$—to an analytic function for all (nonreal) z. The unique continuation which has no essential singularity at $z = \infty$ is the function (3-5). Then, $A(p,\omega)$ is given by the discontinuity of $G(p,z)$ across the real axis, i.e.,

$$A(p,\omega) = i[G(p, \omega + i\epsilon) - G(p, \omega - i\epsilon)] \qquad (3\text{-}6)$$

since

$$\frac{1}{\omega - \omega' + i\epsilon} = P\frac{1}{\omega - \omega'} - \pi i\delta(\omega - \omega')$$

where P denotes the principal value integral and ϵ is an infinitesimal positive number.

The three concepts--equations of motion, boundary conditions, and analytic continuations--form the mathematical basis of all our techniques for determining the Green's functions.

3-2 FREE PARTICLES

Let us illustrate these methods by considering some very simple approximations for G. The most trivial example is that of free particles. Since $v = 0$, the equation of motion (3-2a) is simply

$$\left(i\frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m}\right) G(1,1') = \delta(1 - 1') \tag{3-7}$$

We multiply this equation by

$$\exp\left[-i\mathbf{p}\cdot(\mathbf{r}_1 - \mathbf{r}_{1'}) + i\left(\frac{\pi\nu}{-i\beta} + \mu\right)(t_1 - t_{1'})\right]$$

integrate over all $\mathbf{r}_1$ and all t_1 in the interval 0 to $-i\beta$. Then (3-7) becomes an equation for the Fourier coefficient,

$$\left(z_\nu - \frac{p^2}{2m}\right) G(p,z_\nu) = 1$$

Therefore,

$$G(p,z_\nu) = \frac{1}{z_\nu - (p^2/2m)} \tag{3-8a}$$

The analytic continuation of this formula is

$$G(p,z) = \frac{1}{z - (p^2/2m)} \tag{3-8b}$$

This analytic continuation involves nothing more than replacing $(\pi\nu/-i\beta) + \mu$ by the general complex variable z. The analytic continuations we shall perform will never be more complicated than this. We see directly from (3-6) and (3-8b) that

$$A_0(p,\omega) = 2\pi\delta[\omega - (p^2/2m)]$$

This by-now-familiar result expresses the fact that a free particle with momentum p can only have energy $p^2/2m$. Once we know A we know $G^>$ and $G^<$.

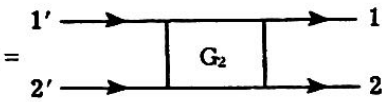
3-3 THE HARTREE APPROXIMATION

To determine G when $v \neq 0$, we must approximate the G_2 that appears in (3-2a). Approximations to G_2 can be physically motivated by the propagator interpretation of $G(1,1')$ and $G_2(12;1'2')$.

The one-particle Green's function, $G(1,1')$, represents the propagation of a particle added to the medium at 1′ and removed at 1. We can represent this pictorially by a line going from 1′ to 1:

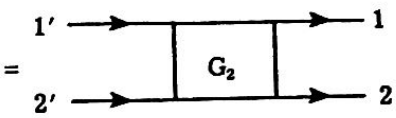
$G(1,1') =$

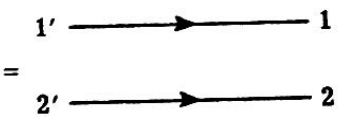
Notice that this line represents propagation through the medium, and not free-particle propagation. Sin.ilarly,

$G_2(12;1'2') =$ 

describes the propagation of two particles added to the medium at 1′ and 2′ and removed at 1 and 2. In general, the motion of the particles is correlated because the added particles interact with each other, either directly or through the intermediary of the other particles in the system.

However, as a first approximation, we may neglect this correlation and assume that the added particles propagate through the medium completely independently of each other. That is, we use the approximation

$G_2(12;1'2') =$ 

$=$ 

$= G(1,1')G(2,2')$ (3-9)

If we then substitute (3-9) into the equation of motion (3-2a), we obtain the approximate equation for G:

$$\left[i\frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} \mp i\int d\mathbf{r}_2\, v(\mathbf{r}_1 - \mathbf{r}_2)G(2,2^+)\right]G(1,1')$$

$$= \left[i\frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} - \int d\mathbf{r}_2\, v(\mathbf{r}_1 - \mathbf{r}_2)\langle n(\mathbf{r}_2)\rangle\right]G(1,1')$$

$$= \delta(1 - 1') \tag{3-10}$$

Equation (3-10) is a Green's function statement of the well-known Hartree approximation. It is the same equation as we would have obtained had we considered a set of independent particles moving through the potential field

$$\mathcal{V}(\mathbf{r}_1) = \int d\mathbf{r}_2\, v(\mathbf{r}_1 - \mathbf{r}_2)\,\langle n(\mathbf{r}_2)\rangle \tag{3-11}$$

The potential field (3-11), called the self-consistent Hartree field, is the average field generated by all the other particles in the system. Thus we see that the Hartree approximation describes the many-particle system as a set of independent particles, each particle, however, moving through the average field produced by all the particles.

For a translationally invariant system, (3-10) is quite trivial. Since $\langle n(\mathbf{r}_2)\rangle$ is independent of the position $\mathbf{r}_2$, the average potential is also constant. Letting $v = \int d\mathbf{r}\, v(\mathbf{r})$, we may write

$$\mathcal{V} = nv$$

Then, by just the same procedure as in the free-particle case, we find from (3-10) the equation for the Fourier coefficient:

$$[z_\nu - (p^2/2m) - nv]\, G(p, z_\nu) = 1$$

The continuation from the z_ν to all complex z of the Fourier coefficient is, therefore,

$$G(p,z) = \frac{1}{z - (p^2/2m) - nv} \tag{3-12}$$

so that in the Hartree approximation

$$A(p,\omega) = 2\pi\delta[\omega - (p^2/2m) - nv] \tag{3-13}$$

Thus the particles move as free particles, except that they each have the added energy nv.

To complete the solution to the Hartree approximation, we must solve for the density of particles in terms of μ, or vice versa. This can be computed from (2-2):

$$n = \pm\, iG^<(\mathbf{r}t,\mathbf{r}t) = \int \frac{d\mathbf{p}}{(2\pi)^3}\frac{d\omega}{2\pi} A(p,\omega) f(\omega) \tag{3-14}$$

which for the Hartree approximation becomes

$$n = \int \frac{d\mathbf{p}}{(2\pi)^3}\frac{d\omega}{2\pi}\frac{1}{e^{\beta[(p^2/2m) + nv - \mu]} \mp 1} \tag{3-15}$$

Similarly we find the energy per unit volume from (2-9):

$$\frac{\langle H\rangle}{\Omega} = \int \frac{d\mathbf{p}}{(2\pi)^3}\left(\frac{p^2}{2m} + \frac{nv}{2}\right)\frac{1}{e^{\beta[(p^2/2m) + nv - \mu]} \mp 1}$$

$$= (1/2)n^2 v + \int \frac{d\mathbf{p}}{(2\pi)^3}\frac{p^2/2m}{e^{\beta[(p^2/2m) + nv - \mu]} \mp 1} \tag{3-16}$$

Finally we may obtain the equation of state of a gas in the Hartree approximation. We do this for simplicity in the low-density limit. We start out by considering the effect of changing the chemical potential by an infinitesimal amount $d\mu$ at fixed temperature. Then the familiar thermodynamic identity,

$$dP = n\, d\mu \tag{3-17}$$

gives the change in the pressure. When (3-15) is taken in the low-density limit ($\beta\mu \to -\infty$), it becomes

$$n = e^{\beta(\mu - nv)} \int \frac{d\mathbf{p}}{(2\pi)^3}\, e^{-\beta(p^2/2m)}$$

Hence at fixed β,

$$dn = \beta n(d\mu - v\, dn)$$

Thus from (3-17),

$$dP = (1/\beta)\, dn + vn\, dn = K_B T\, dn + (1/2)v\, d(n^2)$$

Since at n = 0 the pressure vanishes, we find

$$P - (1/2)n^2 v = nK_B T \tag{3-18}$$

This is in the form of a van der Waals equation,

$$(P - an^2)(\Omega - \Omega_{exc}) = nK_B T$$

but without the volume-exclusion effect. For an interaction whose long-range part is attractive, v is negative, and quite reasonably the pressure is reduced from its free-particle value.

We could never hope to discover a volume-exclusion term from the Hartree approximation. Such a term arises because the particles can never penetrate each others' hard cores. However in deriving the Hartree approximation we have said that the particles move

independently, and therefore this correlation effect has been completely left out. In order to treat hard-core interactions it is necessary to include in the approximation for G_2 the fact that the motion of one particle depends on the detailed positions of the other particles in the medium.

The Hartree approximation is much less trivial when the particles are sitting in an external potential $U(\mathbf{r})$. The system for which Hartree originated his approximation was that of electrons in an atom, under the influence of the central potential of the nucleus.

The equation of motion for G in the presence of an external potential is

$$\left[i\frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} - U(\mathbf{r}_1)\right] G(1,1')$$

$$= \delta(1-1') \pm i \int v(\mathbf{r}_1 - \mathbf{r}_2) G_2(12;1'2^+)\,|_{t_2=t_1}$$

and in the Hartree approximation this reduces to

$$\left[i\frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} - U(\mathbf{r}_1) - \int d\mathbf{r}_2\, v(\mathbf{r}_1 - \mathbf{r}_2)\langle n(\mathbf{r}_2)\rangle\right] G(1,1')$$

$$= \delta(1-1') \qquad (3\text{-}19)$$

Again this equation is the same as we would have obtained had we considered independent particles in the effective potential field

$$U_{\text{eff}}(\mathbf{r}_1) = U(\mathbf{r}_1) + \int d\mathbf{r}_2\, v(\mathbf{r}_1 - \mathbf{r}_2)\langle n(\mathbf{r}_2)\rangle \qquad (3\text{-}20)$$

Since the system is no longer translationally invariant we cannot consider $\langle n\rangle$ or U_{eff} to be independent of position, and the equation cannot be diagonalized by Fourier transforming in space. It can, however, be diagonalized on the basis of normalized eigenfunctions, $\varphi_i(\mathbf{r})$, of the effective single particle Hamiltonian, $H_1(\mathbf{r}) = (-\nabla^2/2m) + U_{\text{eff}}(\mathbf{r})$:

$$H_1(\mathbf{r})\varphi_i(\mathbf{r}) = E_i\varphi_i(\mathbf{r}) \qquad (3\text{-}21)$$

The procedure for solving the equation is to first take Fourier coefficients of the equation of motion, finding

$$[z_\nu - H_1(\mathbf{r})]\,G(\mathbf{r},\mathbf{r}',z_\nu) = \delta(\mathbf{r}-\mathbf{r}') \qquad (3\text{-}22)$$

so that in terms of the φ_i,

$$G(\mathbf{r},\mathbf{r}',z_\nu) = \sum_i \frac{\varphi_i(\mathbf{r})\varphi_i^*(\mathbf{r}')}{z_\nu - E_i}$$

Hence

$$A(\mathbf{r},\mathbf{r}',\omega) = 2\pi \sum_i \varphi_i(\mathbf{r})\varphi_i^*(\mathbf{r}')\,\delta(\omega - E_i) \qquad (3\text{-}23)$$

We see that the single-particle Hamiltonian H_1 defines both the single-particle energies and wave functions of the particles in the system.

Once more, to complete the solution we have to compute the density, since this determines U_{eff}. We have

$$\langle n(\mathbf{r},t)\rangle = \int \frac{d\omega}{2\pi} A(\mathbf{r},\mathbf{r},\omega) f(\omega)$$

$$= \sum_i |\varphi_i(\mathbf{r})|^2 f(E_i) \qquad (3\text{-}24)$$

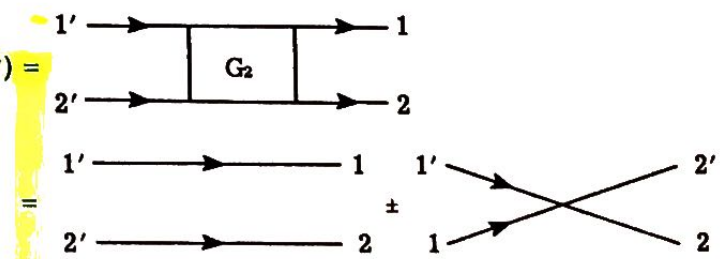
The term $f(E_i)$ gives the average occupation of the i-th single-particle level, while $|\varphi_i(\mathbf{r})|^2$ is obviously the probability of observing at $\mathbf{r}$ a particle in the i-th level.

Notice that to determine $\varphi_i(\mathbf{r})$ it is necessary to solve a nonlinear equation, since $H_1(\mathbf{r})$ itself depends on all the φ_i through its dependence on the density. The process of solving this nonlinear equation is called obtaining a "self-consistent" Hartree solution.

3-4 THE HARTREE-FOCK APPROXIMATION

The Hartree approximation (3-9) for the two-particle Green's function does not take into account the identity of the particles. Since the particles are identical, we cannot distinguish processes in which the particle added at 1′ appears at 1 from processes in which it appears at 2. These processes contribute coherently. To include this possibility of exchange, we can write

$G_2(12;1'2') =$



$$= G(1,1')G(2,2') \pm G(1,2')G(2,1') \qquad (3\text{-}25)$$

This approximation to G_2 leads to the Hartree-Fock approximation. In fixing the relative signs of the two terms in (3-25) we use the fact that $G_2(12;1'2') = \pm G_2(21;1'2')$. This symmetry can

be verified directly from the definition of G_s, (1-7b).

The approximate equation for G resulting from substituting (3-25) into (3-2a) takes the form

$$\left(i\frac{\partial}{\partial t_1} + \frac{\nabla^2}{2m}\right) G(1,1') \mp i\int dr_2 \langle r_1 | \mathcal{V} | r_2 \rangle G(2,1')\Big|_{t_2=t_1}$$

$$= \delta(1-1') \tag{3-26}$$

where

$$\langle r_1 | \mathcal{V} | r_2 \rangle = \delta(r_1 - r_2) \int dr_3\, v(r_1 - r_3) \langle n(r_3) \rangle$$

$$\pm\, iv(r_1 - r_2) G^<(1,2)\Big|_{t_2=t_1} \tag{3-27}$$

again has the interpretation of an average, self-consistent potential field through which the particles move. However, with the inclusion of exchange, $\mathcal{V}$ becomes nonlocal in space.

In the case of a translationally invariant system, we can Fourier-transform (3-26) and (3-27) in space to obtain

$$\left[i\frac{\partial}{\partial t_1} - E(p)\right] G(p, t_1 - t_{1'}) = \delta(t_1 - t_{1'}) \tag{3-28}$$

and

$$E(p) = \frac{p^2}{2m} + nv \pm \int \frac{dp'}{(2\pi)^3}\, v(p - p') \langle n(p') \rangle \tag{3-29}$$

where $v(p) = \int dr\, e^{-ip\cdot r} v(r)$ is the Fourier transform of the potential $v(r)$. Just as before,

$$A(p,\omega) = 2\pi\, \delta(\omega - E(p)) \tag{3-30}$$

so that

$$\langle n(p) \rangle = f(E(p)) = \frac{1}{e^{\beta[E(p) - \mu]} \mp 1} \tag{3-31}$$

The Hartree-Fock single-particle energy E(p) must then be obtained as the solution of (3-29) and (3-31).

To sum up: Both the Hartree and the Hartree-Fock approximations are derived by assuming that there is no correlation between the motion of two particles added to the medium. Thus, these approximations describe the particles as moving independently through an average potential field. The particles then find themselves in perfectly stable single-particle states. There is no possibility for collisions and indeed no mechanism at all for particles moving from one single-particle state to another.

In Chapter 4 we describe a way of introducing the effect of collisions into our Green's function analysis.

This result indicates a close correspondence between our Born collision approximation and the results of an analysis based on a Boltzmann equation with Born approximation collision cross sections. We shall later use a generalization of the Born collision approximation for G to derive this Boltzmann equation.

5 A Technique for Deriving Green's Function Approximations

Up to now we have written approximations for G by relying on the propagator interpretations of G and of the G_2 that appears in the equation of motion for G. We have thus been able to write a few simple approximations for G_2 in terms of the processes that we wished to consider. However, physical intuition can take us just so far. The use of purely imaginary times makes a direct interpretation of these equations difficult. Furthermore it is hard to find physical ways of determining the numerical factors that appear in front of the various terms in the expansion of G_2. We therefore seek a systematic way of deriving approximations for G.

As a purely formal device, we define a generalization of the one-particle Green's function in the imaginary time interval $[0,-i\beta]$:

$$G(1,1';U) = \frac{1}{i}\,\frac{\langle T[S\psi(1)\psi^\dagger(1')]\rangle}{\langle T[S]\rangle} \tag{5-1}$$

Here T means imaginary time ordering and the operator S is given by

$$S = \exp\left[-i\int_0^{-i\beta} d2\; U(2)n(2)\right] \tag{5-2}$$

$n(2) = \psi^\dagger(2)\psi(2)$ and U(2) is a function of space and times in the interval‡ $[0,-i\beta]$.

‡We may regard G(1,1′;U) as a one-particle Green's function, written in the interaction representation, for the system developing in imaginary time in the presence of the scalar potential U. This potential is represented by adding a term $\int dr\; U(r,t)n(r,t)$ to the Hamiltonian. In the interaction representation, all the U dependence

One reason that the Green's function (5-1) is convenient to use is that it satisfies the same boundary condition,

$$G(1,1';U)\,|_{t_1=0} = \pm\, e^{\beta\mu} G(1,1';U)\,|_{t_1=-i\beta} \tag{5-3}$$

as the equilibrium Green's function. The derivation of this boundary condition for G(U) is essentially the same as for the equilibrium functions. The time 0 is the earliest possible time, so that

$$G(1,1';U)\,|_{t_1=0} = \pm\, \frac{1}{i}\, \frac{\langle T[S\psi\dagger(1')]\,\psi(r_1,0)\rangle}{\langle T[S]\rangle}$$

Since the time $-i\beta$ is the latest possible time,

$$G(1,1';U)\,|_{t_1=-i\beta} = \frac{1}{i}\, \frac{\langle \psi(r_1,-i\beta)\, T[S\psi\dagger(1')]\rangle}{\langle T[S]\rangle}$$

The cyclic invariance of the trace that defines the expectation values then implies (5-3).

Another reason this Green's function is convenient is that it obeys equations of motion quite similar to those obeyed by the equilibrium function G. These are

$$\left[i\frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} - U(1)\right] G(1,1';U) = \delta(1-1')$$

$$\pm\, i \int dr_2\, v(r_1 - r_2)\, G_2(12,1'2^+;U)\,|_{t_2=t_1} \tag{5-4a}$$

and

$$\left[-i\frac{\partial}{\partial t_{1'}} + \frac{\nabla_{1'}^2}{2m} - U(1')\right] G(1,1';U) = \delta(1-1')$$

$$\mp\, i \int dr_2\, v(r_2 - r_{1'})\, G_2(12^-,1'2;U)\,|_{t_2=t_1} \tag{5-4b}$$

where

$$G_2(12,1'2';U) = \left(\frac{1}{i}\right)^2 \frac{\langle T[S\psi(1)\psi(2)\psi\dagger(2')\psi\dagger(1')]\rangle}{\langle T[S]\rangle} \tag{5-5}$$

We derive (5-4) in exactly the same way as the equations of motion for the equilibrium function $G(1-1')$. The only new feature is the appearance of the terms UG. To see the origin of these terms, consider, for example,

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is explicit in the S factor, and the field operators are the same as in the absence of the potential.

$$T[S\psi(1)] = T\left\{\exp\left[-i\int_{t_1}^{-i\beta} d2\; U(2)n(2)\right]\right\}$$
$$\times\; \psi(1)T\left\{\exp\left[-i\int_0^{t_1} d2\; U(2)n(2)\right]\right\}$$

Then

$$i\frac{\partial}{\partial t_1}\, T[S\psi(1)] = T\left\{\exp\left[-i\int_{t_1}^{-i\beta} d2\; U(2)n(2)\right]\right\}$$
$$\times\left\{i\frac{\partial\psi(1)}{\partial t_1} + \int dr_2\; U(r_2,t_1)[\psi(1),\, n(r_2,t_1)]\right\}$$
$$\times\; T\left\{\exp\left[-i\int_0^{-i\beta} d2\; U(2)n(2)\right]\right\}$$

Since from (1-5)

$$[\psi(r_1,t_1),\, n(r_2,t_1)] = \delta(r_1 - r_2)\,\psi(r_1,t_1)$$

it follows that

$$i\frac{\partial}{\partial t_1}\,[T(S\psi(1))] = T\left[Si\frac{\partial\psi(1)}{\partial t_1}\right] + T[S\psi(1)]\,U(1) \tag{5-6}$$

Such a calculation is the source of the UG term in (5-4a).

So far we have only succeeded in making things more complicated. We shall learn something by considering the change in G(U) resulting from an infinitesimal change in U. We let

$$U(2) \to U(2) + \delta U(2) \tag{5-7}$$

The change in G resulting from this change in U is

$$\delta G(1,1';U) = \delta\left\{\frac{1}{i}\,\frac{\langle T[S\psi(1)\psi\dagger(1')]\rangle}{\langle T[S]\rangle}\right\} = \frac{1}{i}\left[\frac{\langle T[\delta S\psi(1)\psi\dagger(1')]\rangle}{\langle T[S]\rangle}\right.$$
$$\left. - \frac{\langle T[\delta S]\rangle}{\langle T[S]\rangle}\,\frac{\langle T[S\psi(1)\psi\dagger(1')]\rangle}{\langle T[S]\rangle}\right] \tag{5-8}$$

When δS appears in a time-ordered product, it can be evaluated as

$$\delta S = \delta\left\{\exp\left[-i\int_0^{-i\beta} d2\; U(2)n(2)\right]\right\} = S\frac{1}{i}\int_0^{-i\beta} d2\; \delta U(2)n(2) \tag{5-9}$$

since the T's automatically provide the proper (imaginary) time ordering. On substituting (5-9) into (5-8) we find

$$\delta G(1,1';U) = \int_0^{-i\beta} d2 \left\{ \frac{\langle T[S\psi(1)\psi^\dagger(1')n(2)]\rangle}{i^2\langle T[S]\rangle} - \frac{\langle T[S\psi(1)\psi^\dagger(1')]\rangle}{i\langle T[S]\rangle} \frac{\langle T[Sn(2)]\rangle}{i\langle T[S]\rangle} \right\} \delta U(2)$$

$$= \pm \int_0^{-i\beta} d2 \left[G_2(12,1'2^+;U) - G(1,1';U)\, G(2,2^+;U) \right] \delta U(2) \qquad (5\text{-}10)$$

Since this calculation of δG is just a generalization of the method by which one obtains an ordinary derivative, we call the coefficient of $\delta U(2)$ in (5-10) the functional derivative, or variational derivative, of $G(1,1';U)$ with respect to $U(2)$. It is denoted by $\delta G(1,1';U)/\delta U(2)$, so that

$$\frac{\delta G(1,1';U)}{\delta U(2)} = \pm \left[G_2(12,1'2^+;U) - G(1,1';U)\, G(2,2^+;U) \right] \qquad (5\text{-}11)$$

We may therefore express the G_2 that appears in the equation of motion (5-4) for G in terms of $\delta G/\delta U$. This equation then becomes

$$\left\{ i\frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} - U(1) \mp i \int dr_2\, v(r_1 - r_2) \left[G(r_2 t_1, r_2 t_1^+;U) + \frac{\delta}{\delta U(r_2, t_1^+)} \right] \right\} G(1,1';U) = \delta(1-1') \qquad (5\text{-}12)$$

The Green's function G(U) is thus determined by a single functional differential equation.

Unfortunately there exist no practical techniques for solving such functional differential equations exactly. Equation (5-12) may be used, however, to generate approximate equations for G. We shall begin our discussion by using (5-12) to derive the beginnings of a perturbative expansion of G(U) in a power series in v.

5-1 ORDINARY PERTURBATION THEORY

If there is no interaction between the particles, G(U) is determined by the equation

$$\left[i\frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} - U(1) \right] G_0(1,1';U) = \delta(1-1') \qquad (5\text{-}13)$$

together with the boundary condition (5-3). The function $G_0(1,1';U)$ may be used to convert (5-12) into an integral equation:

$$G(1,1';U) = G_0(1,1';U) \pm i \int_0^{-i\beta} d\bar{1}\, d\bar{2}\, G_0(1,\bar{1};U)\, V(\bar{1}-\bar{2}) \times \left[G(\bar{2},\bar{2}^+;U) + \frac{\delta}{\delta U(\bar{2})} \right] G(\bar{1},1';U) \qquad (5\text{-}14)$$

We have introduced the notation

$$V(1-1') = v(|r_1 - r_{1'}|)\, \delta(t_1 - t_{1'}) \qquad (5\text{-}15)$$

By applying $[i(\partial/\partial t_1) + (\nabla_1^2/2m) - U(1)]$ to (5-14) one can verify that (5-14) is a solution to (5-12). To see that it satisfies the boundary condition (5-3), we observe that

$$G(1,1';U)\big|_{t_1=0} = G_0(1,1';U)\big|_{t_1=0} + \int_0^{-i\beta} d\bar{1}\, G_0(1,\bar{1};U)\big|_{t_1=0} \cdots$$

$$= \pm e^{\beta\mu} \left[G_0(1,1';U)\big|_{t_1=-i\beta} + \int_0^{-i\beta} d\bar{1}\, G_0(1,\bar{1};U)\big|_{t_1=-i\beta} \cdots \right]$$

$$= \pm e^{\beta\mu} G(1,1';U)\big|_{t_1=-i\beta}$$

Notice that (5-14) contains time integrals from 0 to $-i\beta$. This is the ultimate origin of the appearance of such integrals in the Born collision approximation.

To expand G(U) in a power series in V, we need only successively iterate (5-14). To zeroth order $G = G_0$. The first-order term is obtained by substituting $G = G_0$ into the right side of (5-14). Then to first order in V:

$$G(1,1';U) = G_0(1,1';U) \pm i \int_0^{-i\beta} d\bar{1}\, d\bar{2}\, G_0(1,\bar{1};U)\, V(\bar{1}-\bar{2}) \times \left[G_0(\bar{2},\bar{2}^+;U) + \frac{\delta}{\delta U(\bar{2})} \right] G_0(\bar{1},1';U) \qquad (5\text{-}16)$$

We then must compute $(\delta/\delta U(2))G_0(1,1';U)$. Perhaps the simplest way of finding this derivative is to regard $G_0(1,1';U)$ as a matrix in the variables 1 and 1'. The inverse of this matrix, defined by

$$\int_0^{-i\beta} d\bar{1}\; G_0^{-1}(1,\bar{1};U)\, G_0(\bar{1},1';U) = \delta(1-1')$$

is, from (5-13), just

$$G_0^{-1}(1,1';U) = \left[i\frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} - U(1)\right]\delta(1-1') \tag{5-17}$$

Varying both sides of the matrix equation $G_0^{-1}G_0 = 1$ with respect to U implies

$$\delta[G_0^{-1}G_0] = \delta G_0^{-1}G_0 + G_0^{-1}\delta G_0 = 0$$

or

$$\delta G_0 = -G_0\,\delta G_0^{-1} G_0$$

Thus, using (5-17)

$$\frac{\delta G_0(1,1')}{\delta U(2)} = -\int_0^{-i\beta} d3\; d3'\; G_0(1,3)\left[\frac{\delta G_0^{-1}(3,3';0)}{\delta U(2)}\right] G_0(3',1')$$

$$= \int_0^{-i\beta} d3\; G_0(1,3)\,\frac{\delta U(3)}{\delta U(2)}\, G_0(3,1')$$

$$= G_0(1,2)\, G_0(2,1') \tag{5-18}$$

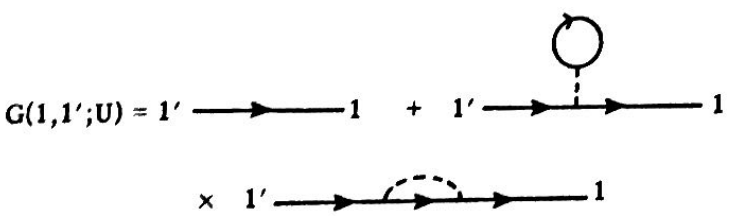
since $\delta U(3)/\delta U(2) = \delta(3-2)$. Substituting (5-18) into (5-16) we find that to first order in V,

$$G(1,1';U) = G_0(1,1';U) \pm i\int_0^{-i\beta} d\bar{1}\; d\bar{2}\; G_0(1,\bar{1};U)\, V(\bar{1}-\bar{2})$$

$$\times\,[G_0(\bar{2},\bar{2}^+;U)\, G_0(\bar{1},1';U)$$

$$\pm\; G_0(\bar{1},\bar{2}^+;U)\, G_0(\bar{2},1';U)] \tag{5-19}$$

We represent this pictorially as



where the lines signify G_0. When U is set equal to zero we have the expansion of $G(1-1')$ to first order in V.

It is instructive to compare this first-order result with the Hartree-Fock approximation, which may be written as

$$\left(i\frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m}\right) G(1-1') = \delta(1-1') \pm i\int_0^{-i\beta} d\bar{2}\; V(\bar{1}-\bar{2})$$

$$\times\,[G(\bar{2}-\bar{2}^+)G(1-1') \pm G(1-\bar{2}^+)G(\bar{2}-1')]$$

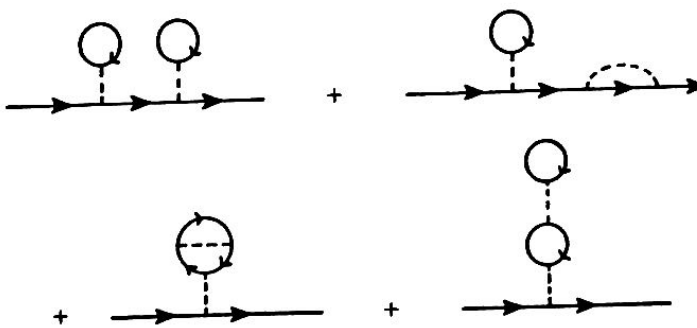
Then

$$G(1-1') = G_0(1-1') \pm i\int_0^{-i\beta} d\bar{1}\; d\bar{2}\; G_0(1-\bar{1})\, V(\bar{1}-\bar{2})$$

$$\times\,[G(\bar{2}-\bar{2}^+)G(\bar{1}-1') \pm G(\bar{1}-\bar{2}^+)G(\bar{2}-1')] \tag{5-20}$$

The first-order solution (5-19) is equivalent to the Hartree-Fock solution expanded to first order in V.

To obtain higher-order terms in V, we substitute (5-19) back into (5-14), and again use (5-18). The GG term gives the second-order contributions



(5-21a)

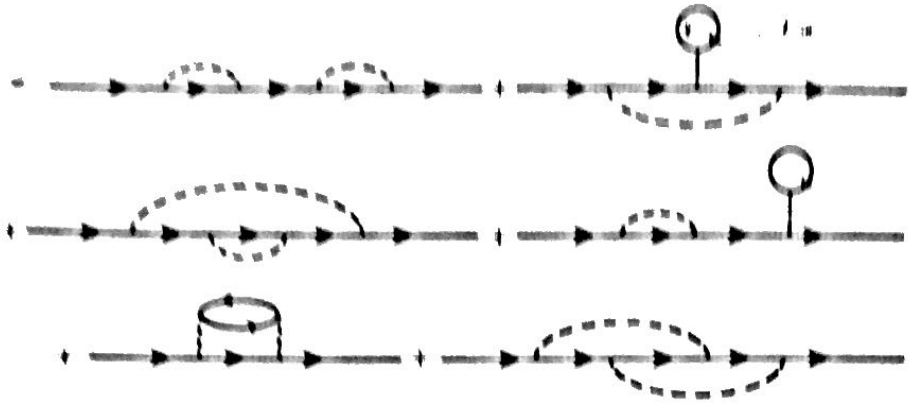
while the second-order contribution from $\delta G/\delta U$ is

$$i\int_0^{-i\beta} d\bar{1}\; d\bar{2}\; G_0(1,\bar{1};U)\, V(\bar{1}-\bar{2})\,\frac{\delta}{\delta U(\bar{2})}$$

$$\times\,\{\pm\, i\int d\bar{3}\; d\bar{4}\; G_0(\bar{1},\bar{3};U)\, V(\bar{3}-\bar{4})$$

$$\times\,[G_0(\bar{4},\bar{4}^+;U)\, G_0(\bar{3}\,1';U)$$

$$\pm\; G_0(\bar{3},\bar{4}^+;U)\, G_0(\bar{3},1';U)]\} \tag{5-21b}$$



All the terms in (5-21a) and the first four terms in (5-21b) arise from an iteration of the Hartree-Fock equation. However, the last two terms do not appear in the Hartree-Fock equation, but are instead the lowest-order contributions of the collision terms in the Born collision approximation. In the appendix we consider this expansion in more detail.

One can iterate further and expand G to arbitrarily high order in V. The general structure of G is given by drawing all topologically different connected diagrams.

We should point out that there are very few situations in which this expansion converges rapidly. Usually the potential is sufficiently large so that the first few orders of perturbation theory give a very poor answer. Furthermore, physical effects such as the $e^{-\Gamma(t-t')}$ behavior of G and the single-particle energy shift cannot appear in finite order in this expansion. Instead, one would find $e^{-\Gamma(t-t')}$ replaced by its power-series expansion

$$1 - \Gamma(t-t') + (1/2)\Gamma^2(t-t')^2 + \cdots$$

which converges slowly for large time differences.

5-2 EXPANSION OF Σ IN V AND G_0

The difficulties of the expansion of G in powers of V may be avoided by either summing infinite classes of terms in the expansion, or equivalently by expanding the self-energy $\Sigma(1,1';U)$ in terms of V. We recall that Σ is defined by

$$\left(i\frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m}\right) G(1-1') - \int_0^{-i\beta} d\bar{1}\ \Sigma(1-\bar{1})\, G(\bar{1}-1') = \delta(1-1') \tag{5-22}$$

in the equilibrium case. In the presence of U we define Σ by the equation

$$\int_0^{-i\beta} d\bar{1}\ [G_0^{-1}(1,\bar{1};U) - \Sigma(1,\bar{1};U)]\, G(\bar{1},1';U) = \delta(1-1') \tag{5-23}$$

If we define the matrix inverse of G by the equation

$$\int_0^{-i\beta} d\bar{1}\ G^{-1}(1,\bar{1};U)\, G(\bar{1},1';U) = \delta(1-1')$$

it is clear that

$$G^{-1}(1,1';U) = G_0^{-1}(1,1';U) - \Sigma(1,1';U) \tag{5-24}$$

To find $\Sigma(U)$, we matrix multiply (5-12) on the right by G^{-1}. Then

$$G^{-1}(1,1';U) = G_0^{-1}(1,1';U) + i\int_0^{-i\beta} d\bar{2}\ V(\bar{1}-\bar{2})\, G(\bar{2},\bar{2}^+)\,\delta(1-1') - i\int_0^{-i\beta} d\bar{2}\, d\bar{1}\ V(1-\bar{2})\left[\frac{\delta G(1,\bar{1};U)}{\delta U(\bar{2})}\right] \times G^{-1}(\bar{1},1';U) \tag{5-24a}$$

so that

$$\Sigma(1,1';U) = \pm i\int d\bar{2}\ V(1-\bar{2})\, G(\bar{2},\bar{2}^+;U)\,\delta(1-1') + i\int d\bar{2}\, d\bar{1}\ V(1-\bar{2})\left[\frac{\delta G(1,\bar{1};U)}{\delta U(\bar{2})}\right] \times G^{-1}(\bar{1},1';U) \tag{5-25a}$$

Using $\delta G \cdot G^{-1} + G\delta G^{-1} = 0$, we find

$$\int_0^{-i\beta} d\bar{1}\left[\frac{\delta G(1,\bar{1};U)}{\delta U(2)}\right] G^{-1}(\bar{1},1';U) = -\int d\bar{1}\ G(1,\bar{1};U)\,\frac{\delta}{\delta U(2)} \times [G_0^{-1}(\bar{1},1';U) - \Sigma(\bar{1},1';U)]$$

$$= G(1,1')\,\delta(2-1') + \int_0^{-i\beta} d\bar{1}\ G(1,\bar{1};U)\,\frac{\delta\Sigma(\bar{1},1';U)}{\delta U(2)}$$

Hence (5-25a) for Σ becomes

$$\Sigma(1,1';U) = \delta(1-1')[\pm i \int d\bar{2}\, V(1-\bar{2})\, G(\bar{2},\bar{2}^+;U)]$$
$$+ iV(1-1')\, G(1,1';U) + i \int d\bar{1}\, d\bar{2}\, V(1-\bar{2})$$
$$\times\, G(1,\bar{1};U)\, \frac{\delta\Sigma(\bar{1},1';U)}{\delta U(\bar{2})} \qquad (5\text{-}25b)$$

This latter equation is very useful for deriving the expansion of Σ in a power series in G_0 and V. To lowest order in V,

$$\Sigma(1,1';U) = \pm i\,\delta(1-1') \int d\bar{2}\, V(1-\bar{2})\, G_0(\bar{2},\bar{2}^+;U)$$
$$+ i\,V(1-1')\, G_0(1,1';U) \qquad (5\text{-}26)$$

This is clearly just the lowest-order approximation to the Hartree-Fock self-energy. The second-order result for Σ is obtained by taking the Hartree-Fock terms in (5-25b) to first order in G, using (5-19). The more interesting second-order terms in Σ result from $\delta\Sigma/\delta U$. To lowest order these terms are

(5-27)

where the lines signify G_0's. Expression (5-27) is just the lowest-order evaluation of the collision term in the Born collision approximation self-energy.

5-3 EXPANSION OF Σ IN V AND G

In the calculations in previous chapters, we have expanded Σ in V and G instead of V and G_0. The primary reason for doing this is that G has a simple physical interpretation, while the physical significance of G_0 in an interacting system is far from clear. We shall therefore indicate how successive iteration of (5-25b) leads to such an expansion in G and V.

The Hartree approximation is derived by neglecting $\delta G/\delta U$ in (5-25a). The Hartree-Fock approximation is derived by neglecting $\delta\Sigma/\delta U$ in (5-25b). This approximation is the first term in the systematic expansion of Σ in a series in V and G:

$$\Sigma_{HF}(1,1';U) = \pm i \int d\bar{2}\, V(1-\bar{2})\, G(\bar{2},\bar{2}^+;U)\, \delta(1-1')$$
$$+ iV(1-1')\, G(1,1';U)$$

The next term comes from approximating $\delta\Sigma/\delta U$ by $\delta\Sigma_{HF}/\delta U$ in (5-25b). Then (5-25b) becomes

$$\Sigma(1,1';U) = \Sigma_{HF}(1,1';U) \pm i^2 \int_0^{-i\beta} d\bar{1}\, d\bar{2}\, V(1-\bar{2})\, G(1,\bar{1};U)$$
$$\times \frac{\delta}{\delta U(\bar{2})} \Big[\int d\bar{3}\, V(\bar{1}-\bar{3})\, G(\bar{3},\bar{3}^-;U)\, \delta(\bar{1}-1')$$
$$\pm V(\bar{1}-1')\, G(\bar{1},1';U) \Big]$$

However, $\delta G = -G \cdot \delta G^{-1} \cdot G$, so that to lowest order,

$$\frac{\delta G(1,1';U)}{\delta U(2)} = G(1,2)\, G(2,1')$$

Therefore, we find to second order in V,

$$\Sigma(1,1';U) - \Sigma_{HF}(1,1';U)$$
$$= \pm i^2 \int d\bar{2}\, d\bar{3}\, V(1-\bar{2})\, V(\bar{3}-1')[G(1,1';U)\, G(\bar{3},\bar{2};U)\, G(\bar{2},\bar{3};U)$$
$$\pm G(1,\bar{3};U)\, G(\bar{3},\bar{2};U)\, G(\bar{2},1';U)]$$

=

(5-28)

where the lines represent G's. Equation (5-28), when U is set equal to zero, is the Born collision approximation.

1. $G_{3/2}$: 1h □
2. Bellaev : 1h •
3. Correzione moto + HF : 2h □
4. Energia : 2h □
5. QBE : 3h

$$\delta n(R,T) = e^{ik\cdot R} U_k \int_{-\infty}^{T} dT' \, \frac{\delta n}{\delta U}(k, T - T') \, e^{\zeta T'}$$

$$\times \int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} \frac{e^{-i\omega T'}}{\omega - i\epsilon}$$

$$= e^{ik\cdot R} U_k \int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} \frac{e^{-i(\omega + i\zeta)T}}{\omega - i\epsilon}$$

$$\times \int_{-\infty}^{0} dT' \, e^{-i(\omega + i\zeta)T'} \frac{\delta n}{\delta U}(k, -T')$$

$$= e^{ik\cdot R} U_k \int_{-\infty + i\zeta}^{\infty + i\zeta} \frac{d\Omega}{2\pi i} \frac{e^{-i\Omega T}}{\Omega - i(\zeta + \epsilon)} \frac{\delta n}{\delta U}(k, \Omega)$$

$$= e^{ik\cdot R} U_k \int_{-\infty + i\zeta}^{\infty + i\zeta} \frac{d\Omega}{2\pi i} \frac{e^{-i\Omega T}}{\Omega - i(\zeta + \epsilon)} \left(\frac{\delta n}{\delta U}\right)_0 (k, \Omega) \, K(k, \Omega)$$

Suppose that K has the pole in the upper half-plane at $\Omega = \Omega_c$, but is otherwise analytic in the upper half-plane. Then, since $\zeta > -i\Omega_c$, $\Rightarrow \Omega - i(\zeta + \epsilon)$ $< \Omega_c + i\epsilon$ we can write the Ω integral as a loop around the pole and an integral from $-\infty$ to ∞ just above the real axis. The contribution to δn from the pole is therefore

$$e^{ik\cdot R} \; e^{-i\Omega_c T} \, (-2\pi i) \, (\text{residue at } \Omega_c)$$

This term increases exponentially in time, which would seem to indicate that the potential U has excited an unstable density fluctuation. It really implies that the random phase approximation is unable to describe the system (except for very short times), and that there are physical processes occurring in the system that call for a better mathematical approximation. The appearance of the pole in the upper half-plane has been suggested as a way of seeing dynamically that the collection of particles with attractive interactions has undergone a transition from a gas to a liquid.†

Later we shall see a similar instability occurring in fermion systems with an attractive short-range interaction. The onset of this instability represents the transition to a "superconducting" phase.

† N. D. Mermin, doctoral thesis, Harvard University, 1961.

8 Relation between Real and Imaginary Time Response Functions

In the last chapter we used the Hartree approximation to describe nonequilibrium phenomena. Unfortunately, we cannot directly write more complicated approximations in the real time domain because we have no simple boundary conditions that can act as a guide in determining $g_2(U)$. Therefore, we have, at this stage, no complete theory for determining the physical response function g(U). [As we saw in Chapter 4, simple physical arguments do not suffice to determine approximations for the two-particle Green's function; it is necessary to use the boundary conditions to determine the range of the time integrations in, e.g., (4-6) and (4-7).]

In Chapter 5 we developed a theory for approximating Σ and therefore $G_2(U)$ in the imaginary time domain. Now we shall discuss the relationship between g(U), the physical response function, and G(U), the imaginary time response function, and show how the theory already developed suffices to determine g(U).

8-1 LINEAR RESPONSE

There is a particularly simple relation between the linear responses of the density in the two time domains. In the imaginary time domain,

$$\frac{\delta G(1,1';U)}{\delta U(2)} = \hbar \, [G_2(12,1'2^+) - G(1,1')G(2,2^+)]$$

Hence the response of the density can be written

$$\hbar i \, \frac{\delta G(1,1^+;U)}{\delta U(2)} = i \, [G_2(12,1^+2^+) - G(1,1^+)G(2,2^+)]$$

$$= \frac{1}{i} \, [\langle T(n(1)n(2))\rangle - \langle n\rangle\langle n\rangle] \qquad (8\text{-}1)$$

In discussing this response it is convenient to define

$$L(1-2) = \pm i \left[\frac{\delta G(1,1^+;U)}{\delta U(2)}\right]_{U=0}$$

$$= \frac{1}{i} \langle T[(n(1) - \langle n\rangle)(n(2) - \langle n\rangle)]\rangle \qquad (8\text{-}2)$$

We should notice that $L(1-2)$ is quite analogous in structure to the one-particle Green's function. Just as $G(1-1')$ is composed of the two analytic functions of time $G^>(1-1')$ and $G^<(1-1')$, so

$$L(1-2) = L^>(1-2) \qquad \text{for } t_1 > t_2$$
$$= L^<(1-2) \qquad \text{for } t_1 < t_2 \qquad (8\text{-}2a)$$

where

$$L^>(1-2) = \frac{1}{i} \langle [n(1) - \langle n\rangle][n(2) - \langle n\rangle]\rangle$$

$$L^<(1-2) = \frac{1}{i} \langle [n(2) - \langle n\rangle][n(1) - \langle n\rangle]\rangle \qquad (8\text{-}2b)$$

As G satisfies the boundary condition,

$$G(1-1')|_{t_1=0} = \pm e^{\beta\mu} G(1-1')|_{t_1=-i\beta}$$

so $L(1-2)$ satisfies the boundary condition

$$L(1-2)|_{t_1=0} = L(1-2)|_{t_1=-i\beta} \qquad (8\text{-}3)$$

Therefore, L can also be written in terms of a Fourier series as

$$L(1-2) = \int \frac{dk}{(2\pi)^3} \sum_\nu (k,\Omega_\nu)\, e^{ik\cdot(r_1-r_2) - i\Omega_\nu(t_1-t_2)} \qquad (8\text{-}4a)$$

where

$$\Omega_\nu = \frac{\pi\nu}{-i\beta} \qquad \nu = \text{even integer} \qquad (8\text{-}4b)$$

In exactly the same way as we establish that the Fourier coefficient for $G(1-1')$ is

$$G(p,z) = \int \frac{d\omega'}{2\pi} \frac{A(p,\omega')}{z-\omega'}$$

$$= \int \frac{d\omega'}{2\pi} \frac{G^>(p,\omega') \mp G^<(p,\omega')}{z-\omega'}$$

we find that

$$L(k,\Omega) = \int \frac{d\omega'}{2\pi} \frac{L^>(k,\omega') - L^<(k,\omega')}{\Omega - \omega'} \qquad (8\text{-}5a)$$

where

$$L^{\gtrless}(k,\omega) = \int dr_1 \int_{-\infty}^{\infty} dt_1\, e^{-ik\cdot(r_1-r_2) + i\omega(t_1-t_2)}$$
$$\times\, iL^{\gtrless}(r_1-r_2,\, t_1-t_2) \qquad (8\text{-}5b)$$

The function $L(k,\Omega)$ is the quantity that is most directly evaluated by a Green's function analysis in the imaginary time domain. The linear response of the density to a physical disturbance can be easily expressed in terms of $L(k,\Omega)$. The physical response is given as:

$$\langle n(1)\rangle_U = \langle \mathcal{U}^\dagger(t_1)\, n(1)\, \mathcal{U}(t_1)\rangle$$

where

$$\mathcal{U}(t) = T\left\{\exp\left[-i \int_{-\infty}^{t_1} d2\, U(2)\, n(2)\right]\right\}$$

and all the times are real. Hence, the linear response of $\langle n(1)\rangle_U$ to U is

$$\delta[\pm ig(1,1^+;U)] = \delta\langle n(1)\rangle_U$$

$$= \frac{1}{i} \int_{-\infty}^{t_1} d2\, \langle [n(1),n(2)]\rangle \delta U(2)$$

$$= \int_{-\infty}^{t_1} d2\, [L^>(1-2) - L^<(1-2)]\, \delta U(2) \qquad (8\text{-}6)$$

These functions $L^>$ and $L^<$ are exactly the same analytic functions as appear in the coefficient of (8-2) of the linear term in the expansion of $G(U)$. This is the fundamental connection between the two linear responses.

If

$$U(R,T) = U_0\, e^{ik\cdot R - i\Omega T} \qquad (8\text{-}7)$$

then

$$\delta\langle n(1)\rangle_U = (\delta n/\delta U)(k,\Omega)\, U(R,T)$$

$$\delta\langle n(1)\rangle_U = \mp\left[(L^>(1-2) - L^<(1-2))\delta(t_1-t_2)\right] \mp [\delta U]$$

where

$$(\delta n/\delta U)(k,\Omega) = \int_{-\infty}^{t_1} dt_2 \int dr_2\, e^{-ik\cdot(r_1 - r_2) + i\Omega(t_1 - t_2)}$$

$$\times [L^{>}(r_1 - r_2, t_1 - t_2) - L^{<}(r_1 - r_2, t_1 - t_2)]$$

$$= \frac{1}{i} \int_{-\infty}^{t_1} dt_2 \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \quad -\frac{1}{i}\int_{-\infty}^{+\infty} d(t_1 - t_2)\, e^{i(\Omega-\omega')(t_1-t_2)}$$

$$\times [L^{>}(k,\omega') - L^{<}(k,\omega')]\, e^{i(\Omega - \omega')(t_1 - t_2)}$$

$$\to (\Omega - \omega' + i\varepsilon)$$

$$= \int \frac{d\omega'}{2\pi} \frac{L^{>}(k,\omega') - L^{<}(k,\omega')}{\Omega - \omega'} \qquad L^{\gtrless}(\omega) = \mathcal{F}[iL^{\gtrless}(t)]$$

$$= -\frac{1}{i}\frac{e^{i(\Omega-\omega')(t_1-t_2)}}{i(\Omega-\omega')}\Big|_{-\infty}^{t_1} = +\frac{1}{\Omega-\omega'}$$

$$\vartheta(t_1 - t_2) = \frac{1}{\Omega - \omega' + i\varepsilon}$$

However, we can recognize this last expression as just $L(k,\Omega)$, so that

$$(\delta n/\delta U)(k,\Omega) = L(k,\Omega) \tag{8-8}$$

Therefore, the Fourier coefficient function $L(k,\Omega)$ is exactly the linear response of $\langle n(1)\rangle_U$ to a disturbance with wavenumber $\mathbf{k}$ and frequency Ω in the upper half-plane.

Let us determine this Fourier coefficient by using the Hartree approximation in the complex time domain. We certainly expect that this approximation has the same physical content as the real time Hartree approximation. Therefore, we anticipate that the linear response $L(\mathbf{k},\Omega)$ computed from this approximation for $G(U)$ should be identical to the $(\delta n/\delta U)(\mathbf{k},\Omega)$ that we computed in the last chapter by means of the random phase approximation.

In the imaginary time domain, the Hartree approximation is

$$G^{-1}(1,1';U) = \left[i\frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} - U_{eff}(1)\right]\delta(1-1')$$

$$= \left[i\frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} - U(1) \mp i\int_0^{-i\beta} d2\, V(1-2)\right.$$

$$\left.\times G^{<}(2,2;U)\right]\delta(1-1')$$

We can compute

$$\mathcal{F}(\vartheta(t)) = i\left(P\frac{1}{\omega} + \pi\delta(\omega)\right)$$

$$\frac{\delta G(1,1';U)}{\delta U(2)} = -\int_0^{-i\beta} d3 \int_0^{-i\beta} d3'\, G(1,3;U)\, G(3,1';U)$$

$$\times \frac{\delta G^{-1}(3,3';U)}{\delta U(2)} \qquad \delta G = -G\,\delta G^{-1}\, G$$

$$= \int_0^{-i\beta} d3\, G(1,3;U)\, G(3,1';U)\, \frac{\delta U_{eff}(3)}{\delta U(2)}$$

$$= G(1,2;U)\, G(2,1';U) \pm i\int_0^{-i\beta} d3 \int_0^{-i\beta} d4$$

$$\times G(1,3;U)\, G(3,1';U)\, V(3-4)\, \frac{\delta G(4,4^+;U)}{\delta U(2)} \tag{8-9}$$

Therefore, in the Hartree approximation,

$$L(1-2) \equiv \pm i\left[\frac{\delta G(1,1^+;U)}{\delta U(2)}\right]_{U=0}$$

$$= \pm iG(1-2)\, G(2-1) + \int_0^{-i\beta} d3 \int_0^{-i\beta} d4$$

$$\times [\pm iG(1-3)\, G(3-1)]\, V(3-4)\, L(4-2)$$

If we define

$$L_0(1-2) = \pm i\, G(1-2)\, G(2-1) \tag{8-10}$$

we can write this approximation as

$$L(1-2) = L_0(1-2) + \int_0^{-i\beta} d3 \int_0^{-i\beta} d4$$

$$\times L_0(1-3)\, V(3-4)\, L(4-2) \tag{8-11}$$

By employing the boundary conditions on G

$$G(1-2)|_{t_1=0} = \pm e^{\beta\mu} G(1-2)|_{t_1=-i\beta}$$

$$G(1-2)|_{t_2=0} = \pm e^{-\beta\mu} G(1-2)|_{t_2=-i\beta}$$

we can see that L_0 satisfies the same boundary condition (8-3) as L. Thus, L_0 may also be expanded in a Fourier series of the form

(8-4a), with a Fourier coefficient $L_0(k,\Omega_\nu)$. From (8-10) it follows that

$$L_0^>(1-2) = \pm iG^>(1-2)G^<(2-1)$$

$$L_0^<(1-2) = \pm iG^<(1-2)G^>(2-1)$$

and hence

$$L_0^{\gtrless}(k,\omega) = \int \frac{dp'}{(2\pi)^3}\frac{d\omega'}{2\pi} G^{\gtrless}(p'+k/2,\omega'+\omega/2) \times G^{\lessgtr}(p'-k/2,\omega'-\omega/2)$$

so that

$$L_0^>(k,\omega) - L_0^<(k,\omega) = \int \frac{dp'}{(2\pi)^3}\frac{d\omega'}{2\pi} A(p'+k/2,\omega'+\omega/2) \times A(p'-k/2,\omega'-\omega/2)\{[1 \pm f(\omega'+\omega/2)] \times f(\omega'-\omega/2) - f(\omega'+\omega/2) \times [1 \pm f(\omega'-\omega/2)]\}$$

Because (8-11) is derived by differentiating the Hartree approximation, the G's that appear in (8-10) must be the Hartree Green's functions, and for these

$$A(p,\omega) = 2\pi\delta(\omega - E(p))$$

$$= 2\pi\delta(\omega - p^2/2m - nv)$$

Therefore, $L_0^> - L_0^<$ takes the simple form

$$L_0^>(k,\omega) - L_0^<(k,\omega) = \int \frac{dp}{(2\pi)^3} 2\pi\delta(\omega - E(p+k/2) + E(p-k/2)) \times [f(E(p-k/2)) - f(E(p+k/2))]$$

It follows then that the Fourier coefficient $L_0(k,\Omega)$ is

$$L_0(k,\Omega) = \int \frac{d\omega'}{2\pi}\frac{L_0^>(k,\omega') - L_0^<(k,\omega')}{\Omega - \omega'}$$

$$= \int \frac{dp}{(2\pi)^3}\frac{f(E(p-k/2)) - f(E(p+k/2))}{\Omega - k\cdot p/m} \qquad (8\text{-}12)$$

If we compare (8-12) with (7-23), we see that

$$L_0(k,\Omega) = \left(\frac{\delta n}{\delta U}\right)_0 (k,\Omega) \qquad (8\text{-}12a)$$

The latter function is the quantity that appears in the solution of the real time Hartree approximation.

Now it is trivial to solve (8-11). We multiply it by $e^{-ik\cdot(r_1 - r_2) + i\Omega_\nu(t_1 - t_2)}$ and integrate over all r_1 and all t_1 between 0 and $-i\beta$. In this way, we pick out the Fourier coefficients on both sides of the equation and find:

$$L(k,\Omega_\nu) = L_0(k,\Omega_\nu)[1 + v(k)L(k,\Omega_\nu)]$$

and therefore

$$L(k,\Omega) = L_0(k,\Omega)[1 + v(k)L(k,\Omega)]$$

Thus

$$L(k,\Omega) = \frac{L_0(k,\Omega)}{1 - v(k)L_0(k,\Omega)}$$

or

$$L(k,\Omega) = \frac{(\delta n/\delta U)_0(k,\Omega)}{1 - v(k)(\delta n/\delta U)_0(k,\Omega)} \qquad (8\text{-}13)$$

We recognize this expression for $L(k,\Omega)$ as exactly that derived for $(\delta n/\delta U)(k,\Omega)$ in the random phase approximation [cf. (7-18)]. Therefore, we see that $(\delta n/\delta U)(k,\Omega)$ can be determined equally well from the imaginary time theory. One just has to solve for $L(k,\Omega)$, using an approximation for $G(U)$, to find the physical response $(\delta n/\delta U)(k,\Omega)$.

Unfortunately, this procedure for determining the physical response from the imaginary time response is very difficult to employ for approximations fancier than the Hartree approximation. It is only for this approximation that we can solve exactly for the response and hence obtain an exact solution for the Fourier coefficient. In other situations, we cannot obtain an explicit form for $L(k,\Omega)$ from the imaginary time Green's function approximation, and hence we cannot employ the simple analysis that we have developed here.

8-2 CONTINUATION OF IMAGINARY TIME RESPONSE TO REAL TIMES

We should really like to have approximate equations of motion for $g(U)$. However, these are hard to obtain directly, because $g_2(U)$ satisfies a somewhat complicated boudary condition. Instead of working with $g_2(U)$ directly, we shall show how $g_2(U)$ may be derived from $G_2(U)$. We have a theory, developed in Chapter 5, for determining the latter function. By expressing $g_2(U)$ in terms of $G_2(U)$, we obtain a theory of the physical response function.

We begin this analysis by introducing an essentially trivial generalization of $G(U)$ and $G_2(U)$. These functions were originally defined as for pure imaginary times in the interval $0 < it, it' < \beta$. However, there is nothing very special about the time zero. We could just as well define Green's functions in the interval $[t_0, t_0 - i\beta]$, i.e.,

$$0 < i(t - t_0) < \beta \qquad (t_0 \text{ real}) \tag{8-14}$$

For times in this interval, we write

$$G(1,1';U;t_0) = \frac{1}{i}\,\frac{\langle T[S\psi(1)\psi\dagger(1')]\rangle}{\langle T[S]\rangle} \tag{8-15a}$$

where

$$S = \exp\left[-i\int_{t_0}^{t_0-i\beta} d2\; U(2)\,n(2)\right] \tag{8-15b}$$

Here T orders according to the size of $i(t - t_0)$; operators with larger values of $i(t - t_0)$ appear on the left. When $t_0 = 0$, the $G(U;t_0)$ defined by (8-15) reduces to the $G(U)$ discussed in Chapter 5.

The theory of $G(U;t_0)$ is identical to the theory of $G(U)$. This generalized response function satisfies the boundary condition

$$G(1,1';U;t_0)\,|_{t_1=t_0} = \pm e^{\beta\mu}\,G(1,1';U;t_0)\,|_{t_1=t_0-i\beta}$$

instead of

$$G(1,1';U)\,|_{t_1=0} = \pm\, e^{\beta\mu}\,G(1,1';U)\,|_{t_1=-i\beta}$$

Therefore, the only change that has to be made in the formulas of Chapter 5 to make them apply to $G(U;t_0)$ is to replace all time integrals over the interval $[0, -i\beta]$ by integrals over $[t_0, t_0 - i\beta]$. In particular, $G(U;t_0)$ satisfies the equations of motion:

$$\left[i\frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} - U(1)\right] G(1,1';U;t_0)\int_{t_0}^{t_0-i\beta} d\bar{1}$$

$$\times\, \Sigma\,(1,\bar{1};U;t_0)\,G(\bar{1},1';U;t_0) = \delta(1-1') \tag{8-16a}$$

and

$$\left[-i\frac{\partial}{\partial t_{1'}} + \frac{\nabla_{1'}^2}{2m} - U(1')\right] G(1,1';U;t_0) - \int_{t_0}^{t_0-i\beta} d\bar{1}$$

$$\times\, G(1,\bar{1};U;t_0)\,\Sigma\,(\bar{1},1';U;t_0) = \delta(1-1') \tag{8-16b}$$

We shall now establish a relationship between $G(U;t_0)$ and $g(U)$ in order that we may convert (8-16) into equations of motion for $g(U)$. To do this, we consider the case $i(t_1 - t_0) < i(t_{1'} - t_0)$. Then

$$\begin{aligned} G(1,1';U;t_0) &= G^<(1,1';U;t_0) \\ &= \pm\frac{1}{i}\,\frac{\langle T[S\psi\dagger(1')\psi(1)]\rangle}{\langle T[S]\rangle} \\ &= \pm(1/i)\,\langle u(t_0, t_0 - i\beta)[u\dagger(t_0,t_{1'})\psi\dagger(1')\,u(t_0,t_{1'})] \\ &\quad\times u\dagger(t_0,t_1)\psi(1)\,u(t_0,t_1)\rangle / \langle u(t_0, t_0 - i\beta)\rangle \end{aligned} \tag{8-17}$$

where

$$u(t_0,t_1) = T\left\{\exp\left[-i\int_{t_0}^{t_1} d2\; U(2)\,n(2)\right]\right\} \tag{8-17a}$$

For comparison we write the physical response function, which is defined for real times. For example,

$$\begin{aligned} g^<(1,1';U) &= \pm(1/i)\,\langle\psi_U\dagger(1')\psi_U(1)\rangle \\ &= \pm(1/i)\,\langle[u\dagger(t_{1'})\psi\dagger(1')\,u(t_{1'})] \\ &\quad\times[u\dagger(t_1)\psi(1)\,u(t_1)]\rangle \end{aligned} \tag{8-18}$$

where

$$u(t_1) = T\left\{\exp\left[-i\int_{-\infty}^{t_1} d2\; U(2)\,n(2)\right]\right\} \tag{8-18a}$$

Let us consider the case in which $U(1)$ is an analytic function of $t_{1'}$ for $0 > \text{Im}\, t_1 > -\beta$, which satisfies

$$\lim_{\mathrm{Re}\, t_1 \to -\infty} U(t_1) = 0 \tag{8-19}$$

For example, $U(R,T)$ might be $U_0 e^{i\mathbf{k}\cdot\mathbf{r} - i\Omega T}$ where $\mathrm{Im}\,\Omega > 0$. If $U(R,T)$ is an analytic function of the time, then $\mathcal{U}(t_0,t_1)$ and $\mathcal{U}(t_0)$ are analytic functions of their time variables in the sense that every matrix element of each term in their power-series expansions is analytic. If all sums converge uniformly, as we shall assume, $G^<(1,1';U;t_0)$ and $g^<(1,1';U)$ are then each analytic functions of their time arguments. The analytic functions $\mathcal{U}(t_0,t_1)$ and $\mathcal{U}(t_0)$ can also be defined by

$$i(\partial/\partial t_1)\,\mathcal{U}(t_1) = \int d\mathbf{r}_1\, n(1)\, U(1)\, \mathcal{U}(1)$$

$$\mathcal{U}(-\infty) = 1 \tag{8-20}$$

and

$$i(\partial/\partial t_1)\,\mathcal{U}(t_0,t_1) = \int d\mathbf{r}_1\, n(1)\, U(1)\, \mathcal{U}(t_0,t_1)$$

$$\mathcal{U}(t_0,t_0) = 1$$

Because of this analyticity it follows that

$$\lim_{t_0 \to -\infty} \mathcal{U}(t_0,t_1) = \mathcal{U}(t_0)$$

and, because of (8-19)

$$\lim_{t_0 \to -\infty} \mathcal{U}(t_0, t_0 - i\beta) = 1$$

Therefore, the analytic functions $G^<(1,1';U;t_0)$ and $g^<(1,1';U)$ are connected by

$$\lim_{t_0 \to -\infty} G^<(1,1';U;t_0) = g^<(1,1';U) \tag{8-21a}$$

and, similarly,

$$\lim_{t_0 \to -\infty} G^>(1,1';U;t_0) = g^>(1,1';U) \tag{8-21b}$$

In order to have a simple confirmation of the result that we have just obtained, let us compute $\pm iG^<(1,1';U;t_0)$ and $\pm ig^<(1,1;U)$ to first order in U. These are

$$\pm iG^<(1,1;U;t_0)$$

$$= \langle n\rangle + \int_{t_0}^{t_0 - i\beta} d2\, (1/i)\, \langle T\{[n(1) - \langle n\rangle][n(2) - \langle n\rangle]\}\rangle\, U(2)$$

$$= \langle n\rangle + \int_{t_0}^{t_1} d2\, (1/i)\, \langle [n(1) - \langle n\rangle]\,[n(2) - \langle n\rangle]\rangle\, U(2)$$

$$- \int_{t_0 - i\beta}^{t_1} d2\, (1/i)\, \langle [n(2) - \langle n\rangle]\,[n(1) - \langle n\rangle]\rangle\, U(2)$$

$$= \langle n\rangle + \int_{t_0}^{t_1} d2\, L^>(1-2)\, U(2)$$

$$- \int_{t_0 - i\beta}^{t_1} d2\, L^<(1-2)\, U(2) \tag{8-22}$$

Since $L^>$ and $L^<$ are analytic functions of their time variables, when U is also analytic, the right side of (8-22) is clearly an analytic function of t_1 and t_0. If we take the limit $t_0 \to -\infty$, (8-22) becomes

$$\lim_{t_0 \to -\infty} [\pm iG^<(1,1;U;t_0)] = \langle n\rangle + \int_{-\infty}^{t_1} d2$$

$$\times\, [L^>(1-2) - L^<(1-2)]\, U(2) \tag{8-22a}$$

This should be compared with (8-6), which indicates that the physical response is

$$\langle n(1)\rangle_U = \pm ig^<(1,1;U)$$

$$= \langle n\rangle + \int_{-\infty}^{t_1} d2\, [L^>(1-2) - L^<(1-2)]\, U(2) \tag{8-22b}$$

This is, of course, the same as (8-22a).

8-3 EQUATIONS OF MOTION IN THE REAL TIME DOMAIN

We now describe how approximate equations of motion for $G(U;t_0)$ may be continued into equations of motion for the physical response function $g(U)$.

Let us begin with the very simple example, the Hartree approximation. In this approximation (8-16a) is

$$\left[i\frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} - U_{eff}(1;t_0)\right] G(1,1';U;t_0) = \delta(1-1') \tag{8-23a}$$

where

$$U_{eff}(R,T;t_0) = U(R,T) \pm i \int dR'\ v(R-R') \times G^<(R'T;R'T;U;t_0) \tag{8-23b}$$

We consider the case in which $i(t_1 - t_0) < i(t_{1'} - t_0)$. Then

$$\left[i\frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} - U_{eff}(1;t_0)\right] G^<(1,1';U;t_0) = 0$$

Using the analyticity of $U(R,T)$, we take the limit $t_0 \to -\infty$ to find

$$U_{eff}(R,T;-\infty) = U(R,T) \pm i \int dR'\ v(R-R') \times g^<(R'T;R'T;U) \tag{8-24a}$$

and

$$\left[i\frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} - U_{eff}(1;-\infty)\right] g^<(1,1';U) = 0 \tag{8-24b}$$

These equations hold for all complex values of t_1 and $t_{1'}$ such that $\beta > \mathrm{Im}(t_1 - t_{1'}) \geq 0$. When they are specialized to the case of real values of the time variables they become just the familiar statement of the real time Hartree approximation.

Our original derivation of the Hartree approximation depended in no way on the analytic properties of $U(R,T)$. In fact, the validity of the equations for $g(U)$ that we shall derive does not depend on the analyticity of U at all. The analytic continuation device is just a convenient way of handling the boundary conditions on the real time response functions. It also gives a particularly simple way of seeing the connection between the imaginary time $G(U)$ and the physical response function $g(U)$.

This same continuation device can be applied in a much more general discussion of the equations of motion for $g(U)$. The self-energy $\Sigma(1,1';U;t_0)$ can be split into two parts as

$$\Sigma(1,1';U;t_0) = \Sigma_{HF}(1,1';U;t_0) + \Sigma_c(1,1';U;t_0) \tag{8-25}$$

where the Hartree-Fock part of Σ is

$$\Sigma_{HF}(1,1';U;t_0) = \delta(t_1 - t_{1'})\{\pm i\delta(r_1 - r_{1'}) \int dr_2\ v(r_1 - r_2) \times G^<(r_2t_1;r_2t_1;U;t_0) + iv(r_1 - r_{1'})G^<(1,1';U;t_0)\} \tag{8-25a}$$

and the collisional part of Σ is composed of two analytic functions of the time variables $\Sigma^>$ and $\Sigma^<$:

$$\Sigma_c(1,1';U;t_0) = \Sigma^>(1,1';U;t_0) \quad \text{for } i(t_1 - t_{1'}) > 0$$
$$= \Sigma^<(1,1';U;t_0) \quad \text{for } i(t_1 - t_{1'}) < 0 \tag{8-25b}$$

For example, in the Born collision approximation

$$\Sigma_c(1,1';U;t_0) = \pm i^2 \int dr_2\, dr_{2'}\ v(r_1 - r_2)v(r_{1'} - r_{2'}) \times \{G(1,1';U;t_0)G(2,2';U;t_0)G(2',2;U;t_0) - G(1,2';U;t_0)G(2,1';U;t_0)G(2',2;U;t_0)\}_{\substack{t_2 = t_1 \\ t_{2'} = t_{1'}}} \tag{8-26a}$$

so that $\Sigma^>$ and $\Sigma^<$ are

$$\Sigma^{\gtrless}(1,1';U;t_0) = \pm i^2 \int dr_2\, dr_{2'}\ v(r_1 - r_2)v(r_{1'} - r_{2'}) \times \{G^{\gtrless}(1,1';U;t_0)G^{\gtrless}(2,2';U;t_0)G^{\lessgtr}(2',2;U;t_0) \pm G^{\gtrless}(1,2';U;t_0)G^{\lessgtr}(2,1';U;t_0) \times G^{\lessgtr}(2',2;U;t_0)\}_{\substack{t_2 = t_1 \\ t_{2'} = t_{1'}}} \tag{8-26b}$$

Since the $G^>$ and $G^<$ are analytic functions of their time variables, so is $\Sigma^{\gtrless}$.

For the sake of simplicity in writing, let us for the moment drop the exchange term in Σ_{HF}, i.e., the term proportional to $v(r_1 - r_{1'})$ in (8-25a). Then (8-16a) becomes

$$\left[i\frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} - U_{eff}(1;t_0)\right] G(1,1';U;t_0) = \delta(1-1') + \int_{t_0}^{t_0 - i\beta} d\bar{1}\ \Sigma_c(1,\bar{1};U;t_0)G(\bar{1},1';U;t_0)$$

For the case $i(t_1 - t_0) < i(t_{1'} - t_0)$, this gives

$$\left[i\frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} - U_{eff}(1;t_0)\right] G^<(1,1';U;t_0)$$

$$= \int_{t_0}^{t_1} d\bar{1}\ \Sigma^>(1,\bar{1};U;t_0)\, G^<(\bar{1},1';U;t_0)$$

$$+ \int_{t_1}^{t_{1'}} d\bar{1}\ \Sigma^<(1,\bar{1};U;t_0)\, G^<(\bar{1},1';U;t_0)$$

$$+ \int_{t_{1'}}^{t_0 - i\beta} d\bar{1}\ \Sigma^<(1,\bar{1};U;t_0)\, G^>(\bar{1},1';U;t_0)$$

$$\int_{t_1}^{t_1'} = \int_{-\infty}^{t_1'} - \int_{-\infty}^{t_1}$$

If we now take the limit $t_0 \to -\infty$, we find that $g^<(U)$ obeys

$$\left[i\frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} - U_{eff}(1)\right] g^<(1,1';U)$$

$$= \int_{-\infty}^{t_1} d\bar{1}\left[\Sigma^>(1,\bar{1};U) - \Sigma^<(1,\bar{1};U)\right] g^<(\bar{1},1';U)$$

$$- \int_{-\infty}^{t_{1'}} d\bar{1}\ \Sigma^<(1,\bar{1};U)\left[g^>(\bar{1},1';U) - g^<(\bar{1},1';U)\right] \qquad (8\text{-}27a)$$

where

$$U_{eff}(1) = U_{eff}(1;-\infty)$$

$$\Sigma^{\gtrless}(1,1';U) = \Sigma^{\gtrless}(1,1';U;-\infty)$$

Applying the same arguments (8-16a) in the case $i(t_1 - t_0) > i(t_{1'} - t_0)$, we find

$$\left[i\frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} - U_{eff}(1)\right] g^>(1,1';U)$$

$$= \int_{-\infty}^{t_1}\left[\Sigma^>(1,\bar{1};U) - \Sigma^<(1,\bar{1};U)\right] g^>(\bar{1},1';U)$$

$$- \int_{-\infty}^{t_{1'}} \Sigma^>(1,\bar{1};U)\left[g^>(\bar{1},1';U) - g^<(\bar{1},1';U)\right] \qquad (8\text{-}27b)$$

Similarly, (8-16b) implies

$$\left[-i\frac{\partial}{\partial t_{1'}} + \frac{\nabla_{1'}^2}{2m} - U_{eff}(1')\right] g^<(1,1';U)$$

$$= \int_{-\infty}^{t_1} d\bar{1}\left[g^>(1,\bar{1};U) - g^<(1,\bar{1};U)\right]\ \Sigma^<(\bar{1},1';U)$$

$$- \int_{-\infty}^{t_{1'}} g^<(1,\bar{1};U)\left[\Sigma^>(\bar{1},1';U) - \Sigma^<(\bar{1},1';U)\right] \qquad (8\text{-}28a)$$

and

$$\left[-i\frac{\partial}{\partial t_{1'}} + \frac{\nabla_{1'}^2}{2m} - U_{eff}(1')\right] g^>(1,1';U)$$

$$= \int_{-\infty}^{t_1} d\bar{1}\left[g^>(1,\bar{1};U) - g^<(1,\bar{1};U)\right]\ \Sigma^>(\bar{1},1';U)$$

$$- \int_{-\infty}^{t_{1'}} d\bar{1}\ g^>(1,\bar{1};U)\left[\Sigma^>(\bar{1},1';U) - \Sigma^<(\bar{1},1';U)\right] \qquad (8\text{-}28b)$$

When $\Sigma^>(U;t_0 = -\infty)$ and $\Sigma^<(U;t_0 = -\infty)$ are expressed in terms of $g^>(U)$ and $g^<(U)$, then (8-27) and (8-28) can be used to determine the real time response functions $g^>(U)$ and $g^<(U)$. For example, the Born collision approximation for $g(U)$ is derived by using (8-26b) to find

$$\Sigma^{\gtrless}(1,1';U) \equiv \Sigma^{\gtrless}(1,1';U;t_0 = -\infty)$$

$$= \pm\, i^2 \int d\mathbf{r}_2\, d\mathbf{r}_{2'}\, v(\mathbf{r}_1 - \mathbf{r}_2)\, v(\mathbf{r}_{1'} - \mathbf{r}_{2'})$$

$$\times \left[g^{\gtrless}(1,1';U)\, g^{\gtrless}(2,2';U)\, g^{\lessgtr}(2',2;U) \pm g^{\gtrless}(1,2';U)\right.$$

$$\times \left.\left[g^{\gtrless}(2,1';U)\, g^{\gtrless}(2',2;U)\right]\right]_{t_2 = t_{1'},\, t_{2'} = t_{1'}} \qquad (8\text{-}29)$$

Equations (8-27) and (8-28) are exact, except for the trivial omission of the exchange term in Σ_{HF}. In Chapter 9 we shall discuss how these equations may be used to describe transport. In particular, we shall use the approximation (8-29) to derive a generalization of the Boltzmann equation. We shall also use these equations to discuss sound propagation in many-particle systems.