§ 15. THE PERTURBATION THEORY SERIES FOR THE THERMODYNAMIC POTENTIAL

There are cases when it proves more convenient to find the thermodynamic potential Ω directly, rather than indirectly, via an evaluation of the Green functions.

The correction to the thermodynamic potential is given in terms of the average of the $\mathcal{S}$-matrix by (see (12.11))

$$\Delta\Omega = -T \ln \langle \mathcal{S} \rangle, \quad \mathcal{S} = \exp\left\{-\int_0^{1/T} \hat{H}_{int}(\tau)\,d\tau\right\}. \tag{15.1}$$

The logarithm can in fact be taken in the ordinary form in (15.1); or, more precisely, a diagram technique can be developed for dealing directly with Ω.

It is obvious from the foregoing that the diagrams which describe the perturbation theory series for Ω are made up of closed loops. Typical diagrams are shown for both variants of a two-particle interaction in Fig. 48*a*, *b*, and for interaction with phonons in Fig. 49 (the diagram in Fig. 49, I, is in fact equal to zero).

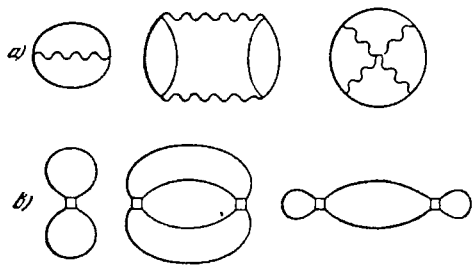

Fig. 48

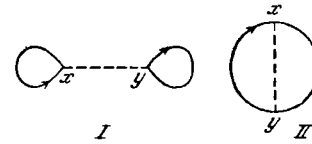

Fig. 49

The diagrams of a given order of the perturbation theory series will include both types — connected and unconnected. The latter consist of two or more closed loops, with no lines joining them. Connected diagrams are obtained if, when describing a term of the series for $\langle \mathcal{S} \rangle$ in accordance with Wick's theorem,

$$\frac{(-1)^n}{n!} \int_0^{1/T} \cdots \int_0^{1/T} d\tau_1 \cdots d\tau_n \langle T_\tau \{\hat{H}_{int}(\tau_1) \cdots \hat{H}_{int}(\tau_n)\}\rangle, \tag{15.2}$$

we can start the pairing with an operator appearing in $\hat{H}_{int}(\tau_1)$ then return to $\hat{H}_{int}(\tau_1)$ without passing over any of the $\hat{H}_{int}$. In any other case, the diagram must be unconnected.

Suppose an nth order unconnected diagram consists of k closed loops, and, for a start, that every one of these loops contains a different number

of vertices. The corresponding expression will be

$$\frac{(-1)^n}{n!}\int d\tau_1^{(1)}\cdots d\tau_{m_1}^{(1)}\langle T_\tau\{\hat{H}_{int}(\tau_1^{(1)})\cdots\hat{H}_{int}(\tau_{m_1}^{(1)})\}\rangle_c$$
$$\times\int d\tau_1^{(2)}\cdots d\tau_{m_2}^{(2)}\langle T_\tau\{\hat{H}_{int}(\tau_1^{(2)})\cdots\hat{H}_{int}(\tau_{m_2}^{(2)})\}\rangle_c$$
$$\cdots\int d\tau_1^{(k)}\cdots d\tau_{m_k}^{(k)}\langle T_\tau\{\hat{H}_{int}(\tau_1^{(k)})\cdots\hat{H}_{int}(\tau_{m_k}^{(k)})\}\rangle_c, \quad (15.3)$$

where

$$m_1+m_2+\cdots+m_k=n\ (m_1\neq m_2\neq\cdots\neq m_k),$$

and the symbol $\langle\cdots\rangle_c$ denotes the averaging corresponding to a given connected diagram. We now sum all the topologically equivalent diagrams containing k loops of the type selected. Obviously this can be done simply by multiplying (15.3) by the number of such diagrams F_k. This number is the same as the number of methods by which we can accomodate n operators $\hat{H}_{int}$ in k different "cells" $\langle\cdots\rangle_c$, containing respectively $m_1, m_2, \ldots, m_k$ places, i.e.

$$F_k=\frac{n!}{m_1!\,m_2!\cdots m_k!}.$$

We get as a result:

$$\frac{(-1)^m}{m_1!}\int d\tau_1^{(1)}\cdots d\tau_{m_1}^{(1)}\langle T_\tau\{\hat{H}_{int}(\tau_1^{(1)})\cdots\hat{H}_{int}(\tau_{m_1}^{(1)})\}\rangle_c$$
$$\times\frac{(-1)^{m_2}}{m_2!}\int d\tau_1^{(2)}\cdots d\tau_{m_2}^{(2)}\langle T_\tau\{\hat{H}_{int}(\tau_1^{(2)})\cdots\hat{H}_{int}(\tau_{m_2}^{(2)})\}\rangle_c$$
$$\cdots\frac{(-1)^{m_k}}{m_k!}\int d\tau_1^{(k)}\cdots d\tau_{m_k}^{(k)}\langle T_\tau\{\hat{H}_{int}(\tau_1^{(k)})\cdots\hat{H}_{int}(\tau_{m_k}^{(k)})\}\rangle_c. \quad (15.4)$$

Notice that we did not really need the assumption that each averaging $\langle\cdots\rangle_c$ corresponds to a connected diagram of a definite type; instead, we could have simply assumed that $\langle\cdots\rangle_c$ is the sum of all the connected diagrams with a given number of vertices. It may be concluded from this that the sum of all the unconnected diagrams containing k closed loops with $m_1, m_2, \ldots, m_k$ vertices respectively is of the form

$$\Xi_{m_1}\Xi_{m_2}\cdots\Xi_{m_k},$$

where

$$\Xi_m=\frac{(-1)^m}{m!}\int d\tau_1\cdots d\tau_m\langle T_\tau\{\hat{H}_{int}(\tau_1)\cdots\hat{H}_{int}(\tau_m)\}\rangle_c \quad (15.5)$$

is nothing but the sum of all the connected diagrams of order m for $\langle\mathcal{S}\rangle$. Obviously,

$$1+\Xi_1+\Xi_2+\cdots=\langle\mathcal{S}\rangle_c. \quad (15.6)$$

If some of the numbers $m_1, m_2, \ldots$ are the same, so that the diagram splits up into $p_1+p_2+\cdots+p_k$ closed loops, containing respectively

$m_1, m_2, \ldots, m_k$ ($m_1 \neq \cdots m_k$) vertices, it can be shown that expression (15.5) must be replaced by(†)

$$\frac{1}{p_1!}\Xi_{m_1}^{p_1}\frac{1}{p_2!}\Xi_{m_2}^{p_2}\cdots\frac{1}{p_k!}\Xi_{m_k}^{p_k} \tag{15.7}$$

or, what amounts to the same thing, by

$$\frac{1}{p_1!}\Xi_1^{p_1}\frac{1}{p_2!}\Xi_2^{p_2}\cdots\frac{1}{p_l!}\Xi_l^{p_l}, \tag{15.8}$$

where the p_l ($p_l = 0, 1, 2, \ldots$) indicate how many closed loops of order l are contained in all the unconnected diagrams. On summing (15.8) over all p_l (the summations over different p_l are obviously independent), we get

$$\begin{aligned}\langle\mathfrak{S}\rangle &= \sum_{p_1,p_2,\ldots}\frac{1}{p_1!}\Xi_1^{p_1}\frac{1}{p_2!}\Xi_2^{p_2}\cdots = \sum_{p_1}\frac{1}{p_1!}\Xi_1^{p_1}\sum_{p_2}\frac{1}{p_2!}\Xi_2^{p_2}\cdots \\ &= e^{\Xi_1}e^{\Xi_2}\cdots = \exp\{\Xi_1+\Xi_2+\cdots\}. \end{aligned}\tag{15.9}$$

Finally, on substituting (15.9) in (15.1), we get

$$\Delta\Omega = -T(\Xi_1+\Xi_2+\cdots) = -T\{\langle\mathfrak{S}\rangle_c - 1\}. \tag{15.10}$$

A very important result has been obtained: to find the corrections to the thermodynamic potential, we only need to find the contribution of the connected diagrams for $\langle\mathfrak{S}\rangle$.

As already remarked, the diagrams for $\langle\mathfrak{S}\rangle$ are in the form of closed loops, and these can be evaluated in accordance with essentially the same rules as for $\mathfrak{G}$-functions. The only difference lies in the factor in front of the diagram.

We mentioned in § 12 that the factor $1/n!$ in the perturbation theory series (12.13) for the $\mathfrak{G}$-functions cancels out if we take into account the contribution of all the topologically equivalent diagrams, the number of which is in fact equal to $n!$ The situation is different when we evaluate $\langle\mathfrak{S}\rangle_c$. The number of equivalent diagrams that give the nth term of series (12.12) will be equal(‡) to $(n-1)!$, so that a factor $1/n$ appears

(†) This can be proved as follows. When some of the $m_1, \ldots, m_k$ are the same, the F_k mentioned above is the same as the number of ways in which $p_1m_1 + p_2m_2 + \cdots + p_km_k = n$ operators $\hat{H}_{int}$ can be allocated to $p_1 + p_2 + \cdots + p_k$ cells $\langle\cdots\rangle_c$, containing $m_1, m_2, \ldots, m_k$ places where, respectively, $p_1, p_2, \ldots, p_k$ of the cells are the same. In this case F_k is equal to

$$F_k = \frac{n!}{p_1!(m_1!)^{p_1}p_2!\,(m_2!)^{p_2}\cdots p_k!(m_k!)^{p_k}}.$$

(‡) All the equivalent diagrams follow by taking all possible permutations of the $n-1$ operators H_{int} in (12.12). One of the H_{int} must be regarded as fixed. When evaluating $\mathfrak{G}$. the beginning and end of the external lines were fixed, i.e. the operators $\psi_\alpha(\boldsymbol{r}_1, \tau_1)$, $\bar{\psi}_\beta(\boldsymbol{r}_2, \tau_2)$ in (12.13).

in front of each diagram (assuming that only topologically non-equivalent diagrams are distinct). The presence of a factor dependent on the order n makes the perturbation theory series for Ω very awkward, especially in cases when we cannot confine ourselves to a finite number of terms but have to sum infinite sequences of diagrams.

We quote some examples of finding the corrections $\Delta\Omega$, and confine ourselves for brevity to interaction with phonons. Only the connected diagram of Fig. 49, II, is non-zero in the second order of perturbation theory. We find its contribution from Wick's theorem, putting $\Omega_2 = -T\Xi_2$ (we use a four-dimensional notation):

$$\Omega_2 = \pm\frac{1}{2}Tg^2\int \mathrm{d}^4x\mathrm{d}^4y\,\mathcal{G}^{(0)}_{\alpha\beta}(x-y)\,\mathcal{G}^{(0)}_{\beta\alpha}(y-x)\,\mathfrak{D}^{(0)}(x-y).$$

It turns out that Ω_2 is proportional to the volume V of the system, as may easily be verified by introducing the new variable $x' = x - y$ in the integral. The situation is the same in any approximation; this is to be expected, since the potential Ω is well known to have the form

$$\Omega = -VP(\mu, T),$$

where P is the pressure expressed as a function of the chemical potential and the temperature. In future, therefore, we shall always give the formulae for $\Delta P (P = P_0(\mu, T) + \Delta P$, where P_0 is the pressure in the system of free particles).

We have for ΔP_2:

$$\Delta P_2 = \mp\frac{1}{2}g^2\int \mathrm{d}^4x\,\mathcal{G}^{(0)}_{\alpha\beta}(x)\,\mathcal{G}^{(0)}_{\beta\alpha}(-x)\,\mathfrak{D}^{(0)}(x). \qquad (15.11)$$

If we change to the momentum representation, we have

$$\Delta P_2 = \pm\frac{1}{2}g^2\frac{T^2}{(2\pi)^6}(2s+1)\sum_{\omega_1,\omega_2}\int \mathrm{d}^3p\,\mathrm{d}^3k \times \frac{1}{i\omega_1 - \varepsilon_0(p)+\mu}\,\frac{1}{i(\omega_1+\omega_2)-\varepsilon_0(p+k)+\mu}\,\frac{\omega_0^2(k)}{\omega_2^2+\omega_0^2(k)}.$$

The corresponding diagram is shown in Fig. 50.

Let us take any diagram of order $2n$. It contains $3n$ lines and $2n$ vertices. However, one of the $2n$ conservation laws turns out to be an identity, provided the remaining $2n-1$ laws are fulfilled. Thus there are altogether $n+1$ independent integrations in a $2n$th order diagram. The extra law of conservation leads to the appearance in the diagram for $\langle\mathfrak{S}\rangle$ of an extra factor $\delta(p=0)$, proportional to the volume V of the system (†).

(†) By definition,

$$\delta(p=0) = \frac{1}{(2\pi)^3}\int \mathrm{d}^3r = \frac{V}{(2\pi)^3}.$$

The rules by which the individual elements of the diagrams are associated with the Green functions (and the vertex parts, in the case of

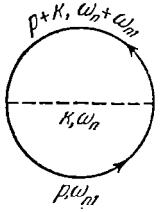

Fig. 50

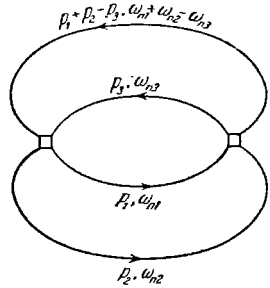

Fig. 51

other interactions) remain the same as for the diagrams for $\mathfrak{G}$. The factor in front of the diagram of order $2n$ for the correction ΔP is equal to

$$M_n = \frac{(-1)^{n+1}}{2n} - g^{2n}\left(\frac{T}{(2\pi)^3}\right)^{2n} (\mp 1)^F (2s+1)^F,$$

where F is the number of closed loops, formed by single $\mathfrak{G}$-lines of the particles.

We quote in addition the expression for ΔP for the case of binary interactions. When the interaction has the form (13.7), the second order correction to the pressure, corresponding to the diagram of Fig. 51, is

$$-\frac{1}{4}\frac{T^3}{(2\pi)^9}\sum_{\omega_1\omega_2\omega_3}\int \mathrm{d}^3p_1\mathrm{d}^3p_2\mathrm{d}^3p_3\,\frac{1}{i\omega_1-\varepsilon_0(p_1)+\mu}\,\frac{1}{i\omega_2-\varepsilon_0(p_2)+\mu}$$
$$\times\frac{1}{i\omega_3-\varepsilon(p_3)+\mu}\,\frac{1}{i(\omega_1+\omega_2-\omega_3)-\varepsilon_0(p_1+p_2-p_3)+\mu}$$
$$\times\mathcal{T}^{(0)}_{\alpha\beta;\gamma\delta}(p_1,p_2;p_1+p_2-p_3,p_3)\,\mathcal{T}^{(0)}_{\gamma\delta;\beta\alpha}(p_1+p_2-p_3,p_3;p_2,p_1).$$

§ 16. DYSON EQUATION. MANY-PARTICLE GREEN FUNCTIONS

1. Dyson equation

As in the absolute zero case, statistical problems at $T \neq 0$ virtually always involve finding several of the first terms of the perturbation theory series as corrections to the Green functions. Within the framework of almost any physical problem which is correctly stated, the formal parameter of the expansion of the diagram technique, namely the interaction Hamiltonian $\hat{H}_{int}$, is not small; as a result, several infinite sequences of terms of the perturbation theory series will give contributions of the same order of magnitude.

We saw in the previous chapter that a summation of infinite series is carried out by the diagram method in the field theory technique.