CHAPTER III

APPLICATION

A Simplified Cluster Expansion for the Classical Real Gas[1]

Synopsis

Mayer's expansion of the partition function of a classical real gas in terms of irreducible cluster integrals is derived by a simpler and more direct method. The two principal features of this method are the following.

(i) The partition function is expanded in an infinite product rather than a series. As a result the exponential form is obtained immediately : there is no need to sum up infinite sets of graphs. Disconnected graphs never enter.

(ii) The calculation leads directly to the canonical N-particle partition function. Neither the fugacity nor the reducible cluster integrals are introduced.

The first approximation (second virial coefficient)

In classical theory the problem of finding the equation of state of a real monatomic gas amounts to evaluating the configurational partition function

$$Q_N = \int e^{-a(u_{12}+u_{13}+\cdots u_{N-1,N})}\, d\bar{r}_1\, d\bar{r}_2 \ldots d\bar{r}_N$$

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[1] N.G. Van Kampen, Physica, 27 (1961), 783

The domain of this 3N-dimensional integral is determined by the fact that each particle may move throughout the volume V, irrespective of the positions of the others. Hence the integral may also be regarded as an average over N-particle configurations,

$$Q_N = V^N \overline{\psi_{12}\ \psi_{13}\ \cdots\ \psi_{N-1,N}} \qquad \text{-----(3.1)}$$

where $\psi_{12} = e^{-au_{12}}$ etc., and the bar denotes the average over all positions of the particles inside V.

The ψ's are functions of the random variables $\bar{r}_1, \ldots, \bar{r}_N$ and $\psi_{12} \longrightarrow 1$ as $|\bar{r}_1 - \bar{r}_2| \longrightarrow \infty$. It is clear that ψ_{12} and ψ_{34} are statistically independent, and also ψ_{12} and ψ_{13}. Thus

$$\overline{\psi_{12}\ \psi_{23}} = \bar{\psi}_{12}\ \bar{\psi}_{13} = \bar{\psi}_{12}^{\,2} .$$

However, the three functions ψ_{12}, ψ_{13}, ψ_{23} are not mutually independent. Yet one may write

$$\overline{\psi_{12}\psi_{13}\psi_{23}} = \bar{\psi}_{12}\ \bar{\psi}_{13}\ \bar{\psi}_{23} \qquad \text{-----(3.2)}$$

as a first approximation for low density. The rationale is, that this equality would be correct if one of the ψ's were replaced with 1; but the configurations for which all three ψ's differ from 1 are rare if the density is low.

For products of ψ's involving more than three particles a similar argument applies. One is thus led to the first approximation

$$Q_N^{(1)} / V^N = \overline{\psi}_{12}\ \overline{\psi}_{13} \cdots \overline{\psi}_{N-1,N} = (\overline{\psi}_{12})^{\frac{1}{2}N(N-1)}$$

This yields the usual result for the second virial coefficient in the following way.

$$\frac{Q_N^{(1)}}{V^N} = \left[\int e^{-au_{12}} \frac{d\bar{r}_1}{V} \frac{d\bar{r}_2}{V} \right]^{\frac{1}{2}N(N-1)}$$

$$= \left[1 + \frac{1}{V} \int \left\{ e^{-au(r_{12})} - 1 \right\} d\bar{r}_{12} \right]^{\frac{1}{2}N(N-1)}$$

In the limit of a large system (i.e., $N \to \infty$, $V \to \infty$, $N/V = \rho$ = constant)

$$\lim \frac{(Q_N^{(1)})^{1/N}}{V} = \exp \left[\tfrac{1}{2}\rho \int \left\{ e^{-au(r_{12})} - 1 \right\} d\bar{r}_{12} \right] = \exp \left[\tfrac{1}{2}\rho\beta_1 \right],$$

where β_1 is the Mayer's first irreducible cluster integral. Thus

$$Q_N^{(1)} = V^N \exp \left[\frac{N^2}{2V} \beta_1 \right] \qquad \text{-----(3.3)}$$

This is the familiar first term in the expansion in powers of the density, which leads to the second virial coefficient. It should be noted that the correct exponential form is obtained without summing over an infinite set of graphs with cumbersome combinatorial factors.

The second approximation (order n^2).

The above method of arriving at the second virial coefficient is not new; however, our real problem is to find the higher orders in the expansion. This will be done by supplying successive correction factors, rather than additive terms. These correction factors describe successively the statistical correlations between the ψ's, which have been neglected in the first approximation.

It is reasonable to expect (and it will be verified by the result) that the next approximation involves three-particle correlations. The triplet of particles 1,2,3 gave rise in the first approximation to the factor (3.2). To make up for the error committed there one has to multiply by the correction factor

$$\frac{\overline{\psi_{12}\,\psi_{13}\,\psi_{23}}}{\bar{\psi}_{12}\,\bar{\psi}_{13}\,\bar{\psi}_{23}} = \frac{\overline{\psi_{12}\,\psi_{13}\,\psi_{23}}}{\bar{\psi}^{3}_{12}} \; . \qquad \text{-----(3.4)}$$

As there are $\binom{N}{3}$ triplets of particles, this factor has to be raised to the power $\binom{N}{3}$. Writing, as usually, $\psi_{ij} = 1 + f_{ij}$ one finds for the total second order correction factor to Q_N

$$\left[\frac{1 + 3\bar{f}_{12} + 3\overline{f^2_{12}} + \overline{f_{12}f_{13}f_{23}}}{1 + 3\bar{f}_{12} + 3\bar{f}^2_{12} + \bar{f}^3_{12}}\right]^{\frac{1}{6}N(N-1)(N-2)}$$

Now $\bar{f}_{12}$ is proportional to V^{-1}, and $\overline{f_{12}f_{13}f_{23}}$ to V^{-2}. Hence the configurational partition function per particle, $(Q_N)^{1/N}$, is

$$\left[1+V^{-2}\ \overline{f_{12}f_{13}f_{23}} + O(V^{-3})\right]^{\frac{1}{6}(N-1)(N-2)}$$

In the limit $N \to \infty$, which constant ρ, one has, in the familiar notation,

$$\exp\left[\tfrac{1}{6}\rho^2\ \overline{f_{12}f_{13}f_{23}}\right] = \exp\left[\tfrac{1}{3}\rho^2\beta_2\right]$$

Collecting results, we have found as a second approximation

$$Q_N^{(2)} = V^N \exp\left[\frac{1}{2}\frac{N^2}{V}\beta_1 + \frac{1}{3}\frac{N^3}{V^2}\beta_2\right] \qquad \text{-----(3.5)}$$

It should be noted that we were led directly to the irreducible cluster integrals β_k, without the detour via the reducible cluster integrals b_k. The reason is that the method enables one to evaluate the canonical partition function itself, without the aid of the grand canonical (or some alternative) formalism.

The total expansion of the partition function

In order to find the term of degree k-1 in the density ρ, consider a group of k particles 1,2,...,k, and take all factors ψ whose subscripts are taken from this group. The correction factor to be computed is

$$\frac{\overline{\psi_{12}\psi_{13}\cdots\psi_{k-1,k}}}{D}$$

where the denominator D is the previous approximation to the same product. Write the numerator in terms of f's and expand

$$\frac{1}{D}\overline{(1+f_{12})(1+f_{13})\ldots(1+f_{k-1,k})}=\frac{1}{D}\left\{1+\overline{f}_{12}+\ldots+\overline{f_{12}f_{13}\ldots f_{k-1,k}}\right\} \qquad \text{-----(3.6)}$$

The several terms in this expansion may be arranged in three classes :

(i) terms involving less than k particles ;

(ii) terms that involve all k particles but are reducible (in the sense that they factorize, each factor involving less than k particles);

(iii) irreducible terms involving all k particles.

All terms of classes (i) and (ii) belong to lower approximations and are therefore also present in D. The terms of class (iii) are necessarily of order $V^{-(k-1)}$. There are also corresponding terms in D, that is, terms made up with the same factors f but erroneously treated as reducible. It is clear that such terms are of order V^{-k} or smaller. In general, each term in D is identical with a term of class (i) or (ii) in the numerator, or else $O(V^{-k})$. Hence (3.6) becomes

$$1+\sum_{(k)}\overline{f_{12}f_{13}\ldots}+O(V^{-k}), \qquad \text{-----(3.7)}$$

where the summation extends over all irreducible k-particle terms. This is just the usual irreducible cluster integral:

$$\sum_{(k)}\overline{f_{12}f_{13}\ldots}=\frac{(k-1)!}{V^{k-1}}\,\beta_{k-1} \qquad \text{-----(3.8)}$$

The total correction factor to the configurational partition function per particle, $(Q_N)^{1/N}$, is obtained by raising (3.6) to the power

$$\frac{1}{N}\binom{N}{k} \longrightarrow \frac{N^{k-1}}{k!} .$$

The result is

$$\exp\left[\left(\frac{N}{V}\right)^{k-1} \frac{\beta_{k-1}}{k}\right].$$

Combining these correction factors with the first approximation (3.3) one obtains the familiar result

$$Q_N = V^N \exp\left[N \sum_{k=1}^{\infty} \left(\frac{N}{V}\right)^k \frac{\beta_k}{k+1}\right] \qquad \text{-----(3.9)}$$

or

$$Q_N = V^N \exp\left[N \sum_{k=1}^{\infty} \rho^k \frac{\beta_k}{k+1}\right] \qquad \text{-----(3.10)}$$

Fourier Transform

If we begin with the complex exponential form of a Fourier series,

$$f(x) = \sum_{n=-\infty}^{\infty}{}' C_n e^{in\pi x/l} \qquad \text{-----(3.11)}$$

$$C_n = \frac{1}{2l} \int_{-l}^{l} f(x)\, e^{-in\pi x/l}\, dx \qquad \text{-----(3.12)}$$

and substitute C_n into f(x), we obtain

$$f(x) = \sum_{n=-\infty}^{\infty}{}' \left[\frac{1}{2l} \int_{-l}^{l} f(x)\, e^{-in\pi x/l}\, dx\right] e^{in\pi x/l}$$

$$= \sum_{n=-\infty}^{\infty}{}' \left[\frac{1}{2\pi} \int_{-l}^{l} f(x)\, e^{in\pi x/l}\, dx\right] e^{-in\pi x/l} \cdot \frac{\pi}{l}$$

Now let us denote the frequency of the general component by

$$p_n \equiv \frac{n\pi}{l}$$

and the difference in frequency between consecutive harmonics by

$$\Delta p \equiv \frac{\pi}{l}$$

Then f(x) can be written

$$f(x) = \sum_{n=-\infty}^{\infty}{}' \left[\frac{1}{2\pi} \int_{-l}^{l} f(x)\, e^{ip_n x}\, dx \right] e^{-ip_n x}\, \Delta p$$

In this form, f(x) appears as the sum of the products of the infinitesimal Δp times the value of the function of p,

$$\left[\frac{1}{2\pi} \int_{-l}^{l} f(x)\, e^{ipx}\, dx \right] e^{-ipx}$$

at a point p_n in each interval Δp. The limit of such a sum is a definite integral, and thus as $l \longrightarrow \infty$ and f(x) becomes aperiodic, we can write

$$f(x) = \int_{-\infty}^{\infty} \left[\frac{1}{2\pi} \int_{-\infty}^{\infty} f(x)\, e^{ipx}\, dx \right] e^{-ipx}\, dp \qquad \text{----(3.13)}$$

This is one form of what is called a Fourier integral.

The Fourier integral can be written in various forms. For instance we can write

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{f}(p)\, e^{-ipx}\, dp \qquad \text{----(3.14)}$$

where

$$\hat{f}(p) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x)\, e^{ipx}\, dx \qquad \text{-----(3.15)}$$

Equation (3.14) and (3.15) are known as Fourier transform pair.

In the case of 3-dimensions, we have the following relations:-

$$f(x) \longrightarrow f(\bar{r})$$

$$f(\bar{r}) = \frac{1}{(2\pi)^{3/2}} \iiint_{-\infty}^{\infty} \hat{f}(\bar{p})\, e^{-i\bar{p}.\bar{r}}\, d\bar{p} \qquad \text{-----(3.16)}$$

$$\hat{f}(\bar{p}) = \frac{1}{(2\pi)^{3/2}} \iiint_{-\infty}^{\infty} f(\bar{r})\, e^{i\bar{p}.\bar{r}}\, d\bar{r} \qquad \text{-----(3.17)}$$

Theorem If $u(r) = \dfrac{e^2\, z_a z_b}{\epsilon r}$, then $\hat{u}(p) = \dfrac{z_a z_b}{(2\pi)^{3/2}} \cdot \dfrac{e^2}{\epsilon} \cdot \dfrac{4\pi}{p^2}$

Proof Let $a = \dfrac{e^2 z_a z_b}{\epsilon}$

$$\therefore\ u(r) = \frac{a}{r} \equiv \lim_{\alpha \to 0} \frac{a}{r} e^{-\alpha r}$$

Use spherical coordinate

$$d\bar{r} = r^2 \sin\theta\, dr\, d\theta\, d\phi$$

$$\hat{u}(p) = \frac{1}{(2\pi)^{3/2}} \int_0^{\infty} r^2 e^{-\alpha r} dr \int_0^{\pi} \frac{a}{r} e^{iprcos\theta} \sin\theta d\theta \int_0^{2\pi} d\phi$$

$$= \frac{1}{(2\pi)^{3/2}} \cdot (2\pi) \int_0^{\infty} r^2 e^{-\alpha r}\, dr \int_0^{\pi} \frac{a}{r} e^{iprcos\theta}\, d(-\cos\theta)$$

$$= \frac{1}{(2\pi)^{3/2}} \cdot (2\pi) \int_0^{\infty} r^2 dr \; e^{-\alpha r} \left[\frac{e^{ipr} - e^{ipr}}{ipr^2} \right] a$$

$$= \frac{(2\pi)}{(2\pi)^{3/2}}(a) \lim_{\alpha \to 0} \int_0^{\infty} \frac{1}{ip} \left[e^{(ip-\alpha)r} - e^{-(ip+\alpha)r} \right] dr$$

$$= \frac{(2\pi)}{(2\pi)^{3/2}}(a) \lim_{\alpha \to 0} \frac{1}{ip} \left[\frac{e^{(ip-\alpha)r}}{(ip-\alpha)} + \frac{e^{-(ip+\alpha)r}}{(ip+\alpha)} \right]_0^{\infty}$$

$$= \frac{(2\pi)}{(2\pi)^{3/2}}(a) . \frac{1}{ip} \lim_{\alpha \to 0} \left[\frac{2ip}{p^2+\alpha^2} \right]$$

$$\hat{u}(p) = \frac{z_a z_b}{(2\pi)^{3/2}} \cdot \frac{e^2}{\epsilon} \cdot \frac{4\pi}{p^2} \qquad \text{-----(3.18)}$$

Theorem of Fourier transform on graph

Define the connected graph without additional line of t+1 vertices by

$$F(\bar{r}_1 - \bar{r}_{t+1}) = \int \cdots \int K(\bar{r}_1 - \bar{r}_2) K(\bar{r}_2 - \bar{r}_3) \ldots K(\bar{r}_t - \bar{r}_{t+1}) d\bar{r}_2 \ldots d\bar{r}_t \qquad \text{-----(3.19)}$$

If $\bar{r}_{t+1} \longrightarrow \bar{r}_1$, we have a ring,

$$F(\bar{0}) = \int \cdots \int K(\bar{r}_1 - \bar{r}_2) K(\bar{r}_2 - \bar{r}_3) \ldots K(\bar{r}_t - \bar{r}_1) d\bar{r}_2 \ldots d\bar{r}_t \qquad \text{-----(3.20)}$$

Let

$\bar{r}_1 \longrightarrow \bar{r}$, $\bar{r}_{t+1} \longrightarrow \bar{0}$, equation (3.19) becomes

$$F(\bar{r}) = \int\cdots\int K(\bar{r}-\bar{r}_2)K(\bar{r}_2-\bar{r}_3)\cdots K(\bar{r}_t)d\bar{r}_2\cdots d\bar{r}_t$$

Multiplying both sides by $\frac{1}{(2\pi)^{3/2}}.e^{i\bar{p}.\bar{r}}$ and integrating with respect to $d\bar{r}$, we have

$$\frac{1}{(2\pi)^{3/2}}\int F(\bar{r})\, e^{i\bar{p}.\bar{r}}\, d\bar{r} = \frac{1}{(2\pi)^{3/2}}\int\cdots\int e^{i\bar{p}.\bar{r}}K(\bar{r}-\bar{r}_2)$$

$$K(\bar{r}_2-\bar{r}_3)\cdots K(\bar{r}_t)d\bar{r}d\bar{r}_2\cdots d\bar{r}_t$$

By Jacobian transformation; $d\bar{r}_1 d\bar{r}_2 \longrightarrow d(\bar{r}_1-\bar{r}_2)\, d\bar{r}_2$

$$d\bar{r}d\bar{r}_2\cdots d\bar{r}_t \longrightarrow d(\bar{r}-\bar{r}_2)d(\bar{r}_2-\bar{r}_3)\cdots d(\bar{r}_{t-1}-\bar{r}_t)\, d\bar{r}_t$$

$$\therefore\quad \frac{1}{(2\pi)^{3/2}}\int F(\bar{r})e^{i\bar{p}.\bar{r}}\, d\bar{r} = \frac{1}{(2\pi)^{3/2}}\left[\int K(\bar{r}-\bar{r}_2)e^{i\bar{p}.(\bar{r}-\bar{r}_2)}\, d(\bar{r}-\bar{r}_2)\right]\cdots$$

$$\left[\int K(\bar{r}_t)\, e^{i\bar{p}.\bar{r}_t}\, d\,\bar{r}_t\right] \qquad ----(3.21)$$

By the definition of Fourier transform, let

$$\hat{K}(\bar{p}) = \frac{1}{(2\pi)^{3/2}}\int K(\bar{r})\, e^{i\bar{p}.\bar{r}}\, d\bar{r} \qquad ----(3.22)$$

$$\hat{F}(\bar{p}) = \frac{1}{(2\pi)^{3/2}}\int F(\bar{r})\, e^{i\bar{p}.\bar{r}}\, d\bar{r} \qquad ----(3.23)$$

Thus, equation (3.21) becomes

$$\hat{F}(\bar{p}) = \frac{1}{(2\pi)^{3/2}}\left[(2\pi)^{3/2}\hat{K}(\bar{p})\right]^t \qquad ----(3.24)$$

and

$$F(\bar{r}) = \frac{1}{(2\pi)^{3/2}}\int \hat{F}(\bar{p})\, e^{-i\bar{p}.\bar{r}}\, d\bar{p} \qquad ----(3.25)$$

For a ring $\bar{r} \longrightarrow \bar{0}$

$$F_t(\bar{0}) = \frac{1}{(2\pi)^{3/2}} \int \hat{F}(\bar{p})d\bar{p} = \frac{1}{(2\pi)^3} \int \left[(2\pi)^{3/2} \hat{K}(\bar{p})\right]^t d\bar{p} \quad \text{--(3.26)}$$

We also define

$$A_t = \int F_t(\bar{0})\, d\bar{r}_1 = V\, F_t(\bar{0}) \quad \text{-----(3.27)}$$

For the connected graph with additional lines, we define,

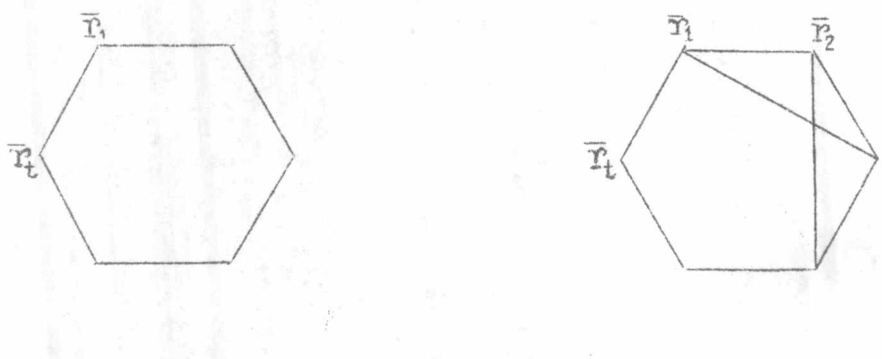
$$G(\bar{r}_1-\bar{r}_{t+1}) = \int\cdots\int K(\bar{r}_1-\bar{r}_2)K(\bar{r}_2-\bar{r}_3)K(\bar{r}_1-\bar{r}_3)\ldots K(\bar{r}_t-\bar{r}_{r+1})d\bar{r}_2\ldots d\bar{r}_t \quad \text{-----(3.28)}$$

If $\bar{r}_{t+1} \longrightarrow \bar{r}_1$, it becomes a ring with additional lines

$$G(\bar{0}) = \int\cdots\int K(\bar{r}_1-\bar{r}_2)K(\bar{r}_2-\bar{r}_3)K(\bar{r}_1-\bar{r}_3)\ldots K(\bar{r}_t-\bar{r}_1)d\bar{r}_2\ldots d\bar{r}_t \quad \text{-----(3.29)}$$

We also define

$$B = \int G(\bar{0})\, d\bar{r}_1 = V\, G(\bar{0}) \quad \text{-----(3.30)}$$



(a) A ring without additional line (b) A ring with additional lines

Figure 4, The ring diagram

We now consider the terms $f_{12}f_{23}f_{13}$, $f_{12}f_{23}f_{34}f_{14}$, in the irreducible cluster integral which we have

$$f_{ij} = e^{-u(r_{ij})/kT} - 1 = e^{-\beta u_{ij}} - 1$$

where $u(r_{ij}) = u_{ij}$, $\beta = 1/kT$.

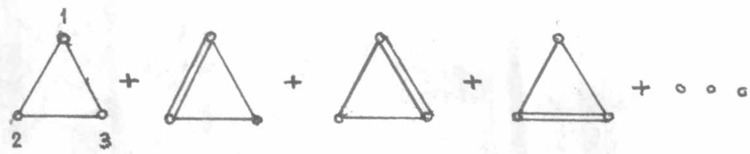
For 3-particles ring

$$f_{12}f_{13}f_{23} = (e^{-\beta u_{12}}-1)(e^{-\beta u_{23}}-1)(e^{-\beta u_{13}}-1)$$

$$= (-\beta)^3(u_{12}u_{23}u_{13}) + \text{higher order terms}$$

We can write in the ring diagram

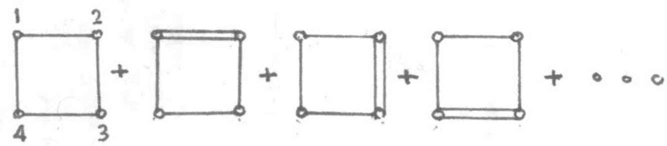
$f_{12}f_{13}f_{23}$ =



For 4-particles ring

$$f_{12}f_{23}f_{34}f_{41} = (-\beta)^4 (u_{12}u_{23}u_{34}u_{41}) + \text{higher order terms}$$

$f_{12}f_{23}f_{34}f_{41}$ =



For the real gas with electrostatic interaction, we know that the interaction potential between molecules i and j is defined by

$$u(r) = \frac{e^2 z_i z_j}{\epsilon r} \qquad \text{----(3.31)}$$

But equation (3.18), we have

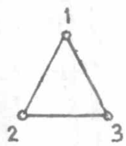
$$\hat{u}(p) = \frac{z_i z_j}{(2\pi)^{3/2}} \cdot \frac{e^2}{\epsilon} \cdot \frac{4\pi}{p^2} = \frac{C}{p^2} \qquad \text{-----(3.32)}$$

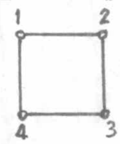
By the theorem of Fourier transform on graph, a ring of t-particles is defined by

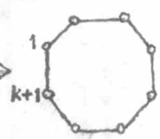
$$F_t(\bar{0}) = \int \hat{u}(p)\, d\bar{p} = \int \left(\frac{1}{p^2}\right)^t (C)^t\, d\bar{p} \qquad \text{----}(3.33)$$

We find that the higher order terms of the irreducible integral have negligible values in comparison with the leading term, therefore, we can neglect these higher order terms.

Therefore, in what follows we shall neglect the ring with additional lines. For examples, we retain only such terms as.

$f_{12}f_{23}f_{13} \longrightarrow$ 

$f_{12}f_{23}f_{34}f_{14} \longrightarrow$ 

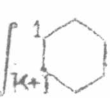
$f_{12}f_{23}\cdots f_{k+1,1} \longrightarrow$ 

By the definition of the irreducible cluster integral, we have Eq.(2.66)

$$\beta_k = \frac{1}{k!V}\int\cdots\int \sum_{k+1 \geq i > j \geq 1} f_{ij}\, d\bar{r}_1 \cdots d\bar{r}_{k+1},$$

All products with more than singly connected.

Now we define β_{ko} is a ring without additional line which contributed to β_k.

$$\beta_{ko} = \frac{1}{k!}\,\frac{1}{V}(-\beta)^{k+1}\,\frac{(k+1)!}{(k+1)(2)} \int_{k+1}^{1}$$  $$d\bar{r}_{k+1} \qquad \text{----}(3.34)$$

The factor $\frac{(k+1)!}{(k+1)(2)}$ is due to the way to count for the ring in the irreducible cluster integral.

By the definition of Fourier transform on graph, we obtain

$$\beta'_{ko} = \frac{1}{2V} (-\beta)^{k+1} V F_{k+1}(\bar{0})$$

$$\beta'_{ko} = \frac{1}{2} (-\beta)^{k+1} \frac{1}{(2\pi)^3} \int \left[(2\pi)^{3/2} \hat{u}(\bar{p}) \right]^{k+1} d\bar{p} \quad \text{----(3.35)}$$

From the equation (3.10), we have

$$Q_N = V^N \exp \left[N \sum_{k=1}^{\infty} \frac{\beta_k \rho^k}{k+1} \right] \quad \text{----(3.36)}$$

Let $S(\rho') = \sum_{k=1}^{\infty} \beta_k \rho'^k$

$$\int_0^\rho S(\rho')d\rho' = \sum_{k=1}^{\infty} \frac{\beta_k \rho^{k+1}}{k+1} = \rho \sum_{k=1}^{\infty} \frac{\beta_k \rho^k}{k+1}$$

$$\frac{1}{\rho} \int_0^\rho S(\rho')d\rho' = \sum_{k=1}^{\infty} \frac{\beta_k \rho^k}{k+1}$$

$$\therefore \quad Q_N = V^N \exp \left[\frac{N}{\rho} \int_0^\infty S(\rho') \, d\rho' \right] \quad \text{----(3.37)}$$

For a ring without additional line, we define

$$S_o(\rho) = \sum_{k=1}^{\infty} \beta'_{ko} \rho^k \quad \text{----(3.38)}$$

$$S_o(\rho) = \sum_{k=1}^{\infty} \frac{1}{2} \frac{\rho^k}{(2\pi)^3} (-\beta)^{k+1} \int \left[(2\pi)^{3/2} \hat{u}(p) \right]^{k+1} d\bar{p}$$

$$= \frac{1}{2} \frac{1}{(2\pi)^3} \int \sum_{k=1}^{\infty} \rho^k \left[(2\pi)^{3/2} (-\beta) \hat{u}(p) \right]^{k+1} d\bar{p}$$

Let $a = \left[(2\pi)^{3/2} (-\beta) \hat{u}(p) \right]$

$$S_o(\rho) = \frac{1}{2}\frac{1}{(2\pi)^3}\int \sum_{k=1}^{\infty} \rho^k \, a^{k+1} \, d\bar{p}$$

$$= \frac{1}{2}\frac{1}{(2\pi)^3} \rho \, a^2 \int \sum_{k=1}^{\infty} \rho^{k-1} \, a^{k-1} \, d\bar{p}$$

$$= \frac{1}{2}\frac{1}{(2\pi)^3} \rho \, a^2 \int \sum_{k=o}^{\infty} \rho^k a^k \, d\bar{p}$$

$$S_o(\rho) = \frac{1}{2}\frac{1}{(2\pi)^3} \rho \, a^2 \int \frac{1}{(1-\rho a)} \, d\bar{p}$$

$$= \frac{1}{2} \beta^2 \rho \int \frac{\hat{u}(p)^{\;2}}{1+(2\pi)^{3/2}\beta\rho\,\hat{u}(p)} \cdot d\bar{p}$$

Substitute $\hat{u}(p) = \frac{z_i z_j \, e^2}{(2\pi)^{3/2}\epsilon} \cdot \frac{4\pi}{p^2}$ from Eq. (3.18),

$$S_o(\rho) = \frac{z_i^2 z_j^2 \, e^4 \beta^2 \rho}{\pi \, \epsilon^2} \int \frac{1/p^4}{1+\rho\beta\left(\frac{z_i z_j 4\pi \, e^2}{\epsilon}\right)\frac{1}{p^2}} \, d\bar{p}$$

Use the symmetrical spherical coordinate, we have

$$d\bar{p} = 4\pi \, p^2 \, dp$$

Thus,

$$S_o(\rho) = \frac{4 z_i^2 \, z_j^2 \, e^4 \, \beta^2 \rho}{\epsilon^2} \int_o^{\infty} \frac{1}{p^2 + \rho\beta\left(\frac{z_i z_j 4\pi e^2}{\epsilon}\right)} \, dp$$

$$= \left(\frac{z_i z_j \beta}{\epsilon}\right)^{3/2} e^3 \, \pi^{\frac{1}{2}} \, \rho^{\frac{1}{2}} \qquad \text{-----(3.39))}$$

$$S_o \, (\rho) \approx \sqrt{\rho} \qquad \text{-----(3.40)}$$