July 30, 1980

I would like next to get some idea of the Green's functions that go along with the grand canonical ensemble.

Consider an Ising model. A state is described by giving the spin s_x at each site x. On[redacted] the set of states one has the Bolzmann prob. measure. The Green's functions are then the moments

$$\left\langle \prod_x s_x^{n_x} \right\rangle$$

where [redacted] $n_x = 0$ except for a finite number of x.

This Ising situation can be generalized as follows. One has a field described by variables ϕ_x at each site x. To be specific, think of ϕ_x as a real scalar; (it could be a vector). Then we have a partition function

$$Z = \int e^{-\beta S(\phi)} \mathcal{D}\phi \qquad \text{and Bolzmann measure} \quad \frac{e^{-\beta S(\phi)}}{Z}$$

on the set of configurations. The Green's functions are the moments of the Bolzmann measure and can be obtained from the generating function

$$Z(J) = \int e^{\beta \sum_x J_x \phi_x - \beta S(\phi)} \mathcal{D}\phi \Big/ \int e^{-\beta S(\phi)} \mathcal{D}\phi$$

(Perhaps β should be absorbed into S and J.)

Consider now the grand partition function

$$Z = \sum \frac{z^n}{n!} \int e^{-\beta U_n} \, dq_1 \cdots dq_n .$$

We can interpret this as a sum over configurations, provided we define a configuration to be a finite sequence of points $q_1, \ldots, q_n$ modulo changing the order. A better way to say this is a configuration is a [redacted] positive divisor $\sum n_q q$ on q-space.

Consequently we have a field [redacted] $n(q)$ over q-space taking the values $0, 1, 2, \ldots$, with only finitely many $n(q) > 0$. A configuration is a set of $n(q)$ and we have the [redacted] Boltzmann measure on this set of configurations. It is clear now what the Green's functions are from this viewpoint. They are expectation values of monomials in the variables $n(q)$.

What is a generating function? Let's take a simple example where

(*) $$U_n(q_1, \ldots, q_n) = \sum_{i=1}^{n} f(q_i)$$

Then

$$\frac{z^n}{n!} \int e^{-\beta U_n} dq_1 \ldots dq_n = \frac{1}{n!}\left(\int z e^{-\beta f(q)} dq\right)^n$$

so to get a generating function it seems like we want to replace z by a function of q. Thus our generating function is something like

$$\tilde{Z} = \sum_n \frac{1}{n!} \int z(q_1) \cdots z(q_n)\, e^{-\beta U_n(q_1, \ldots, q_n)} dq_1 \ldots dq_n .$$

Maybe we should put $z(q) = e^{\beta \mu(q)}$ where $\mu(q)$ = chemical potential at q. Then assuming (*) we have

$$\tilde{Z} = \exp\left(\int e^{\beta\mu(q) - \beta f(q)} dq\right) .$$

Thus $\tilde{Z}$ is a function of the variables $\mu(q)$, i.e. a function of the function μ. Perhaps I should think of $\tilde{Z}$ as a power series in the variables [redacted] $z(q) = e^{\beta\mu(q)}$.

Now fix a site q_0 and consider the moments $\langle n(q_0)^r \rangle$. In the independent particle model (*) we see that formally

$$\tilde{Z} = \exp\left([redacted]\ z(q_0) e^{-\beta f(q_0)} + \text{stuff independent of } z(q_0) \right).$$

Since

$$\langle n(q_0)^r \rangle = \frac{1}{\tilde{Z}} [redacted] \left(z(q_0) \frac{\partial}{\partial z(q_0)} \right)^r \tilde{Z}$$

we should understand what sort of prob. distribution on $\mathbb{N}$ belonging to a partition function of the form

$$[redacted]\ e^{za+b} = e^b \sum \frac{z^n a^n}{n!}$$

Clearly we get a Poisson distribution

$$p_n = e^{-za} \frac{(za)^n}{n!}$$

So therefore we see that in the independent particle model [redacted] the variable $n(q_0)$ is governed by a Poisson distribution with mean $e^{\beta(\mu(q_0) - f(q_0))}$.

This is like the formulas

$$\langle n_\alpha \rangle = e^{\beta\mu - \beta\varepsilon_\alpha}$$

$$= \frac{1}{e^{\beta(\varepsilon_\alpha - \mu)} \mp 1} \qquad \begin{array}{l} - \text{ Bose statistics} \\ + \text{ FD } \quad " \end{array}$$

and suggests refining the latter to an understanding of the actual probality distribution.

In the FD case $n=0$ or 1 and the probabilities are

$$\frac{p_0}{p_1} = \frac{p_0}{1-p_0} = e^{+\beta(\varepsilon-\mu)} \qquad p_0 = \frac{e^{\beta(\varepsilon-\mu)}}{e^{\beta(\varepsilon-\mu)}+1}$$

$$p_1 = \frac{1}{e^{\beta(\varepsilon-\mu)}+1}$$

so the mean $\langle n \rangle = p_1$ completely specifies the distribution.

In the BE case the probabilities form a geometric series.

$$p_n = \left(e^{-\beta(\varepsilon-\mu)}\right)^n / Z \qquad Z = \frac{1}{1-e^{-\beta(\varepsilon-\mu)}}$$

Thus $\quad p_n = r^n - r^{n+1} \quad$ where $\quad r = e^{-\beta(\varepsilon-\mu)}$.

and $\quad \langle n \rangle = r - r^2 + 2(r^2 - r^3) + \cdots = r + r^2 + r^3 + \cdots = \frac{r}{1-r}$

specifies the distribution, provided we assume it has this geometric form.

One of the ideas I really want to explore is the possibility of obtaining amplitudes for some quantum theory as integrals over discrete configurations.

Given a measure $d\mu$ on R one has its moments

$$c_n = \frac{\int x^n \, d\mu}{\int d\mu} = \frac{1}{Z}\frac{d^n Z}{dJ^n}\bigg|_{J=0}$$

where $\quad Z(J) = \int e^{Jx} d\mu \Big/ \int d\mu$

One also has reduced moments

$$b_n = \frac{d^n}{dJ^n} \log Z \bigg|_{J=0}$$

Thus $\quad b_0 = 0 \qquad b_1 = c_1$

$$b_2 = \frac{d^2}{dJ^2}\log Z\Big|_{J=0} = \frac{d}{dJ}\left(Z^{-1}\frac{dZ}{dJ}\right) = Z^{-1}\frac{d^2Z}{dJ^2} - Z^{-1}\frac{dZ}{dJ}\,Z^{-1}\frac{dZ}{dJ}\Big|_{J=0}$$

$$= c_2 - c_1^2 \qquad \text{i.e.} \quad \langle x^2\rangle - \langle x\rangle^2$$

$$b_3 = Z^{-1}\frac{d^3Z}{dJ^3} - 3Z^{-1}\frac{dZ}{dJ}\,Z^{-1}\frac{d^2Z}{dJ^2} + 2Z^{-1}$$ [redacted] $$\frac{dZ}{dJ}\,Z^{-1}\frac{dZ}{dJ}\,Z^{-1}\frac{dZ}{dJ}$$

$$= c_3 - 3c_1c_2 + 2c_1^3$$

Examples: 1) Gaussian $\quad d\mu = \frac{1}{\sqrt{2\pi a}}\, e^{-\frac{x^2}{2a}}$

$$Z(J) = \int e^{Jx - \frac{x^2}{2a}}\frac{dx}{\sqrt{2\pi a}} = e^{a\frac{J^2}{2}}$$

$$\therefore \quad \log Z(J) = a\frac{J^2}{2} \quad \text{so} \quad b_2 = a \quad \text{and rest of } b_n = 0.$$

2) Poisson $\quad p_n = e^{-\lambda}\frac{\lambda^n}{n!}$ for $n \in \mathbb{N}$

$$Z(J) = \sum e^{Jn}\, e^{-\lambda}\frac{\lambda^n}{n!} = e^{\lambda(e^J - 1)}$$

$$\log Z(J) = \lambda(e^J - 1) = \sum_{n=1}^{\infty} \lambda \frac{J^n}{n!} \qquad \text{hence all } b_n = \lambda$$

3) FD with $p_1/p_0 = e^{-\beta\varepsilon}$. Then $p_0 = \frac{1}{1+e^{-\beta\varepsilon}} \quad p_1 = \frac{e^{-\beta\varepsilon}}{1+e^{-\beta\varepsilon}}$

so $$Z(J) = \frac{1 + e^{J-\beta\varepsilon}}{1 + e^{-\beta\varepsilon}}$$

4) BE with $p_n/p_{n-1} = e^{-\beta\varepsilon}$. Then

$$Z(J) = \frac{\sum e^{Jn}(e^{-\beta\varepsilon})^n}{\sum (e^{-\beta\varepsilon})^n} = \frac{1 - e^{-\beta\varepsilon}}{1 - e^{J-\beta\varepsilon}}$$

There doesn't seem to be a simple formula for the reduced moments.

<u>July 31, 1980</u>

We are trying to understand the Green's functions belonging to the grand canonical partition function

$$Z_{gr} = \sum_n \frac{z^n}{n!} \int e^{-\beta U_n} dq_1 \cdots dq_n$$

Yesterday we saw the possibility of viewing this as a sum over configurations, where a configuration is defined as a positive divisor in q-space. Thus instead of a spin variable at each site we have an occupation number $n(q)$ which is in $\mathbb{N}$ and is a.e. 0.

Let us simplify by taking q-space to be a finite set, say $q \in \{1, \ldots, R\}$. Then because the weight of a configuration [redacted]

[redacted] $\underbrace{1, 1, \ldots, 1}_{n_1}, \underbrace{2 \cdots 2}_{n_2}, \cdots, \underbrace{R \cdots R}_{n_R}$

is

$$z^{\sum n_q} \frac{1}{\prod n_q!} e^{-\beta \underbrace{U(1,\ldots,1, 2\cdots 2, \ldots, R \cdots R)}_{\| \text{ by defn. of } \tilde{U}}}$$

we can write

$$Z_{gr} = \sum_{n_1, \ldots, n_R} \frac{z^{\sum n_q}}{\prod n_q!} e^{-\beta \tilde{U}(n_1, \ldots, n_R)}$$

A Greens function in analogy with Ising models is a moment of a polynomial $\prod n_q^{\alpha_q}$ in the variables n_q describing the configuration. We can get at these moments by introducing activity variables

z_q at each site q and forming

$$\tilde{Z}_{gr} = \sum_{n_1, \ldots, n_R} \prod_{q=1}^{R} \frac{z_q^{n_q}}{n_q!} e^{-\beta \tilde{\mathcal{U}}(n_1, \ldots, n_R)}$$

Then one has

$$\left\langle \prod n_q^{\alpha_q} \right\rangle = \frac{1}{\tilde{Z}_{gr}} \prod \left(z_q \frac{\partial}{\partial z_q} \right)^{\alpha_q} \tilde{Z}_{gr} \Bigg|_{z_q = z}$$

Look at $\langle n_1^{\alpha_1} \rangle = \frac{1}{\tilde{Z}_{gr}} \left(z_1 \frac{\partial}{\partial z_1} \right)^{\alpha_1} \tilde{Z}_{gr} \Big|_{z_q = z}$

We can write

$$\tilde{Z}_{gr} = \sum_{n_1} \frac{z_1^{n_1}}{n_1!} \sum_{n_2, \ldots, n_R} \frac{z_2^{n_2} \cdots z_R^{n_R}}{n_2! \cdots n_R!} e^{-\beta \tilde{\mathcal{U}}(n_1, n_2, \ldots, n_R)}$$

Let's set $z_2 = \cdots = z_R = z$ in the 2nd sum and observe that it is a partition function for configurations at the sites $q = 2, \ldots, R$ with energy calculated as if n_1 atoms are present at $q = 1$. Put

$$Q(n_1, z) = \sum_{n_2, \ldots, n_R} \frac{z^{n_2 + \cdots + n_R}}{n_2! \cdots n_R!} e^{-\beta \tilde{\mathcal{U}}(n_1, n_2, \ldots, n_R)}$$

Then

$$\tilde{Z}_{gr} \Big|_{z_2 = \cdots = z_R = z} = \sum \frac{z_1^{n_1}}{n_1!} Q(n_1, z)$$

so

$$\langle n_1^{\alpha_1} \rangle = \frac{\sum (n_1)^{\alpha_1} \frac{z_1^{n_1}}{n_1!} Q(n_1, z)}{\sum \frac{z_1^{n_1}}{n_1!} Q(n_1, z)} \Bigg|_{z_1 = z}$$

The denominator is just Z_{gr}

So what we find is that the [redacted] probability distribution for the variable n_1 is given by

$$P(n_1 = m) = \frac{\displaystyle\sum_{n_1 = m,\, n_2 \dots n_g} \frac{z^{\sum n_g}}{\prod n_g!}\, e^{-\beta U(n_1, \dots, n_g)}}{\displaystyle\sum_{n_1, \dots, n_g} \frac{z^{\sum n_g}}{\prod n_g!}\, e^{-\beta U(n_1, \dots, n_g)}}$$

which should have been completely obvious from the beginning – namely you just take the part of the partition function belonging to these occupation numbers.

functional differentiation: Let us consider a functional $F(f)$, that is, a function of the function f. I want to work out the concept of Taylor series for [redacted] F. First we need linear functionals. In good cases a linear functional is of the form

$$F(f) = \int f(x)\, g(x)\, dx$$

i.e. if we think of f as an infinite-dimensional vector with the components $f(x)$, then $F(f)$ is [redacted] the dot product of f with the vector $g = (g(x))$. A quadratic functional is obtained by multiplying two linear fnls.

$$\int f(x) g_1(x)\, dx \int f(x) g_2(x)\, dx$$

$$= \iint f(x_1) f(x_2)\; g_1(x_1) g_2(x_2)\, dx_1\, dx_2$$

$$= \frac{1}{2!} \iint f(x_1) f(x_2) \underbrace{\left[g_1(x_1) g_2(x_2) + g_1(x_2) g_2(x_1) \right]}_{g(x_1, x_2)} dx_1\, dx_2$$

where g is symm.

The [redacted] Taylor series of F [redacted] can be expected to look like

$$(*) \quad F(f) = [\text{redacted}]\; g_0 + \int g_1(x_1) f(x_1)\, dx_1 + \frac{1}{2!} \iint g_2(x_1, x_2) f(x_1) f(x_2)\, dx_1\, dx_2 + \cdots$$

and now what I want is to obtain the coefficient functions $g_n(x_1, \ldots, x_n)$ [redacted] by the process of functional differentiation.

The idea is to define the functional derivative by varying f to $f+\delta f$. Thus

$$F(f+\delta f) = F(f) + \underset{\text{in } \delta f}{\text{linear term}} + O((\delta f)^2)$$

One can be precise by putting $\delta f = \varepsilon\eta$ and then

$$F(f+\varepsilon\eta) = F(f) + \frac{d}{d\varepsilon} F(f+\varepsilon\eta)\Big|_{\varepsilon=0} \cdot \varepsilon + O(\varepsilon^2)$$

In good cases the linear term can be expressed.

$$\frac{d}{d\varepsilon} F(f+\varepsilon\eta)\Big|_{\varepsilon=0} = \int g(x)\,\eta(x)\,dx$$

and one writes [redacted] $g = \nabla F(f)$

so that

$$F(f+\varepsilon\eta) = F(f) + \nabla F(f) \bullet \varepsilon\eta + O(\varepsilon^2)$$

Another notation uses is that

$$\nabla F(f)(x) = \frac{\delta F}{\delta f(x)}(f).$$

The point is that this functional derivative depends on the measure dx used to define the dot product of functions.

It is clear that if ⊛ holds, then we can functionally differentiate

[redacted]

$$\frac{\delta F}{\delta f(x)} = g_1(x) + \int g_2(x,x_1) f(x_1)\,dx_1$$

$$+ \frac{1}{2!}\iint g_3(x,x_1,x_2) f(x_1) f(x_2)\,dx_1\,dx_2 + \cdots$$

In effect

$$\delta \frac{1}{n!} \int \cdots \int g_n(x_1, \ldots, x_n) f(x_1) \cdots f(x_n)\, dx_1 \cdots dx_n$$

$$= \frac{1}{n!} \int \cdots \int g_n(x_1, \ldots, x_n) \left[\delta f(x_1) f(x_2) \cdots f(x_n) + f(x_1)\, \delta f(x_2) f(x_3) \cdots f(x_n) + \cdots \right] dx_1 \cdots dx_n$$

$$+ O((\delta f)^2)$$

By the symmetry of g_n, this is

$$\frac{1}{(n-1)!} \int \cdots \int g_n(x_1, \ldots, x_n)\, \delta f(x_1)\, f(x_2) \cdots f(x_n)\, dx_1 \cdots dx_n$$

so it works.

Therefore by repeated differentiation we obtain

$$\frac{\delta^n}{\delta f(x_1) \cdots \delta f(x_n)} F(f) \Big|_{f=0} = g_n(x_1, \ldots, x_n)$$

Consider next a grand partition fn.

$$\tilde{Z}(z) = \sum_n \frac{1}{n!} \int z(q_1) \cdots z(q_n)\, e^{-\beta U(q_1, \ldots, q_n)}\, dq_1 \cdots dq_n$$

which is evidently a functional of the activity function $z(q)$. We get the usual grand partition function by setting $z(q)$ = the constant z, however we [redacted] can obviously ask questions about energy and density for an arbitrary activity level. Is there a particle density $\rho(q)$ function belonging to a general variable activity level $z(q)$?

Compute

$$\frac{\delta \tilde{Z}}{\delta z(q)} = \sum_n \frac{1}{n!} \int e^{-\beta U(q, q_1, \ldots, q_n)}\, z(q_1) \cdots z(q_n)\, dq_1 \cdots dq_n$$

Is it possible for $z(q)\frac{\delta}{\delta z(q)}\log\tilde{Z}$ to be the particle density at q?

$$\int z(q)\frac{\delta\tilde{Z}}{\delta z(q)}dq = \sum_n \frac{1}{n!}\int e^{-\beta U(q,q_1,\dots,q_n)} z(q)\cdots z(q_n)\, dq\, dq_1\cdots dq_n$$

$$= \sum_n \frac{n}{n!}\int e^{-\beta U(q_1,\dots,q_n)} z(q_1)\cdots z(q_n)\, dq_1\cdots dq_n$$

So when divided by [redacted] $\tilde{Z}$ you get $\langle n\rangle$ the average number of particles.

Therefore

$$\langle n(q)\rangle = z(q)\frac{\delta}{\delta z(q)}\log\tilde{Z}$$

is the particle density at the point q. When all $z(q)=z$ and U is translation invariant, it will be $\frac{N}{V}$ for all q.

Here's an important point about the expansion:

$$F(f) = g_0 + \int g_1(x_1)f(x_1)dx_1 + \frac{1}{2!}\int g_2(x_1,x_2)f(x_1)f(x_2)dx_1\,dx_2 + \dots$$

$$g_n(x_1,\dots,x_n) = \left.\frac{\delta^n}{\delta f(x_1)\cdots\delta f(x_n)}F\right|_{f=0}$$

The point is that the values of g_n for equal values of the arguments $x_1,\dots,x_n$, say $x_i = x_j$, are not really well-defined. Hence there [redacted] may be some sort of problem with

$$z(q_1)\frac{\delta}{\delta z(q_1)}\quad z(q_2)\frac{\delta}{\delta z(q_2)}$$

$$z(x)\,\frac{\delta \tilde{Z}}{\delta z(x)} = \sum_n \frac{z(x)}{n!}\int e^{-\beta U(x,q_1,\dots,q_n)}\, z(q_1)\cdots z(q_n)\, dq_1\cdots dq_n$$

This is a function of x and of z. Now vary z

$$\delta\left(z(x)\,\frac{\delta \tilde{Z}}{\delta z(x)}\right) = \sum_n \frac{\delta z(x)}{n!}\int e^{-\beta U(x,q_1,\dots,q_n)}\, z(q_1)\cdots z(q_n)\, dq_1\cdots dq_n$$

$$+\sum_n \frac{z(x)}{n!}\int e^{-\beta U(x,q_0,\dots,q_n)}\,\delta z(q_0)\, z(q_1)\cdots z(q_n)\, dq_0\cdots dq_n$$

$$\therefore\ \frac{\delta}{\delta z(y)}\left(z(x)\,\frac{\delta \tilde{Z}}{\delta z(x)}\right) = \delta(x-y)\sum_n \frac{1}{n!}\int e^{-\beta U(x,q_1,\dots,q_n)}\, z(q_1)\cdots z(q_n)\, dq_1\cdots dq_n$$

$$+\sum_n \frac{z(x)}{n!}\int e^{-\beta U(x,y,q_1,\dots,q_n)}\, z(q_1)\cdots z(q_n)\, dq_1\cdots dq_n$$

Therefore we obtain the rule

$$\frac{\delta}{\delta z(y)}\big(z(x)\big) = \delta(x-y)$$

because $\quad z(x) = \int \delta(x-y)\, z(y)\, dy$

$$\frac{\delta^2 \tilde{Z}}{\delta z(x)\,\delta z(y)} = \sum \frac{1}{n!}\int e^{-\beta U(x,y,q_1,\dots,q_n)}\, z(q_1)\cdots z(q_n)\, dq_1\cdots dq_n$$

$$\int dx\,dy\; z(x)z(y)\,\frac{\delta^2 \tilde{Z}}{\delta z(x)\,\delta z(y)} = \sum \frac{(n+1)(n+2)}{(n+2)!}\int e^{-\beta U(q_1,q_2,\dots,q_{n+2})}\, z(q_1)\cdots z(q_{n+2})\, dq_1\cdots dq_{n+2}$$

Thus

$$\frac{1}{\tilde{Z}}\int dx\,dy\; z(x)z(y)\,\frac{\delta^2 \tilde{Z}}{\delta z(x)\,\delta z(y)} = \frac{1}{\tilde{Z}}\sum \frac{n(n-1)}{n!}\int e^{-\beta U(q_1,\dots,q_n)}\, z(q_1)\cdots z(q_n)\, dq_1\cdots dq_n$$

$$= \langle n(n-1)\rangle$$

which is consistent with

$$\frac{1}{\tilde{Z}}\int dx\,dy \quad z(x)\frac{\delta}{\delta z(x)}\left(z(y)\frac{\delta}{\delta z(y)}\tilde{Z}\right) = \frac{1}{\tilde{Z}}\int dx\,dy\left(z(x)z(y)\frac{\delta^2 \tilde{Z}}{\delta z(x)\delta z(y)} + \delta(x-y)z(x)\frac{\delta \tilde{Z}}{\delta z(x)}\right)$$

$$= \langle (n)(n-1)\rangle + \langle n\rangle = \langle n^2\rangle.$$

Hence we see that $z(x)\frac{\delta}{\delta z(x)}\left(z(y)\frac{\delta \tilde{Z}}{\delta z(y)}\right)$ is not smooth although $z(x)z(y)\frac{\delta^2 \tilde{Z}}{\delta z(x)\delta z(y)}$ is smooth. It seems that

$$\frac{1}{\tilde{Z}} \quad z(x)\frac{\delta}{\delta z(x)}\left(z(y)\frac{\delta}{\delta z(y)}\tilde{Z}\right) = \langle n(x)\,n(y)\rangle$$

[redacted] has a valid interpretation. Thus

$$\langle n(x)\,n(y)\rangle = \underbrace{\frac{1}{\tilde{Z}}\, z(x)z(y)\frac{\delta^2 \tilde{Z}}{\delta z(x)\delta z(y)}}_{\text{smooth}} + \delta(x-y)\underbrace{\frac{z(y)}{\tilde{Z}}\frac{\delta \tilde{Z}}{\delta z(y)}}_{\langle n(y)\rangle}$$

[redacted] as a distribution [redacted] on the product x,y space. It seems therefore to be effectively meaningless to talk about the moments $\langle n(x)^2\rangle$

Example: $U_n(q_1,\dots,q_n) = \sum_{i=1}^{n} V(q_i)$

Then

$$\tilde{Z} = \exp\left(\int z(x)e^{-\beta V(x)}\,dx\right)$$

$$\langle n(x)\rangle = \frac{\delta}{\delta z(x)}\log\tilde{Z} = e^{-\beta V(x)}$$

$$\frac{\delta}{\delta z(y)}\frac{\delta \tilde{Z}}{\delta z(x)} = \frac{\delta \tilde{Z}}{\delta z(y)}\,e^{-\beta V(x)} = \tilde{Z}\,e^{-\beta V(y)-\beta V(x)}$$

$$\langle n(x)\, n(y) \rangle = e^{-\beta(V(x)+V(y))} + \delta(x-y)\, e^{-\beta V(x)}$$

i.e $$\langle n(x)\, n(y) \rangle = \langle n(x) \rangle \langle n(y) \rangle + \delta(x-y) \langle n(y) \rangle$$

which agrees with the following calculation for the Poisson distribution:

$$\langle n^2 \rangle = \sum_{n\geq 0} \underbrace{n^2}_{n(n-1)+n} \frac{e^{-\lambda}\lambda^n}{n!} = \sum \frac{n(n-1)}{n!} e^{-\lambda}\lambda^n + \sum \frac{n}{n!} e^{-\lambda}\lambda^n$$

$$= \lambda^2 + \lambda = \langle n \rangle^2 + \langle n \rangle$$

August 2, 1980

We consider a classical grand partition function with variable activity $z(q)$:

$$\tilde{Z}(z) = \sum \frac{1}{n!} \int dq_1 \cdots dq_n \, z(q_1) \cdots z(q_n) \, e^{-\beta U_n(q_1, \ldots, q_n)}$$

We can think of this as a partition function where there is one configuration for each positive divisor $\{n(q)\}$ on q-space. Then [redacted] a point q gives a function $n(q)$ on the set of [redacted] configurations. We want to think of $n(q)$ as a random variable on the space of configurations, but this doesn't work because the probability of there being [redacted] a particle exactly at q is zero.

Our probability space looks as follows: X is q-space

$$pt \amalg X \amalg \left(X^2/\Sigma_2 \right) \amalg \cdots\cdots \quad = SP(X)$$

Suppose we have a subset [redacted] A of X with complement $\bar{A}$. Then

$$SP(X) = SP(A) \times SP(\bar{A})$$

and so we get a map

$$SP(X) \longrightarrow SP(A)$$

and hence an induced probability measure on [redacted] $SP(A)$.

$\tilde{Z}$ can be written

$$\tilde{Z} = \sum_{m,n} \frac{1}{m!\,n!} \int_{A^m} dq_1 \cdots dq_m \prod_{i=1}^{m} z(q_i) \int_{\bar{A}^n} dq_1' \cdots dq_n' \prod_{i=1}^{n} z(q_i') \, e^{-\beta U_{m+n}(q_1 \cdots q_n')}$$

If I take A to be a point, then dq restricted to A

gives 0, hence all the terms with $m>0$ vanish. On the other hand when we decompose

$$SP_n(X) = \coprod_{m=0}^{n} SP_m(A) \times SP_{n-m}(\bar{A})$$

the pieces with $m>0$ have measure 0, so the induced probability measure on $SP(A) = \mathbb{N}$ is the δ measure at 0.

So to get something interested we must assume A has positive measure in X, say A is a nice region.

First note how the prob. measure on $SP(X)$ arises. On X^n we have the measure

$$\frac{1}{n!} dq_1 \cdots dq_n \prod_{i=1}^{n} z(q_i)\, e^{-\beta U_n(q_1,\cdots q_n)}$$

and we push it via $X^n \longrightarrow SP_n(X)$ to get a measure $d\mu_n$ on $SP_n(X)$. Then we have measures on each $SP_n(X)$ and we have to normalize the sum measure on $SP(X) = \coprod SP_n(X)$ to be a prob. measure. This means dividing by

$$\sum_n \int d\mu_n = Z.$$

Now look what happens in the case of $SP(A)$. We have

$$SP_n(X) = \coprod SP_m(A) \times SP_{n-m}(\bar{A})$$

and the measure $d\mu_n$ decomposes as follows. On $A^m \times \bar{A}^{n-m}$ we have

$$\frac{1}{m!}\frac{1}{(n-m)!} dq_1 \cdots dq_m \prod z(q_i)\; dq_1' \cdots dq_{n-m}' \prod z(q_i')\, e^{-\beta U(q,q')}$$

and pushing this via $A^m \times \bar{A}^{n-m} \longrightarrow SP_m(A) \times SP_{n-m}(\bar{A})$ gives a measure $d\mu_{m,n-m}$ on the latter. Clearly

$$d\mu_n = \coprod_{m=0}^{n} d\mu_{m,n-m}$$

So now it is clear what kind of measure is obtained on $SP(A)$. On the piece $SP_m(A)$ we get

$$\sum_{n=0}^{\infty} d\mu_{m,n} \text{ pushed via } SP_m(A)\times SP_n(\bar{A}) \xrightarrow{pr_1} SP_m(A).$$

Thus we get

$$\frac{1}{m!}\, dq_1 \cdots dq_m \text{ [redacted] } \prod_{i=1}^{m} z(q_i) \sum_n \frac{1}{n!} \int_{\bar{A}^n} \text{[redacted]}\, dq_1' \cdots dq_n' \prod z(q_j')\, e^{-\beta \mathcal{U}(q_1,\dots,q_m,q_1',\dots,q_n')}$$

What this means is that we have a measure on $SP(A)$ based on a factor like $e^{-\beta \mathcal{U}(q)}$ which is computed by summing over the [redacted] possible configurations in $\bar{A}$. We could normalize and divide by the partition function for $\bar{A}$ if we want. Let's put:

$$\mathcal{U}_{m+n}(q,q') = \mathcal{U}_m(q) + \tilde{\mathcal{U}}_{m,n}(q,q') + \mathcal{U}_n(q').$$

Then upon dividing by $\tilde{Z}$ for $\bar{A}$ we get

$$\frac{1}{m!}\, d^m q \prod z(q_i)\, e^{-\beta \mathcal{U}_m(q)} \underbrace{\frac{\sum_n \frac{1}{n!} \int_{\bar{A}^n} d^n q' \prod z(q_j')\, e^{-\beta \mathcal{U}_n(q')}\, e^{-\beta \tilde{\mathcal{U}}_{m,n}(q,q')}}{\sum_n \frac{1}{n!} \int_{\bar{A}^n} d^n q' \prod z(q_j')\, e^{-\beta \mathcal{U}_n(q')}}}_{\text{average of } e^{-\beta \tilde{\mathcal{U}}_{m,n}(q,\underset{\text{variable}}{q'})} \text{ over } \bar{A}.}$$

So we see that the ~~probability~~ measure on $SP(A)$ is a grand measure associated to [redacted] a weighting which involves averaging out over the possible configurations in $\bar{A}$.

Let's consider the simple case of independent particles $\mathcal{U}_n(q) = \sum_{i=1}^{n} V(q_i)$. Then

$$\tilde{Z}_X = \exp\left\{ \int z(q) e^{-\beta V(q)} dq \right\}$$

$$\tilde{Z}_{\bar{A}} = \exp\left\{ \int_{\bar{A}} z(q') e^{-\beta V(q')} dq' \right\}.$$

so it's clear that we get the grand probability measure on $SP(A)$ with partition function

$$\tilde{Z}_A = \exp\left\{ \int_A z(q) e^{-\beta V(q)} dq \right\}.$$

Let's look at this as A shrinks to a point q_0

$$\int_A z(q) e^{-\beta V(q)} dq \sim vol(A) . z(q_0) e^{-\beta V(q_0)}$$

Look at the function n_A = number of particles on A. This is a random variable on the probability space $SP(A)$, and we have that its distribution is a Poisson distribution

$$p_n = e^{-\lambda} \frac{\lambda^n}{n!}$$

where $\lambda = \int_A z(q) e^{-\beta V(q)} dq \sim vol A . const.$ Thus

$$\langle n_A^2 \rangle = \lambda^2 + \lambda,$$

and although we can make sense of

$$\lim_{A \downarrow q_0} \frac{\langle n_A \rangle}{vol(A)} \quad \text{as density at } q_0$$

it is not possible to make sense of

$$\lim_{A \downarrow q_0} \left\langle \frac{n_A^2}{vol(A)^2} \right\rangle.$$

Therefore we have $\langle n(x) \rangle$ defined but not $\langle n(x)^2 \rangle$, although it seems that

$$\langle n(x_1) \cdots n(x_n) \rangle$$

can be interpreted as distributions on X^n.

Let $f(x)$ be a smooth function on X. Then the quantities

$$\int \langle n(x) \rangle f(x)\, dx$$

$$\int \langle n(x) n(y) \rangle f(x) f(y)\, dx\, dy \qquad \text{etc.}$$

make sense, which suggests that they are moments of a random variable

$$\int n(x) f(x)\, dx$$

on $SP(X)$. For example $n_A = \int n(x) \chi_A(x)\, dx$ might be true. Perhaps the value of $\int n(x) f(x)\, dx$ at a configuration $(q_1, \ldots, q_n)$ should be $\sum_{i=1}^{n} f(q_i)$. Maybe

$$n(x) = \sum_i \delta(x - q_i) \qquad \text{at the configuration } (q_1, \ldots, q_n).$$

Therefore $n(x)$ is random-variable-valued distribution in the sense that for any test function $f(x)$ the express $\int n(x) f(x)\, dx$ ~~is~~ a random-variable. Compare with $\phi(x)$ in field theory being an operator-valued distribution, in the sense that $\int \phi(x) f(x)\, dx$ is an operator.

$$SP(X) = pt \amalg X \amalg X^2/\Sigma_2 \amalg \cdots\cdots$$

On $SP_n(X)$ we have the measure $\frac{1}{n!} dx_1 \cdots dx_n$; this means we take this measure on X^n and push it to $SP_n(X)$, so that $\frac{1}{n!}\int f(x_1,\dots,x_n)\, dx_1 \cdots dx_n$ is the integral of a function f on $SP_n(X)$. Now given a function $f(x)$ on X we can extend it to a "1-particle" function on $SP(X)$ given by

$$\tilde{f}(x_1,\dots,x_n) = \sum_{i=1}^{n} f(x_i)$$

For example if $f = \delta_q$ i.e. $f(x) = \delta(x-q)$, then we get the gadget $n(q)$ [redacted]

$$n(q)(x_1,\dots,x_n) = \sum \delta(x_i - q).$$

We can think of $n(q)$ as a random-variable on $SP(X)$ with distribution values (distributions on X), or as a distribution on X with values in random-variables on $SP(X)$. In the latter interpretation, given a test fn. $f(x)$ we can smear it to get

$$\int f(x)\, n(x)\, dx$$

which is a function on $SP(X)$, namely the function $\tilde{f}$ above. Thus

$$\int f(x)\, n(x)\, dx = \tilde{f} \qquad \text{because} \qquad n(x) = \tilde{\delta}_x .$$

$\tilde{f}$ is a real-valued function on $SP(X)$ and hence it gives rise to a distribution on $\mathbb{R}$. Let's compute its char. fn.

$$\int e^{J\tilde{f}} \underbrace{d\mu}_{\text{measure on } SP(X)} = \sum_n \frac{1}{n!} \int e^{Jf(x_1)+\cdots+Jf(x_n)} dx_1 \cdots dx_n$$

$$= \exp\left\{\int e^{Jf(x)}dx\right\}$$

Now $\displaystyle\int d\mu = \sum \frac{1}{n!}V^n = e^V$, $\quad V = \int dx.$

hence the characteristic function of $\tilde{f}$ as a random variable on the probability space X is

$$W = \exp\left\{\int (e^{Jf(x)} - 1)\, dx\right\}$$

There's no way I can see how to let $f \longrightarrow \delta_g$ in this expression.

Look at the reduced moments

$$b_n = \frac{d^n}{dJ^n}\log(W)\Big|_{J=0}$$

$$\log W = \int (e^{Jf(x)} - 1)\, dx = J\int f(x)dx + \frac{J^2}{2!}\left(\int f(x)^2 dx\right) + \cdots$$

Thus $\displaystyle b_n = \int f(x)^n dx \qquad n \geq 1$

Let's return to the problem of the Green's fns. belonging to the grand partition fn.

$$\tilde{Z} = \sum_n{}' \frac{1}{n!}\int d^n q \prod^n z(q_i)\, e^{-\beta U_n(q)}$$

Then

$$\frac{\delta \tilde{Z}}{\delta z(x)} = \sum_n{}' \frac{1}{n!}\int d^n q \prod z(q_i)\, e^{-\beta U_{n+1}(x,q)}$$

and similarly for higher derivatives. So there is no problem with defining the functions.

$$\frac{\delta^n \tilde{Z}}{\delta z(x_1)\cdots\delta z(x_n)}$$

and these will be nice smooth fns. on X^n. If we use the identity

$$\frac{\delta}{\delta z(x)} z(y) = \delta(x-y)$$

then we can make sense of

$$\prod_{i=1}^{n}\left(z(x_i)\frac{\delta}{\delta z(x_i)}\right)\tilde{Z}$$

as a distribution on X^n. It should be possible to justify the formula

$$\langle n(x_1)\cdots n(x_n)\rangle = \frac{1}{\tilde{Z}}\prod_{i=1}^{n}\left(z(x_i)\frac{\delta}{\delta z(x_i)}\right)\tilde{Z}$$

as distributions on X^n. How?

What we have with the grand configuration space $SP(X)$ is an analogue of the set of classical field configurations ϕ which occur in the Feynman amplitude formula. In this example, there is no problem with the existence of the measure $\mathcal{D}\phi$, because we have the measure $d\mu = \sum \frac{1}{n!} d^n x$ on $SP(X)$. So the formula

$$Z(J) = \int e^{-S(\phi) + \int J\phi\, dx}\, \mathcal{D}\phi$$

of field theory becomes

$$Z(J) = \int e^{-\beta\tilde{u} + \int J n\, dx}\, d\mu$$

which is to be interpreted as

$$Z(J) = \sum_{n \geq 0} \frac{1}{n!} \int d^n q \; e^{-\beta U_n(q) + \sum_{j=1}^{n} J(q_j)}$$

consistent with the formula

$$\int J(x)\, n(x)\, dx = \sum_j J(q_j) \qquad \text{at} \quad q = (q_1, \dots, q_n)$$

At least formally the Green's functions (= moments of the $n(x)$) will be given by

$$\langle n(x_1) \cdots n(x_k) \rangle = \frac{1}{Z(J)} \frac{\delta^n Z(J)}{\delta J(x_1) \cdots \delta J(x_k)}$$

$$= \frac{\int n(x_1) \cdots n(x_k)\, e^{-\beta \tilde{U} + \int J n\, dx}\, d\mu}{\int e^{-\beta \tilde{U} + \int J n\, dx}\, d\mu}$$

Let's try:

$$\int n(x)\, e^{-\beta \tilde{U} + \int J n\, dx}\, d\mu = \sum \frac{1}{n!} \int d^n q \sum \delta(x - q_j)\, e^{-\beta U_n(q) + \sum J(q_j)}$$

$$= \sum_{n \geq 1} \frac{1}{(n-1)!} \int d^{n-1} q \; e^{-\beta U_n(x, q) + J(x) + \sum J(q_j)}$$

$$= \frac{\delta Z}{\delta J(x)} \qquad \text{OK}$$

$$\int n(x)\, n(y)\, e^{-\beta \tilde{U} + \int J n\, dx}\, d\mu = \sum \frac{1}{n!} \int d^n q \sum_{i,j} \delta(x - q_i)\, \delta(y - q_j)\, e^{-\beta U_q + \sum J(q_j)}$$

Break up: $\sum_{i,j} \delta(x - q_i)\, \delta(y - q_j) = \sum_{i \neq j} + \sum_{i = j}$

The $i \neq j$ part is

$$\sum \frac{1}{n!}\, n(n-1) \int d^{n-2}q\, e^{-\beta U_n(x,y,q) + J(x)+J(y)+\sum J(q_i)}$$

$$= z(x)z(y)\frac{\delta^2 Z}{\delta z(x)\,\delta z(y)} \qquad \text{where} \quad z(x) = e^{J(x)}$$

The $i=j$ part is

$$\sum \frac{1}{n!}\, n \int dq_0\, \delta(x-q_0)\,\delta(y-q_0) \int d^{n-1}q\, e^{-\beta U_n(q_0, q) + J(q_0) + \sum J(q_i)}$$

The point is that

$$\int dq_0\, \delta(x-q_0)\,\delta(y-q_0)\, F(q_0) = \delta(y-x)\, F(x)$$

using the fundamental property of $\int dq_0\, \delta(x-q_0)(?)$.
Hence the $i=j$ part becomes

$$\delta(y-x) \sum \frac{1}{n!} \int d^n q\; e^{-\beta U_{n+1}(x, q) + J(x) + \sum J(q_i)}$$

$$= \delta(y-x)\, \frac{\delta Z}{\delta J(x)}$$

Hence we end up with the familiar formula.

$$\frac{\int n(x)n(y)\, e^{-\beta \tilde{U} + \int J n\, dx}\, d\mu}{\int e^{-\beta \tilde{U} + \int J n\, dx}\, d\mu} = \frac{1}{Z}\left(z(x)\, z(y) \frac{\delta^2 Z}{\delta z(x)\,\delta z(y)} + \delta(x-y)\, z(x) \frac{\delta Z}{\delta z(x)} \right)$$

So now it is clear that we can define distributions by.

$$\langle n(x_1) \cdots n(x_k) \rangle = \frac{1}{Z}\, \frac{\delta^n Z(J)}{\delta J(x_1) \cdots \delta J(x_k)}$$

and that in principle we can compute them in terms of pieces belonging to the different strata of $SP_k(X)$.

Suppose we have a two particle function, i.e. an $F(x_1,x_2)$ defined on $SP_2(X)$. Then we can extend it to $SP(X)$ by

$$\tilde{F}(q_1,\dots,q_n) = \frac{1}{2}\sum_{i\neq j} F(q_i,q_j),$$

and average it over the grand canonical ensemble.

$$\frac{1}{Z}\int \tilde{F} e^{-\beta\tilde{U} + \int J n\,dx}\,d\mu = \sum_n \frac{1}{n!}\int d^n q\, \tilde{F}(q) e^{-\beta\tilde{U}(q) + \tilde{J}(q)} \Big/ Z$$

$$= \frac{1}{2}\sum_n \frac{n(n-1)}{n!}\int d^n q\, F(q_1,q_2) e^{-\beta\tilde{U}(q) + \tilde{J}(q)} \Big/ Z$$

$$= \frac{1}{2}\sum_n \frac{1}{n!}\int dx\,dy\, d^n q\, F(x,y) e^{-\beta U(x,y,q) + J(x) + J(y) + \sum J(q_i)} \Big/ Z$$

$$= \frac{1}{2}\int dx\,dy\, F(x,y)\langle n(x)n(y)\rangle'.$$

this $'$ means the diagonal part is omitted

Thus $$\langle n(x)n(y)\rangle' = \frac{1}{2}\, z(x)z(y)\frac{\delta^2 Z}{\delta z(x)\delta z(y)}$$

Let's denote this by $g^{(2)}(x,y)$, or simply $g(r)$ assuming it depends only on $|x-y| = r$. Then we get

$$\langle U\rangle = \frac{1}{2}\int dx\,dy\, U(r)g(r)$$

$$= \frac{V}{2}\int_0^\infty 4\pi r^2 dr\, U(r)g(r)$$

August 4, 1980

Green's functions for grand partition function

$$Z(z) = \sum \frac{1}{n!} \int d^n q \; e^{-\beta U_n(q)} \prod_{i=1}^{n} z(q_i)$$

$$= \int d\mu \; e^{-\beta \tilde{U} + \int J n \, dx} \qquad z(x) = e^{J(x)}$$

$$G_1(x) = \langle n(x) \rangle = z(x) \frac{\delta}{\delta z(x)} \log Z \Big|_{\text{all } z(x) = z}$$

$$= \frac{z \sum \frac{z^n}{n!} \int d^n q \; e^{-\beta U_{n+1}(x, q)}}{\sum \frac{z^n}{n!} \int d^n q \; e^{-\beta U_n(q)}}$$

$$G_2(x, y) = z(x) z(y) \frac{\delta^2 Z}{\delta z(x) \delta z(y)} \Big|_{\text{all } z(x) = z}$$

$$= \frac{z^2 \sum \frac{z^n}{n!} \int d^n q \; e^{-\beta U_{n+2}(x, y, q)}}{\sum \frac{z^n}{n!} \int d^n q \; e^{-\beta U_n(q)}}$$

So now I want to assume z adjusted so that the dominant term method can be used. First note that under the assumption of translation invariance for the energy, we

$$\int d^{n-1} q \; e^{-\beta U_n(x, q)} = \frac{1}{V} \overbrace{\int d^n q \, e^{-\beta U(q)}}^{Z_N}$$

so consequently

$$G_1(x) = \sum n \frac{z^n}{n!} \frac{1}{V} Z_n \Big/ \sum \frac{z^n}{n!} Z_n$$

$$= \frac{N}{V}$$ assuming that the series $\sum \frac{z^n}{n!} Z_n$

has dominant term at $n = N$.

Similarly in the expression for $G_2(x,y)$ if the dominant term in the partition function occurs at $n = N$, then we expect the same is true for the numerator in

$$G_2(x,y) \approx \frac{\frac{z^N}{(N-2)!} \int d^{N-2}q \, e^{-\beta U_N(x,y,q)}}{\frac{z^N}{N!} \int d^N q \, e^{-\beta U_N(q)}}$$

$$= N(N-1) \frac{\int d^{N-2}q \, e^{-\beta U_N(x,y,q)}}{\int d^N q \, e^{-\beta U_N(q)}}$$

Better approach. Write partition function in the form

$$Z = \sum \frac{1}{n!} \int d^n q \, e^{-\beta U_n(q)} \prod_{j=1}^{n} z(q_j)$$

and define the Green's functions to be

$$G_n(x_1, \ldots, x_n) = \frac{1}{Z} \frac{\delta^n Z}{\delta z(x_1) \cdots \delta z(x_n)}$$

and the connected Green's functions by

$$G_n^c(x_1, \ldots, x_n) = \frac{\delta^n}{\delta z(x_1) \cdots \delta z(x_n)} \log Z$$

For an ideal gas all $U_n(q) = 0$, so

$$Z = \sum \frac{1}{n!} \int d^n q \prod z(q_j) = \exp\left\{ \int z(q) \, dq \right\}$$

hence $\begin{cases} G_n^c = 0 & \text{for } n \geq 2 \\ G_1^c(x) = 1. & \text{for all } x \end{cases}$

Also
$$G_2(x_1, x_2) = \frac{1}{Z} \sum_n{}' \frac{1}{n!} \int d^n q \; e^{-\beta U_{n+2}(x,y,q)} \prod z(q_j)$$
$$= 1$$

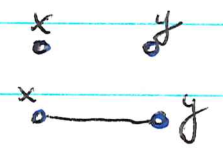
and more generally $G_n(x_1, \ldots, x_n) = 1$ for all n in this notation.

Now we want to express these Green's fns. in terms of diagrams. Recall $U_n(q) = \frac{1}{2} \sum_{i \neq j} u(r_{ij})$ and

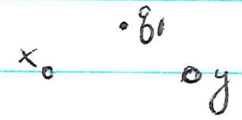
$$e^{-\beta U_n(q)} = \prod_{i<j} (1 + f_{ij}) \qquad f_{ij} = e^{-\beta u(r_{ij})} - 1.$$

The numerator for $G_2(x_1, x_2)$ represents a sum over diagrams with two fixed vertices which get labelled by x, y.

n=0



n=1

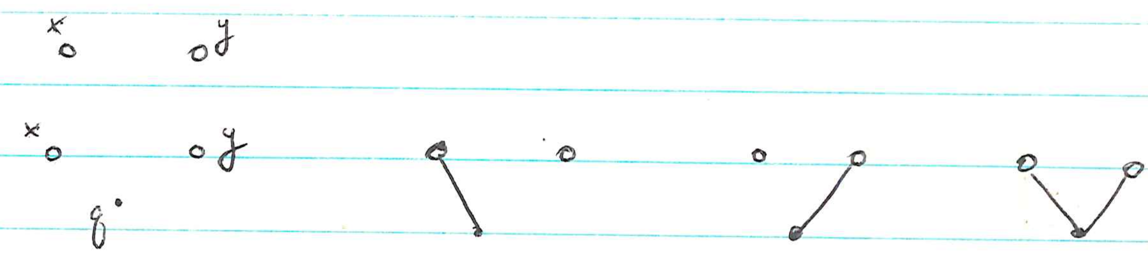


8 possible diagrams.

We can simplify a little bit by taking out the factor $e^{-\beta u(x,y)}$ common to all the terms of $G_2(x,y)$. This means we may assume x, y are not connected by an edge. Hence we get

n=0

n=1

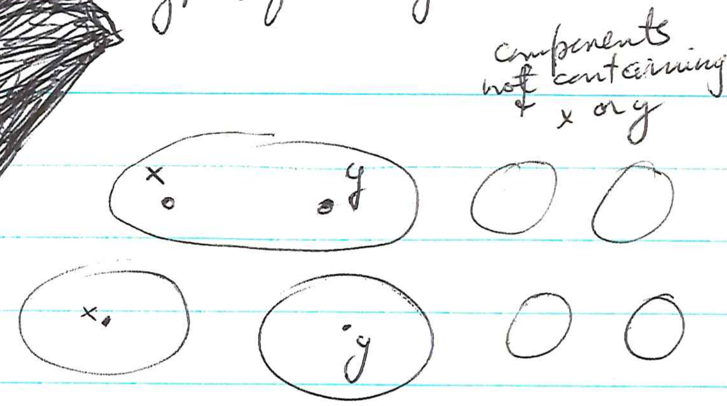


Next suppose we use the connected diagram decomposition. Then we get [redacted] two types of diagrams

[redacted]

x, y in same component:

x, y in diff. components:

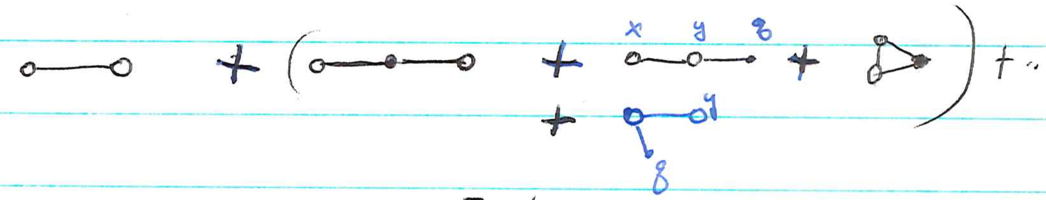


[redacted] When we divide by Z we cancel the components not containing x or y and we find

$$G_2(x,y) = G_2^c(x,y) + G_1^c(x)\, G_1^c(y)$$

So now it's clear that

$G_2^c(x,y) =$



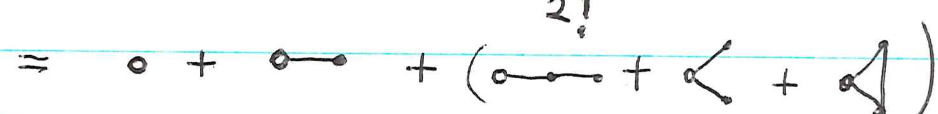
Let's compute carefully.

$$G_1(x) = \frac{1}{Z}\frac{\delta Z}{\delta z(x)}\bigg|_{z(x)=z} = \frac{\overbrace{\sum_n \frac{z^{n-1}}{n!}\, n \int d^{n-1}q\, e^{-\beta U_n(x,q)}}^{Z_n/V}}{\sum_n \frac{z^n}{n!}\underbrace{\int d^n q\, e^{-\beta U_n(q)}}_{Z_n}}$$

$$= \frac{1}{z}\frac{\langle n \rangle}{V} = \rho/z$$

According to page 961 one has

$$\rho/z = 1 + F_2 z + F_3 \frac{z^2}{2!} + \cdots$$



$$= 1 + az + (3a^2 + b)\frac{z^2}{2} + \cdots$$

where $$a = \int f(|q|)\, dq = \frac{1}{V} \int f_{12}\, dq_1 dq_2$$

$$b = \int f_{12} f_{13} f_{23}\, dq_2 dq_3 \quad \text{where } q_1 = 0.$$