January 29, 1981

Review J-matrices and the KdV flows.

[redacted] Start with a bdd. self-adjoint operator A on $\mathcal{H}$ and a cyclic vector e_1 with $\|e_1\| = 1$. Apply Gram-Schmidt to the sequence $e_1, Ae_1, A^2e_1, \ldots$ to obtain an orthonormal basis $e_1, e_2, e_3, \ldots$ for $\mathcal{H}$. One has then

$$Ae_n = a_n e_{n+1} + b_n e_n + c_n e_{n-1} + \cdots$$

with $a_n > 0$. Since $\langle e_j | Ae_n \rangle = \langle Ae_j | e_n \rangle = 0 \quad j \le n-2$ no terms beyond $c_n e_{n-1}$ occur; also $c_n = \langle e_{n-1} | A e_n \rangle = \langle A e_{n-1} | e_n \rangle = a_{n-1}$. Thus

$$Ae_n = a_n e_{n+1} + b_n e_n + a_{n-1} e_{n-1}$$

so the matrix of A relative to this orthonormal basis is a J-matrix.

$$\begin{pmatrix} b_1 & a_1 & & \\ a_1 & b_2 & a_2 & \\ & a_2 & b_3 & \ddots \\ & & \ddots & \ddots \end{pmatrix}$$

Another way to obtain this matrix goes as follows. For λ not in the spectrum of A, $\frac{1}{\lambda - A}$ exists. Put

$$u_n(\lambda) = \langle e_n | \frac{1}{\lambda - A} | e_1 \rangle .$$

This is a sequence in ℓ^2 satisfying

$$\lambda u_n - (a_n u_{n+1} + b_n u_n + a_{n-1} u_{n-1}) = \langle (\bar{\lambda} - A) e_n | \frac{1}{\lambda - A} | e_1 \rangle = \langle e_n | e_1 \rangle = \delta_{n1}$$

for $n > 1$

and

$$\lambda u_1 - (a_1 u_2 - b_1 u_1) = 1. \quad \text{Thus}$$

$$\frac{1}{u_1} = \lambda - b_1 - \underbrace{a_1 \frac{u_2}{u_1}}_{a_1^2 / a_1 \frac{u_1}{u_2}} \qquad a_{n-1} \frac{u_{n-1}}{u_n} = \lambda - b_n - \underbrace{a_n \frac{u_{n+1}}{u_n}}_{a_n^2 / a_n \frac{u_n}{u_{n+1}}} \quad n > 1$$

So [redacted] $u_1 = \frac{1}{\lambda-b_1-}\,\frac{a_1^2}{\lambda-b_2-}\,\frac{a_2^2}{\lambda-b_2-}\cdots\cdots\frac{a_{n-1}^2}{\left(a_{n-1}\frac{u_{n-1}}{u_n}\right)}$.

Thus

$$\boxed{\langle e_1|\frac{1}{\lambda-A}|e_1\rangle = \frac{1}{\lambda-b_1-}\,\frac{a_1^2}{\lambda-b_2-}\,\frac{a_2^2}{\lambda-b_3-}\cdots\cdots}$$

The KdV flows: It's simplest to work with doubly-infinite matrices. Then a J-matrix can be written

$$A = aT + b + T^{-1}a$$

where a, b are diagonal matrices and

$$(aTu)_n = a_n(Tu)_n = a_n u_{n+1} \qquad \Rightarrow \quad (Tu)_n = u_{n+1}$$

is the backwards shift. Let $f(x)$ be a polynomial, with real coeffs. say x^m; [redacted] then $f(A)$ can be put in the form

$$f(A) = p(T) + p(T)^*$$

where $p = \alpha_0 + \alpha_1 T + \cdots + \alpha_m T^m$ is a polynomial and the α_i are diagonal matrices. Put

$$B = \tfrac{1}{2}(p - p^*)$$

Then

$$[B,A] = [p,A] \quad \Rightarrow [B,A] \text{ of form } \beta_{-1}T^{-1}+\beta_0+\beta_1 T+\cdots$$

$$= [-p^*,A] \quad \Rightarrow \quad \text{———} \quad \beta_1' T + \beta_0' + \beta_1' T^{-1}+\cdots$$

hence $[B,A]$ is a J-matrix. Therefore we obtain a D.E. on J-matrices associated to the polynomial f.

$$\partial_t A = [B,A]$$

Let's compute the effect on $\langle e_1|\frac{1}{\lambda-A}|e_1\rangle$: We have

$$\partial_t\left(\frac{1}{\lambda-A}\right) = \left[B, \frac{1}{\lambda-A}\right]$$

(this reduces to $\partial_t(A^m) = [B, A^m]$ which follows using the derivation property of both sides.) Then

$$\partial_t \langle e_1 | \frac{1}{\lambda - A} | e_1 \rangle = \underbrace{\langle e_1 | B}_{\langle -Be_1 |} \frac{1}{\lambda - A} | e_1 \rangle - \langle e_1 | \frac{1}{\lambda - A} B | e_1 \rangle .$$

and the point is that $-2Be_1$ is very close to $f(A)e_1$. To see this note that when we write $A = aT + b + T^{-1}a$ we think of $a = (a_n)$, $b = (b_n)$ as zero in entries $n \leq 0$, hence each of the terms aT, b, $T^{-1}a$ is supported for $(m,n) \geq 0$. The same is true for the matrices $p(T)$, $p(T)^*$. Hence

$$p(T)e_1 = ce_1 \qquad c \text{ real since } f \text{ is.}$$

for some c. Thus we have

$$f(A)e_1 = p(T)^* e_1 + ce_1$$

$$\langle e_1 | f(A) e_1 \rangle = c + \langle e_1 | p(T)^* e_1 \rangle = c + \langle p(T) e_1 | e_1 \rangle$$

$$= 2c$$

$$\boxed{\cancel{Be_1 = \tfrac{1}{2}(p(T)^* e_1 + ce_1) = \tfrac{1}{2}(f(A)e_1 - 2ce_1)}}$$

$$Be_1 = \tfrac{1}{2}(p - p^*)e_1 = \tfrac{1}{2}(ce_1 - fe_1 + ce_1)$$

$$\text{or} \quad -2Be_1 = f(A)e_1 - \langle e_1 | f(A) | e_1 \rangle e_1$$

Thus we have

$$\partial_t \langle e_1 | \frac{1}{\lambda - A} | e_1 \rangle = \langle e_1 | \frac{f(A)}{\lambda - A} | e_1 \rangle - \langle e_1 | f(A) | e_1 \rangle \langle e_1 | \frac{1}{\lambda - A} | e_1 \rangle$$

which can be interpreted as follows. We have

$$\langle e_1 | \frac{1}{\lambda - A} | e_1 \rangle = \int \frac{d\mu(x)}{\lambda - x} \qquad \text{where } d\mu \text{ is}$$

a measure supported on the spectrum of A with

$$\int d\mu = 1.$$

If we define a family of prob. measures by

$$(\bigstar) \qquad d\mu_t(x) = e^{tf(x)}\, d\mu(x) \Big/ \int e^{tf(x)} d\mu(x)$$

then we have

$$\boxed{\cancel{\partial_t \int \frac{d\mu_t(x)}{\lambda - x} = \int \frac{f(x)\, d\mu_t(x)}{\lambda - x}}}$$

$$\partial_t \big(d\mu_t(x)\big) = f(x)\, d\mu_t(x) - \frac{e^{tf(x)} d\mu(x) \int f(x) e^{tf(x)} d\mu(x)}{\left(\int e^{tf(x)} d\mu(x)\right)^2}$$

or

$$\partial_t (d\mu_t) = \big(f - \langle f \rangle_t\big)\, d\mu_t$$

hence

$$\partial_t \int \frac{d\mu_t}{\lambda - x} = \int \big(f - \langle f \rangle_t\big) \frac{d\mu_t}{\lambda - x}$$

Comparing with $\partial_t \langle e_1 | \frac{1}{\lambda - A} | e_1 \rangle = \langle e_1 | \frac{f(A) - \langle e_1 | f(A) | e_1 \rangle}{\lambda - A} | e_1 \rangle$

we see that the path $(\bigstar)$ gives the integral curve for the KdV flow belonging to f.

<u>February 1, 1981</u>

It seems that doubly-infinite J matrices can be treated as a one-sided J-matrix whose entries are 2×2 blocks. Hence I ought to consider the operator situation

$$A = aT + b + T^{-1}a^*$$

where $a = (a_n)$, $b = (b_n)$ are sequences of operators on a fixed space W $(a_n > 0)$. Let's pick a basis e^i for W and then consider the bases e_n^i $n \geq 1$ for the space on which A acts. This time we have a matrix spectral measure $d\mu_{ij}(x)$ such that

$$\int \frac{d\mu_{ij}(x)}{\lambda - x} = \langle e_1^i \,|\, \frac{1}{\lambda - A} \,|\, e_1^j \rangle$$

Let's be more precise. We have a self-adjoint bounded operator A on a Hilbert space $\mathcal{H}$, and a subspace W such that the subspaces $A^n W$ $n \geq 0$ are independent and span $\mathcal{H}$. Think of $e_1 : \mathbb{C}^r \xrightarrow{\sim} W$ as unitary isomorphism. From this data we can construct unitary embeddings $e_n : \mathbb{C}^r \hookrightarrow \mathcal{H}$ such that the spaces $e_n(\mathbb{C})^r$ are orthogonal exhausting $\mathcal{H}$ as follows. Take $A e_1$ followed by projection $\perp$ to W:

$$Ae_1 - e_1 e_1^* A e_1 : \mathbb{C}^r \longrightarrow \mathcal{H}$$

and factor it into an embedding $e_2 : \mathbb{C}^r \hookrightarrow \mathcal{H}$ following a positive-definite operator a_1. Thus

$$Ae_1 = e_1 \underbrace{(e_1^* A e_1)}_{b_1} + e_2 a_1$$

It's pretty clear that we thereby grind out a sequence a_n, b_n of operators on $\mathbb{C}^r$. Now our matrix measure $d\mu(x)$ is defined by

$$\int \frac{d\mu(x)}{\lambda - x} = e_1^* \frac{1}{\lambda - A} e_1 .$$

If we start with a matrix measure $d\mu(x)$ such that the inner product on $\mathbb{C}[x]^n$ is non-degenerate then by completion we get $A, \mathcal{H}, e_1$ etc. Note that

$$A\Big(\sum{}' e_n u_n\Big) = \sum A e_n u_n = \sum (e_{n+1}a_n + e_n b_n + e_{n-1}a_{n-1}) u_n$$

$$= \sum_n e_n(a_n u_{n+1} + b_n u_n + a_{n-1}u_{n-1})$$

so that under the isom $u=(u_n) \longmapsto \sum e_n u_n$, $\ell^2\otimes\mathbb{C}^n \xrightarrow{\sim} \mathcal{H}$ we have $A = aT + b + T^{-1}a$. $(ae_n = e_n a_n$, etc.$)$

Next consider the KdV flow belong to $B = \frac{1}{2}(aT - T^{-1}a)$. We have

$$\partial_t \frac{1}{\lambda-A} = \Big[B, \frac{1}{\lambda-A}\Big] = \Big[-T^{-1}a, \frac{1}{\lambda-A}\Big]$$

hence

$$\partial_t e_1^* \frac{1}{\lambda-A}e_1 = -\underbrace{e_1^* T^{-1}}_{\substack{0 \text{ since } T \text{ is} \\ \text{backward shift}}} a\frac{1}{\lambda-A}e_1 + e_1^*\frac{1}{\lambda-A}\underbrace{T^{-1}ae_1}_{\substack{(A-b-aT)e_1 \\ = Ae_1 - e_1b_1}}$$

Thus

$$\partial_t e_1^*\frac{1}{\lambda-A}e_1 = e_1^*\frac{1}{\lambda-A}(Ae_1 - e_1b_1)$$

On the level of the measure we can proceed as follows: set

$$d\mu_t(x) = e^{tx}d\mu_t(x)\Big(\int e^{tx}d\mu_t\Big)^{-1}$$

Then

$$\partial_t d\mu_t(x) = x\,d\mu_t(x) - d\mu_t(x)\cdot\int x\,d\mu_t(x).$$

so it all works.

For correct formulas see p.370-371

February 6, 1981

Let's correct the error made in trying to understand one-sided J-matrices with operator entries. First review the situation. We start with a Hilbert space W. Then we consider a triple consisting of a Hilbert space $\mathcal{H}$, together with a bounded self-adjoint operator A, and an embedding $e_1 : W \to \mathcal{H}$, $e_1^* e_1 = id$, such that one has an injection

$$\mathbb{C}[z] \otimes W \hookrightarrow \mathcal{H}$$
$$z^n \otimes w \longmapsto A^n e_1 w$$

with dense image. From such a triple one can construct a J-matrix $aT + b + T^* a$ on the Hilbert space $\ell^2_{\geq 1} \hat{\otimes} W$. Also one gets a positive operator-valued measure $d\mu(x)$ such that

$$e_1^* \frac{1}{\lambda - A} e_1 = \int \frac{d\mu(x)}{\lambda - x} . \qquad \text{Note } \int d\mu(x) = id_W$$

In the following we identify $\mathcal{H}$ with $\ell^2_{\geq 1} \hat{\otimes} W$ and A with the J-matrix $aT + b + T^* a$. We want to describe the flow

$$\partial_t A = [B, A] \qquad B = \frac{1}{2}(aT - T^* a)$$

in terms of the spectral measure $d\mu$.

$$\partial_t e_1^* \frac{1}{\lambda - A} e_1 = e_1^* \left[B, \frac{1}{\lambda - A}\right] e_1 = e_1^* \Big[\underbrace{B - \frac{A}{2}}_{-\frac{b}{2} - T^* a}, \frac{1}{\lambda - A}\Big] e_1$$

$$= -\frac{1}{2} b_1 \, e_1^* \frac{1}{\lambda - A} e_1 - \underbrace{e_1^* T^*}_{0} a \frac{1}{\lambda - A} e_1 + e_1^* \frac{1}{\lambda - A} \underbrace{\left(\frac{b}{2} + T^* a\right) e_1}_{A - \left(\frac{b}{2} + aT\right) e_1}$$

$$\boxed{\partial_t e_1^* \frac{1}{\lambda - A} e_1 = e_1^* \frac{A}{\lambda - A} e_1 - \frac{1}{2} b_1 \left(e_1^* \frac{1}{\lambda - A} e_1\right) - \frac{1}{2}\left(e_1^* \frac{1}{\lambda - A} e_1\right) b_1}$$

We can realize this flow on measures $d\mu$ as follows. Put

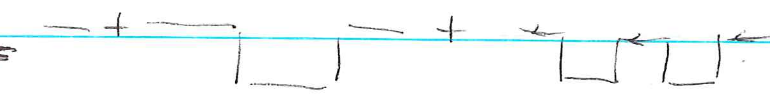
$$d\mu_t(x) = \left(\int e^{tx} d\mu\right)^{-1/2} e^{tx} d\mu(x) \left(\int e^{tx} d\mu\right)^{-1/2}$$

so that $d\mu_t(x)$ is a hermitian operator measure which is >0. It's clear this works.

Let take a 2-sided infinite J-matrix A and to simplify suppose the entries a_n, b_n are just real numbers. Then A operates on $\ell^2_{\mathbb{Z}} = \ell^2_{\leq 0} \oplus \ell^2_{\geq 1}$ and hence has the form

$$A = \left(\begin{array}{c|c} A^- & |e_0\rangle a_0 \langle e_1| \\ \hline |e_1\rangle a_0 \langle e_0| & A^+ \end{array}\right)$$

so we can compute the resolvent $\frac{1}{\lambda - A}$ by diagrams. Put $f_+ = \langle e_+ | \frac{1}{\lambda - A_+} | e_+\rangle$ where $e_+ = e_1$, and similarly define f_- where $e_- = e_0$. Then

$$\langle e_+ | \frac{1}{\lambda - A} | e_+ \rangle =$$ 

$$= f_+ + f_+ a_0 f_- a_0 f_+ + f_+ a_0 f_- a_0 f_+ a_0 f_- a_0 f_+ + \cdots$$

$$= \frac{f_+}{1 - a_0 f_- a_0 f_+}$$

Similarly we find

$$\left\langle \begin{matrix} e_+ \\ e_- \end{matrix} \right| \frac{1}{\lambda - A} \left| \, e_+ \ e_- \right\rangle = \begin{pmatrix} \dfrac{f_+}{1 - a_0 f_- a_0 f_+} & \dfrac{f_+ a_0 f_-}{1 - a_0 f_+ a_0 f_-} \\[2ex] \dfrac{f_- a_0 f_+}{1 - a_0 f_+ a_0 f_-} & \dfrac{f_-}{1 - a_0 f_+ a_0 f_-} \end{pmatrix}$$

This matrix is symmetric and has the special property that its determinant is

$$\frac{f_+ f_-}{1 - a_0 f_+ a_0 f_-}$$

which is the constant $(a_0)^{-1}$ times the off-diagonal entries.

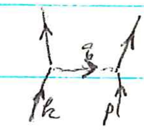
<u>Problem</u>: Can you find a condition on the measure $d\mu(x)$ which says when it comes from a 2-sided J-matrix. Here W is spanned by $e_1 = e_+$ and $e_0 = e_-$ and the point is to find out when the block J-matrix $\underline{a}T + \underline{b} + T^*\underline{a}$ is such that $\underline{a}_n$ is diagonal $n \geq 1$ and $\underline{b}_n$ is diagonal for $n \geq 2$.

February 7, 1981

It's time to understand Hartree-Fock approximation in the interacting Fermi gas. It would be nice to obtain this approximation as a Gaussian approximation to Grassman path integral.

The situation: One has a Fermi gas described by

$$H = \sum \omega_k a_k^* a_k + \frac{1}{2} \sum V_q a^*_{k-q} a^*_{p+q} a_p a_k$$



and one wants to compute the propagator

$$G(k,t) = -i \langle T[a_k(t) a_k^*] \rangle$$

The Heisenberg operators $a_k(t) = e^{+iHt} a_k e^{-iHt}$ satisfy an equation of motion

$$\partial_t a_k = [iH, a_k]$$

$p+q=k$ or $l-q=k$

$$= i\Big\{ -\omega_k a_k + \frac{1}{2} \sum V_q a^*_{l-q} a_{k-q} a_l$$

Since $V_{-q} = V_q$,

$$- \frac{1}{2} \sum V_{-q} a^*_{l+q} a_l a_{k+q} \Big\}$$

$$\boxed{\partial_t a_k = i\Big\{ -\omega_k a_k + \sum_{q,l} V_q a^*_{l-q} a_{k-q} a_l \Big\}}$$

What one does is to approximate $a_l^* a_m a_n$ by

$$\langle a_l^* a_m \rangle a_n - \langle a_l^* a_n \rangle a_m$$

and this should be valid provided the fluctuation of $a_l^* a_m$ around $\langle a_l^* a_m \rangle$ is small.

So I want to try to see if this approximation has a nice interpretation from the path integral viewpoint. First I want to consider the boson setup with a similar Hamiltonian.

Let's review the formulas.

$$\int e^{-a\bar{z}z}\,dx\,dy = \int e^{-2a\left(\frac{x^2}{2}+\frac{y^2}{2}\right)}dx\,dy = \left(\frac{\sqrt{2\pi}}{\sqrt{2a}}\right)^2 = \frac{\pi}{a}$$

$$\int e^{-z^*Az}\,d^nx\,d^ny = \frac{\pi^n}{\det(A)} \qquad \text{provided} \quad Re(A) = \frac{A+A^*}{2} > 0$$

$$-\frac{\partial}{\partial a_{ji}}\log\int e^{-\bar{z}_i a_{ij} z_j} = \frac{\partial}{\partial a_{ji}}\log\det(A) = \frac{(ij)\text{-th cofactor}}{\det} = \left(A^{-1}\right)_{ij}$$

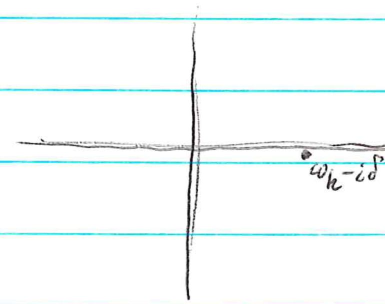
$$\therefore \quad \boxed{\frac{\int e^{-z^*Az}\, z_i\bar{z}_j}{\int e^{-z^*Az}} = \left(A^{-1}\right)_{ij}}$$

The free propagator is

$$G^0(k,t) = -i\left\langle T\left[\overset{e^{-i\omega_k t}a_k}{a_k(t)}\,a_k^*\right]\right\rangle$$

$$= -ie^{-i\omega_k t}\,\theta(t)$$

$$= \int \frac{d\omega}{2\pi}\,\frac{e^{-i\omega t}}{\omega-\omega_k+i\delta}$$



so $$G^0(k,\omega) = \frac{1}{\omega-\omega_k+i\delta}$$

(Think of δ as $1/$lifetime, where lifetime $\sim\infty$).

The free propagator satisfies

$$\left(i\partial_t - \omega_k\right)G^0(k,t) = \delta(t) \qquad G^0 = \frac{1}{i\partial_t - H_0}$$

and so at least formally we have

$$\frac{\int e^{-\int\psi^*(i\partial_t - H_0)\psi\,dt}\,\psi\psi^*}{\int e^{-\int\psi^*(i\partial_t-H_0)\psi\,dt}} = G^0$$

Let's look at the exponent in this Gaussian integral. Here ψ is to run over all $\mathbb{C}$-valued functions of k,t or we can F.T.

$$\psi_k(t) = \int \frac{d\omega}{2\pi} e^{-i\omega t} \psi_{k\omega}$$

and then

$$\int \psi^*(i\partial_t - H_0)\psi \, dt = \sum_{k\,\omega} (\omega - \omega_k)|\psi_{k\omega}|^2 .$$

So it's clear this Gaussian integral isn't well-defined, and so probably one has to resort to imaginary time in some way.

However it seems I have chosen A wrong. I want

$$\frac{\int e^{-\psi^* A \psi} \psi(t)\psi^*(t')}{\int e^{-\psi^* A \psi}} = \langle T[\psi(t)\psi^*(t')]\rangle$$

$$\| $$

$$\frac{1}{\partial_t + iH_0}$$

and so therefore the Gaussian integral I should be looking at is

$$\int e^{-\int \psi^*(\partial_t + iH_0)\psi \, dt}$$

Now

$$-\int \psi^*(\partial_t + iH_0)\psi \, dt = -\sum_{k,\omega} (-i\omega + i\omega_k)|\psi_{k\omega}|^2$$

$$= i \sum_{k\,\omega} (\omega - \omega_k)|\psi_{k\omega}|^2$$

and if each ω_k is replaced by $\omega_k - i\delta$ we get a nice negative-definite real part. $\blacksquare$

February 8, 1981

The basic formula is

$$\frac{\int e^{-\psi^* A \psi}\, \psi_i \psi_j^*}{\int e^{-\psi^* A \psi}} = (A^{-1})_{ij}$$

and it's valid both for boson and fermion cases. We want the left side to give a time-ordered product

$$\langle T[\psi_i(t)\psi_j^*]\rangle = G_{ij}(t)$$

which satisfies $\left(\frac{d}{dt} + iH_0\right) G = \delta(t)$, hence we want to take

$$A = \partial_t + iH_0$$

which means we have the exponential

$$e^{-\int \psi^*(\partial_t + iH_0)\psi\, dt} = e^{i\int \psi^*(i\partial_t - H_0)\psi\, dt}$$

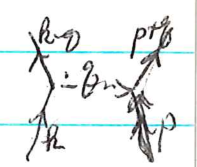
and hence the action

$$S = \int \psi^*(i\partial_t - H_0)\psi\, dt$$

To handle the interacting system $\psi^* H_0 \psi$ has to be replaced by the interacting Hamiltonian.

Let's consider the interacting fermi-gas

$$H = \sum \varepsilon_k a_k^* a_k + \frac{1}{2}\sum_{q,p,k} V_q\, a_{k-q}^* a_{p+q}^* a_p a_k$$



When the action is computed we replace a_k by $\psi_k(t) = \sum_\omega e^{-i\omega t}\psi_{k\omega}$ and we integrate over time. Let's compute the action carefully.

$$\int \psi^* H_0 \psi = \int dt \sum_k \varepsilon_k \psi_k(t)^* \psi_k(t) = \sum_{k,\omega} \varepsilon_k |\psi_{k\omega}|^2$$

$$\frac{1}{2}\int dt \sum V_q \, \psi^*_{k-q}(t)\, \psi^*_{p+q}(t)\, \psi_p(t)\, \psi_k(t)$$

What this becomes is a sum of the same type, but where frequency is added

$$\frac{1}{2}\sum V_{q\omega''}\, \psi^*_{k\omega-q\omega''}\, \psi^*_{p\omega'+q\omega''}\, \psi_{p\omega'}\, \psi_{k\omega}$$

and where in this case because V is time-independent, we have $V_{q\omega''} = V_q \cdot$ [redacted] ?

So one should look at a simpler example. Let's take

$$H = \sum_k \varepsilon_k a^*_k a_k + \sum_{kl} V_{kl}(t)\, a^*_k a_l$$

Here the total action is

$$\int \psi^*(i\partial_t - H_0)\psi \, dt - \int \psi^* V \psi \, dt$$

where $\psi = \{\psi_k(t)\}$. We have formally in the fermion case

$$\frac{\int e^{i\int \psi^*(i\partial_t - H)\psi\, dt}}{\int e^{i\int \psi^*(i\partial_t - H_0)\psi\, dt}} = \frac{\det(\partial_t + iH)}{\det(\partial_t + iH_0)} = \det(1 - G_0 V)$$

where $G_0 = \dfrac{1}{i\partial_t - H_0}$. For boson's we get $\det(1-G_0V)^{-1}$.

However we are interested in the propagator

$$iG_{kl}(t,t') = \frac{\int e^{i\int \psi^*(i\partial_t - H_{\text{[redacted]}})\psi\, dt}\, \psi_k(t)\, \psi_l(t')^*}{\int e^{i\int \psi^*(i\partial_t - H)\psi\, dt}} = \langle T[\psi_k(t)\psi_l(t')]^* \rangle$$

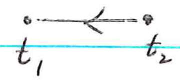
$$\frac{1}{\partial_t + iH_0} = \frac{i}{i\partial_t - H_0}$$

We can compute this as

$$iG(t,t') = \frac{\int e^{-i\int \psi^*(i\partial_t - H_0)\psi\, dt}\; e^{-i\int \psi^* V \psi\, dt}\, \psi(t)\psi(t')^*}{\int e^{i\int \psi^*(i\partial_t - H_0)\psi\, dt}} \div \frac{\int e^{-i\int \psi^*(i\partial_t - H_0)\psi - i\int \psi^* V \psi}}{\int e^{i\int \psi^*(i\partial_t - H_0)\psi}}$$

The division cancels the disconnected diagrams, so what's left is a sum of terms for each diagram

and the contribution is $-iV(t)$ for a vertex at time t and $iG_0(t_1, t_2)$ for



. Thus we get our familiar series

$$iG = iG_0 + iG_0(-iV)\, iG_0 + \cdots\cdots$$

February 9, 1981

Review:
$$\frac{\int e^{-\psi^* A \psi}\, \psi_k \psi_\ell^*}{\int e^{-\psi^* A\psi}} = \langle k | A^{-1} | \ell \rangle$$
holds both for bosons + fermions. To apply we want $\psi = \{\psi(t)\}$ and we want
$$\langle t | A^{-1} | t' \rangle = \langle T[a(t)\, a^*(t')] \rangle = e^{-iH_0(t-t')}\, \tilde{\theta}(t-t')$$
where $\tilde{\theta}$ is some Heaviside function (jump of $+1$ as t crosses t'). Thus
$$A = \partial_t + i H_0$$
and so
$$-\psi^* A \psi = i \underbrace{\int \psi^* (i\partial_t - H_0)\psi \, dt}_{\text{the action } S}$$

Let's rewrite in terms of frequency
$$iS = i \sum (\omega - \varepsilon_k) |\psi_{k\omega}|^2$$
where $H_0 |k\rangle = \varepsilon_k |k\rangle$. This gives the Green's function
$$\langle \omega | A^{-1} | \omega \rangle = \frac{i}{\omega - \varepsilon_k + i\delta}$$
where the inverse lifetime δ has to be put in to specify the bdry conditions.

Question: What does it mean to do this integral in imaginary time?

The point perhaps is that the Green's function
$$\theta(t-t') \langle a(t)\, a^*(t') \rangle = \theta(t-t') \langle a\, e^{-iH_0(t-t')} a^* \rangle$$
makes sense for $it = \tau > it' = \tau'$. Hence we can construct a Gaussian integral with
$$\langle \tau | A^{-1} | \tau' \rangle = \theta(\tau - \tau')\, e^{-H_0(\tau-\tau')}$$

so this time $\quad A = \partial_\tau + H_0,$ and so the Gaussian exponent is $\quad -\psi^* A \psi = -\int \psi^*(\partial_\tau + H_0)\psi \, d\tau$. Notice that this is obtained if one rewrites formally

$$\tau = it$$

$$i\int \psi^*(i\partial_t - H_0)\,dt = \int \psi^*(-\partial_\tau - H_0)\,d\tau \qquad \partial_\tau = -i\partial_t$$

Now we have a new ~~kind of~~ path integral. So next we can use Fourier transform. The standard thing is to use periodic fns. [redacted] $\psi(\tau)$ of period β

$$\psi(\tau) = \sum \psi_\omega e^{-i\omega\tau} \qquad \omega \in \frac{2\pi}{\beta}\mathbb{Z} \qquad ?$$

The Green's fns. is [redacted] analytic

Question. Can we say something about [redacted] finding a path integral expression for $\langle x | \frac{1}{W-H} | x' \rangle$?

Here H is a Schroedinger operator

$$H = \frac{p^2}{2m} + V(x).$$

If one makes this a 1-particle operator and extends to Fock space, the Green's function is

$$i\,G(xt, x't') = \langle x | e^{-iH(t-t')} | x' \rangle \, \theta(t-t')$$

(Think $G = \frac{1}{i\partial_t - H}$). Hence the Fourier transform is

$$\int dt\, e^{i\omega t} G(xt, x'0) = \int_0^\infty dt\, e^{i\omega t} \frac{1}{i} \langle x | e^{-iHt} | x' \rangle$$

$$= \langle x | \frac{1}{\omega - H} | x' \rangle$$

Now we know that $\langle x | e^{-iHt} | x' \rangle$ is an integral over paths starting at x' at time 0 and ending at x at time t. So $\langle x | \frac{1}{\omega - H} | x' \rangle$ becomes an integral over paths of varying time intervals.

Now ω is normally viewed as complex or at least not in the spectrum of H. However from Hamilton-Jacobi theory it seemed to be natural to fix a real energy E and look at paths in the hypersurface

$$H = \frac{p^2}{2m} + V(x) = E$$

which start over x' and end over x.

February 15, 1981

mean field theory: Consider an Ising model and consider a specific site, say the one with index 0. I want to compute the average spin $\langle s_0 \rangle$ at this site, or better the probability of finding the spin up or down. This probability of a value s_0 for this spin is

$$p_{s_0} = \frac{\sum_{s'} e^{-\beta E(s_0, s')}}{\sum_{s_0} \sum_{s'} e^{-\beta E(s_0, s')}}$$

where $s' = \{s_j\}_{j \geq 1}$ and $s = (s_0, s')$

$$-E(s) = H \sum{}' s_j + \frac{1}{2} \sum{}' J_{ij} s_i s_j$$

$$-E(s_0, s') = H s_0 + s_0 \sum_{j>0} J_{0j} s_j + (-E(s'))$$

In the above expression for p_{s_0} we can divide numerator and denominator by $\sum e^{-\beta E(s')}$ and we get

$$p_{s_0} = \frac{\langle e^{s_0 \beta (H + J_{0j} s'_j)} \rangle}{\sum_{s_0} \langle e^{s_0 \beta (H + J_{0j} s'_j)} \rangle} \qquad J_{0j} s'_j = \sum_{j>0} J_{0j} s_j$$

where $\langle \ \rangle$ denotes average wrt s'. Notice that

$$H + \sum_{j>0} J_{0j} s_j$$

is the local field at the 0-th site due to the external field H and the other spins. Now the idea of mean field theory is to assume that local field doesn't fluctuate very much, and hence one can approximate it by its average value

$$\langle H + \sum{}' J_{0j} s'_j \rangle = H + \sum J_{0j} \langle s'_j \rangle$$

Ignore difference between averages over s' and over s.

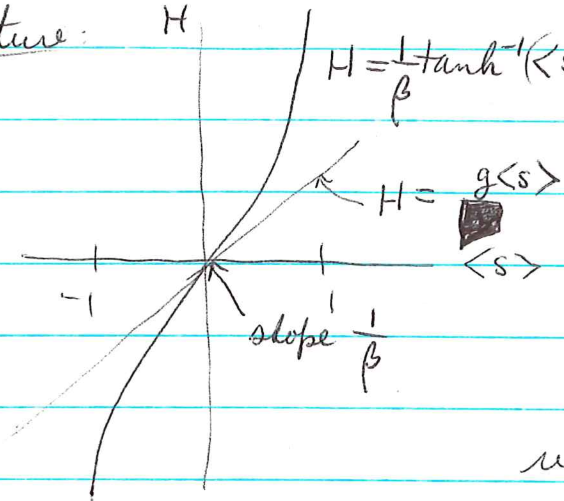
Let's suppose we have a lattice for our sites so that $\langle s_j \rangle$ is independent of j. Then we get

$$\langle H + \sum' J_{0j} s_j \rangle = H + g\langle s \rangle \qquad g = \sum' J_{0j}$$

and so we get the self-consistency equation

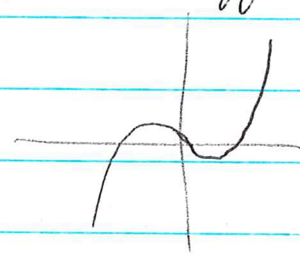
$$\langle s \rangle = \frac{e^{\beta(H+g\langle s\rangle)} - e^{-\beta(H+g\langle s\rangle)}}{e^{\beta(H+g\langle s\rangle)} + e^{-\beta(H+g\langle s\rangle)}} = \tanh \beta(H+g\langle s\rangle)$$

Picture:



$$H = \frac{1}{\beta}\left[\tanh^{-1}\langle s\rangle\right] - g\langle s\rangle$$

Thus this difference will give



when $g > \frac{1}{\beta}$ or $\beta g > 1$

Therefore $\beta g = 1$ gives the critical temperature.

However we know there is no phase transition for the 1-dim'l Ising model, so this approximation can't be very good in this case.

Next I look at the case of an interacting classical gas where mean field theory is supposed to give van der Waals equation of state. The partition fn is

$$Z = \sum_{n \geq 0} \frac{z^n}{n!} \int dx_1 \cdots dx_n \, e^{-\beta U_n(x)}$$

$$U_n(x) = \sum_{i<j} u(x_i, x_j)$$

This is like a continuous Ising model where most of the spins are down and only finitely many are up. The density $\rho(y)$ is what you integrate against to get 1-particle function averages, hence

$$\rho(y) = \frac{1}{Z} \sum_{n\geq 0} \frac{z^{n+1}}{n!} \int dx_1 \cdots dx_n \, e^{-\beta U_{n+1}(y,x)}$$

But $\quad U_{n+1}(y,x) = \sum_1^n U_2(y, x_j) + U_n(x_1, \ldots, x_n)$, hence we have

$$\rho(y) = z \left\langle \underline{x} \longmapsto e^{-\beta \sum U_2(y, x_j)} \right\rangle$$

Let us denote by ξ a typical configuration $x_1, \ldots, x_n$ and by

$$n(x, \xi) = \sum_j \delta(x - x_j) \qquad \text{if } \xi = \{x_j\}$$

Then

$$e^{-\beta \sum_j U_2(y, x_j)} = e^{-\beta \int U_2(y,x)\, n(x,\xi)\, dx}$$

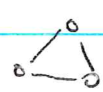
According to the mean field idea, we approximate the average of $\xi \mapsto e^{-\beta \int U_2(y,x)\, n(x,\xi)\, dx}$ by the value this function would have if $\xi \mapsto n(x,\xi)$ is replaced by its average which is $\rho(x)$. Thus using that $\rho(y)$ is independent of y we get the equation

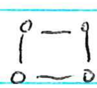
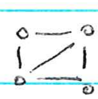
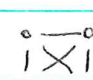
$$\boxed{\rho = z\, e^{-\left(\beta \int U_2(0,x)\, dx\right) \rho} \qquad \text{mean field equation}}$$

Now recall the equations

$$\frac{\rho}{z} = e^{\Gamma_2 \rho + \Gamma_3 \frac{\rho^2}{2!} + \cdots} \qquad \frac{P}{kT} = \rho - \Gamma_2 \frac{\rho^2}{2} - \Gamma_3 \frac{\rho^3}{1!\, 3} \cdots$$

where $\quad \Gamma_2 = \circ\!-\!\circ = \int \left(e^{-\beta U_2(0,x)} - 1\right) dx$

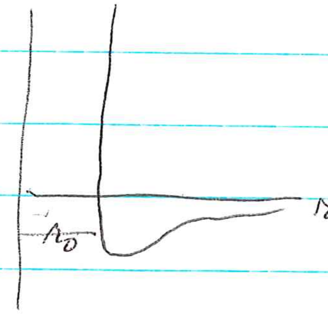
$\Gamma_3 =$ 

$\Gamma_4 =$  $+$  $+$ 

So what the mean field approach does is to forget about $\Gamma_3, \Gamma_4, \dots$ and to replace

$$\Gamma_2 = \int \left(e^{-\beta u_2(0,x)} - 1\right) dx \quad \text{by} \quad -\beta \int u_2(0,x)\, dx$$

It's clear this ignores the hard core part of van der Waals. [redacted] Recall that in the derivation one writes



$$\Gamma_2 = -a + \beta b + \cdots$$

$$a = \frac{4}{3}\pi r_0^3 \qquad b = -\int_{r_0}^{\infty} u_2(0,r)\, 4\pi r^2 dr$$

but that the rest of the derivation also has a fudge:

$$\beta p = \rho - (-a + \beta b)\frac{\rho^2}{2}$$

$$\beta\left(p + b\frac{\rho^2}{2}\right) = \rho\left(1 + \frac{a}{2}\rho\right) = \rho\,\frac{1}{1 - \frac{a}{2}\rho} = \frac{N}{V}\,\frac{1}{1 - \frac{a}{2}\frac{N}{V}}$$

or

$$\left(p + \frac{bN^2}{2V^2}\right)\left(V - \frac{a}{2}N\right) = NkT$$

and that I remember seeing that this fudge is necessary for the phase transition.

So the question becomes whether there is a nice way to do the mean field business in the presence of a hard core, so as to get van der Waals without extra approximations.

Let's proceed as follows. We are trying to find the average of $\xi \longmapsto e^{-\beta \sum_j u_2(0,x_j)}$ over the different configurations of the gas. If it weren't for the hard core it would be reasonable to expect most configurations consist of points x_j spead out with density ρ and so

$$\left\langle e^{-\beta \sum u_2(0,x_j)} \right\rangle \doteq e^{-\beta\left(\int u_2(0,x)\, dx\right)\rho}$$

[redacted]

Because of the hard core the function $e^{-\beta\sum u_2(0,x_j)}$ vanishes if any x_j are in the core $|x_j| \le r_0$. So what we have is a certain subset A of configurations where are x_j are outside of the sphere $V_e: |x| \le r_0$, and on this subset we have a function which we will suppose is nearly constant. Then we get

$$\langle e^{-\beta\sum u_2(0,x_j)}\rangle \doteq \mu(A)\, e^{-\beta\underbrace{\left(\int_{r_0}^{\infty} u_2(r)\, 4\pi r^2 dr\right)}_{\text{call this } -b}\rho}$$

and

$$\mu(A) = \frac{\sum_n \frac{z^n}{n!}\int_{V-V_e} dx_1\ldots dx_n\, e^{-\beta U_n(x)}}{\sum_n \frac{z^n}{n!}\int_V dx_1\ldots dx_n\, e^{-\beta U_n(x)}} \qquad V_e = \text{excluded volume}$$

Approximate this by

$$\mu(A) = \frac{Z(T, V-V_e, z)}{Z(T, V, z)}$$

and recall that $V \sim \infty$, but V_e is fixed, and

$$\frac{\log Z(T,V,z)}{V} = p\beta$$

Thus

$$\log \mu(A) = p\beta(V-V_e) - p\beta V = -p\beta V_e$$

$$\therefore\ \mu(A) \doteq e^{-\beta p V_e}$$

Another derivation is to notice that if we try to remove the volume V_e from the gas we do the work pV_e, and hence the state with gas outside V_e has higher energy; according to Boltzmann the probability of finding this higher energy state is $e^{-\beta p V_e}$

So putting all this together we get the equation

$$\frac{\rho}{z} = e^{-\beta p a + \beta b \rho} \qquad \text{where } a = V_e$$

Let's see if this leads to van der Waals.

$$\underset{-\beta p a + \beta b \rho}{\log\left(\frac{\rho}{z}\right)} = \Gamma_2 \rho + \Gamma_3 \frac{\rho^2}{2!} + \Gamma_4 \frac{\rho^3}{3!} + \cdots$$

$$a \cdot (p\beta) = a\left(\rho - \Gamma_2 \frac{\rho^2}{2!} - 2\Gamma_3 \frac{\rho^3}{3!} - 3\Gamma_4 \frac{\rho^4}{4!} - \cdots\right)$$

$$\therefore \beta b \rho = (\Gamma_2 + a)\rho + (\Gamma_3 - a\Gamma_2)\frac{\rho^2}{2!} + (\Gamma_4 - 2a\Gamma_3)\frac{\rho^3}{3!} + (\Gamma_5 - 3a\Gamma_4)\frac{\rho^4}{4!} + \cdots$$

$$\therefore \Gamma_2 = -a + \beta b \qquad \text{good.}$$

$$\Gamma_3 = a\Gamma_2$$

$$\Gamma_4 = 2a\Gamma_3 = 2!\, a^2 \Gamma_2$$

$$\Gamma_5 = 3!\, a^3 \Gamma_2$$

$$p\beta = \rho - \Gamma_2 \frac{\rho^2}{2!} - 2a\Gamma_2 \frac{\rho^3}{3!} - 3 \cdot 2!\, a^2 \Gamma_2 \frac{\rho^4}{4!} - 4 \cdot 3!\, a^3 \Gamma_2 \frac{\rho^5}{5!} - \cdots$$

$$= \rho - \Gamma_2 \underbrace{\left(\frac{\rho^2}{2} + a\frac{\rho^3}{3} + a^2 \frac{\rho^4}{4} + \cdots\right)}_{\frac{1}{a^2}\left(-\log(1 - a\rho) - a\rho\right)}$$

$$p\beta = \rho + (-a + \beta b)\frac{1}{a^2}\left(\log(1 - a\rho) + a\rho\right)$$

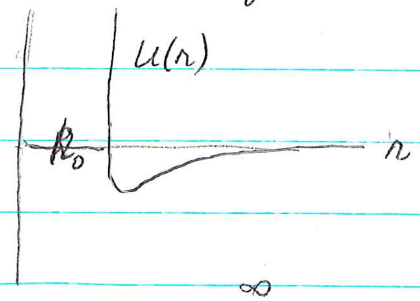
This does not seem to be van der Waals, although if we make the 2nd order approx we get

$$p\beta = \rho + (-a + \beta b)\frac{\rho^2}{2} + \cdots$$

as we should.

February 16, 1981

Take mean field result for classical gas with potential



$$a = \frac{4}{3}\pi r_0^3 \qquad b = -\int_{r_0}^{\infty} U(r)\, 4\pi r^2 dr$$

is

$$\frac{\rho}{z} = e^{-\beta p a + \beta b \rho}$$

also

$$\rho = z\frac{\partial}{\partial z}(p\beta). \quad \text{so}$$

$$\frac{\partial}{\partial\rho}(p\beta) = \underbrace{\frac{\partial}{\partial z}(p\beta)}_{\rho/z}\frac{\partial z}{\partial\rho} = \rho\frac{\partial}{\partial\rho}(\log z) = \rho\frac{\partial}{\partial\rho}(\rho + \beta p a - \beta b\rho)$$

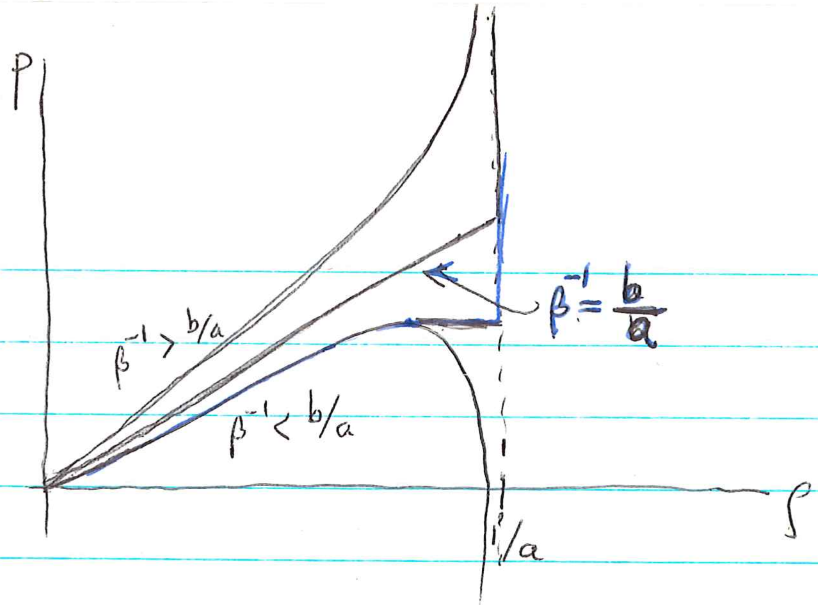
$$(1-a\rho)\frac{\partial}{\partial\rho}(p\beta) = 1 - \beta b\rho$$

$$\frac{\partial}{\partial\rho}(p\beta) = \frac{1-\beta b\rho}{1-a\rho} = \frac{1-\frac{\beta b}{a}}{1-a\rho} + \frac{\beta b}{a}$$

$$\boxed{p\beta = \frac{\beta b}{a}\rho + \left(1-\frac{\beta b}{a}\right)\frac{1}{a}\left(-\log(1-a\rho)\right)}$$

Now one has to plot this and interpret correctly when there is critical behavior. Critical behavior occurs when $\frac{\partial}{\partial\rho}(p\beta) < 0$ at some point. Now we must have $\rho < \frac{1}{a}$ because of the hard cores. Now $1-\beta b\rho$ decreases and so if $1-\frac{\beta b}{a} > 0$ there is no critical behavior. The critical temperature thus is

$$\boxed{\beta = \frac{a}{b} \quad \text{critical temp.}}$$



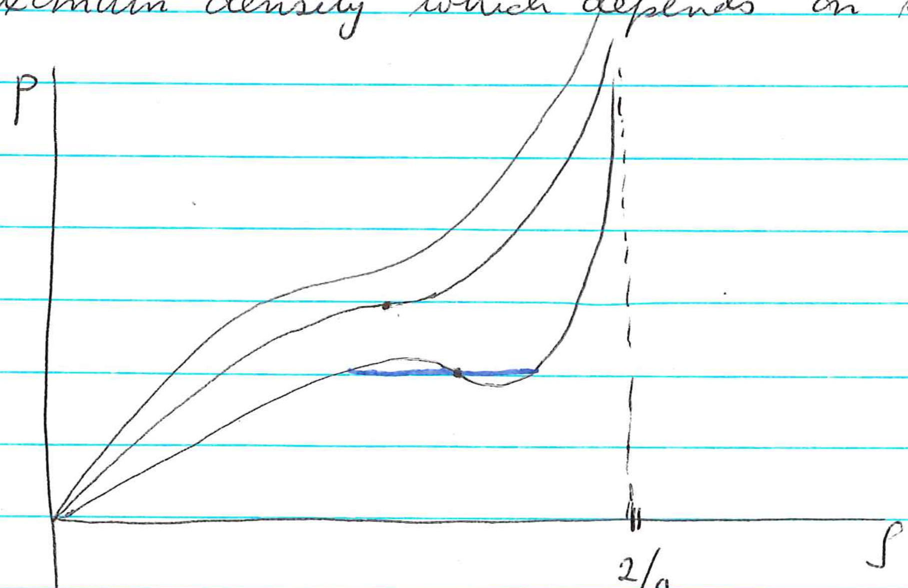
$p \;=\; \frac{1}{\beta}\rho + \cdots$

The van der Waals equation is

$$p\beta = \; - \beta b \frac{\rho^2}{2} + \frac{\rho}{1 - \frac{a}{2}\rho} \qquad \frac{d}{d\rho}(p\beta) = -\beta b \rho + \frac{1}{(1-\frac{a}{2}\rho)^2}$$

~~And you see immediately that if the molecules are separated by at least [illegible] then the excluded volume is [illegible] the critical~~

and the critical density is $\rho = \frac{2}{a}$. This is not the actual maximum density which depends on sphere-packing.



This is a much nicer curve.

Here's how you should have derived van der Waals from the mean field approach. Not quite, but let's pursue this idea. Recall that

$$\frac{\mathcal{S}}{z} = \text{average of } \{x_j\} \longmapsto e^{-\beta \sum u_2(0,x_j)} \text{ over the configurations of the gas.}$$

This function is zero for some x_j in the volume a so we first need to calculate the probability of the gas missing this ball.

Now we can do this in two ways. The expected number of molecules in the volume a is ρa. If the molecules were independent of each other the number of them in the volume a would be governed by Poisson's distribution

$$\frac{(\rho a)^n e^{-\rho a}}{n!} = \text{probability of } n \text{ molecules in the volume } a$$

Thus the probability of no molecules would be $e^{-\rho a}$ and we would get

$$\frac{\mathcal{S}}{z} = e^{-\rho a + \beta b \rho} \qquad \text{i.e. } \Gamma_2 = -a + \beta b$$

and all other $\Gamma_n = 0$.

On the other hand, the molecules aren't going to be independent of each other, and we expect it to be rather unlikely to find more than one molecule in the volume a. The other extreme would be the distribution having only $n=0$, $n=1$ and $\langle n \rangle = \rho a$

$$n=0: \quad 1-\rho a, \qquad n=1: \quad \rho a$$

This gives

$$\boxed{\frac{\mathcal{S}}{z} = (1-\rho a)e^{\beta b \rho}}$$

$$\frac{\partial}{\partial \rho}(p\beta) = \rho \frac{\partial}{\partial \rho} \log z = \rho \frac{\partial}{\partial \rho}\left(\log \rho - \log(1-\rho a) - \beta b \rho\right)$$

$$= 1 - \frac{-\rho a}{1-\rho a} - \beta b \rho = \frac{1}{1-\rho a} - \beta b \rho$$

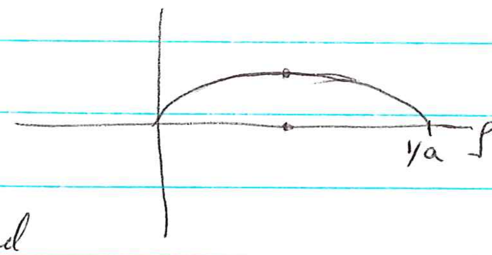
$$p\beta = -\frac{1}{a}\log(1-a\rho) - \beta b \frac{\rho^2}{2} \quad \sim \rho + (a-\beta b)\frac{\rho^2}{2} + \cdots$$

We get phase transitions when there are roots of

$$\frac{\partial}{\partial\rho}(p\beta) = \frac{1}{1-\rho a} - \beta b \rho = 0$$

with $0<\rho<\frac{1}{a}$. This is

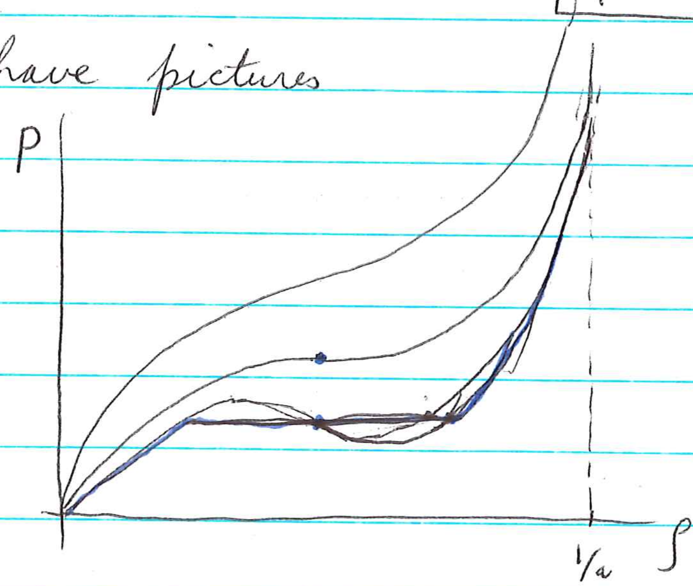
$$\beta b(\rho)(1-a\rho) = 1$$



The critical point has $\boxed{\rho = \frac{1}{2a}}$ and

$$\beta b \frac{1}{2a}\frac{1}{2} = 1 \quad \text{or} \quad \boxed{\beta = \frac{4a}{b}}$$

So we have pictures



so it seems this gives the same qualitative features as the van der Waals law.

$$p\beta = -\frac{1}{a}\log(1-a\rho) - \beta b \frac{\rho^2}{2} \qquad \text{above}$$

$$p\beta = \frac{\rho}{1-\frac{a}{2}\rho} - \beta b \frac{\rho^2}{2}$$

February 17, 1981

I attempt to derive van der Waals by a grand version of what's in Reif's book. Review Reif's argument: Replace $Z_N(T,V)$ by a 1-particle independent particle partition fn.

$$Z_N(T,V) \doteq \frac{1}{N!}\left(\int e^{-\beta u_{eff}(r)}\,dr\right)^N$$

where

$$\int e^{-\beta u_{eff}(r)}\,dr = (V-V_{ex})\,e^{-\beta \bar{u}_{eff}}$$

so that u_{eff} is + infinite over V_{ex} and constant with value $\bar{u}_{eff}$ on the rest of V. Then he argues that with a, b as before

$$V_{ex} = \frac{Na}{2} \qquad \bar{u}_{eff} = -\frac{b}{2}\frac{N}{V}$$

and one gets

$$Z_N \doteq \frac{1}{N!}\left(\left(V-\frac{Na}{2}\right)e^{\beta\frac{b}{2}\frac{N}{V}}\right)^N$$

so

$$p\beta = \frac{\partial}{\partial V}\log Z_N = N\frac{\partial}{\partial V}\left(\log\left(V-\frac{Na}{2}\right)+\beta\frac{b}{2}\frac{N}{V}\right)$$

$$= \frac{N}{V-\frac{Na}{2}} - \beta\frac{b}{2}\frac{N^2}{V^2} = \frac{\rho}{1-\frac{a}{2}\rho} - \beta\frac{b}{2}\rho^2$$

which is the van der Waals equation.

So now do this from the grand viewpt:

$$\mathcal{Z} = \sum \frac{z^N}{N!}Z_N \cong \exp\left\{z\left(V-\frac{Na}{2}\right)e^{\beta\frac{b}{2}\frac{N}{V}}\right\} \quad \times$$

hence

$$p\beta = \frac{\log \mathcal{Z}}{V} \cong z\underbrace{\left(1-\frac{a}{2}\rho\right)e^{\beta\frac{b}{2}\rho}}_{F(\rho)}$$

Now to eliminate z using $\rho = z\frac{\partial}{\partial z}(p\beta)$ or $d(p\beta) = \rho\, d\log z$

$$d\log(p\beta) = d\log z + d\log F = \frac{d(p\beta)}{\rho} + d\log F$$

YUCK.

There seems to be a problem here even when $b=0$. Thus if we have

$$p\beta = \frac{\rho}{1-\frac{a}{2}\rho} = z\left(1-\frac{a}{2}\rho\right)$$

Then

$$d(p\beta) = \frac{(1-\frac{a}{2}\rho)1-\rho(-\frac{a}{2})}{(1-\frac{a}{2}\rho)^2}\,d\rho = \frac{d\rho}{(1-\frac{a}{2}\rho)^2}$$

$$\rho\, d(\log z) = \rho\, d\log\left(\frac{\rho}{(1-\frac{a}{2}\rho)^2}\right) = \rho\left[\frac{d\rho}{\rho} - 2\,\frac{(-\frac{a}{2})d\rho}{(1-\frac{a}{2}\rho)}\right]$$

$$= \left[1+\frac{a\rho}{1-\frac{a}{2}\rho}\right]d\rho = \frac{1+\frac{a}{2}\rho}{1-\frac{a}{2}\rho}\,d\rho$$

so we don't have $d(p\beta) = \rho\, d\log z$, and something is wrong.

Here's the mistake

$$Z_N = \frac{1}{N!}\left(V-N\frac{a}{2}\right)^N \qquad \mathcal{Z} = \sum \frac{z^N}{N!}\left(\overset{\text{not constant}}{V}-N\frac{a}{2}\right)^N$$

obviously this formula can't be used for fixed V and all N. I checked that dominant term for $\mathcal{Z}$ is consistent with $p\beta = \frac{\rho}{1-a\rho}$ in this case

Anyway I still haven't succeeded in deriving van der Waals from mean field idea applied to the grand ensemble.

February 26, 1981

Let's review the many-body formalism. One starts with the grand partition function

$$Z(\beta, V, \mu) = \mathrm{tr}\left(e^{-\beta(H-\mu N)}\right) = \sum_n \left(e^{\beta\mu}\right)^n \mathrm{tr}\left(e^{-\beta H_n}\right)$$

from which thermodynamic quantities can be computed, e.g.

$$p = \frac{1}{\beta}\frac{\partial}{\partial V}\log Z \qquad N = \frac{1}{\beta}\frac{\partial}{\partial \mu}\log Z$$

$$-\frac{\partial}{\partial\beta}\log Z = E - \mu N$$

Then $\quad dQ = dE + p\,dV - \mu\,dN \quad$ is the heat added to the system in a small change and

$$\frac{dQ}{T} = k\Big(\underbrace{\beta\,dE}_{d(\beta E) - E\,d\beta} + \left(\frac{\partial}{\partial V}\log Z\right)dV - \beta\mu\,dN\Big)$$

$$= k\left\{d(\beta E) + \left(\frac{\partial}{\partial\beta}\log Z - \mu N\right)d\beta + \left(\frac{\partial}{\partial V}\log Z\right)dV - \beta\mu\,dN\right\}$$

$$= k\left\{d(\beta E + \log Z) - \mu N\,d\beta - \beta\mu\,dN - \underbrace{\left(\frac{\partial}{\partial\mu}\log Z\right)}_{N\beta}d\mu\right\}$$

$$= k\left\{d\left(\beta E + \log Z - \beta\mu N\right)\right\}$$

Thus the entropy is

$$S = k\left\{\beta E + \log Z - \beta\mu N\right\}.$$