Forest-Root Formulas in Statistical Physics

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An interpolation formula

$$f(0) = -\int_0^\infty f'(t)dt$$

We'd better assume f goes to zero at infinity. Note the minus sign!

Generalization: Chevron interpolation

Consider a 2-particle version with

$$f(t_1, t_2, t_{12})$$

Interpret t_1 and t_2 as the position of 2 particles on the half line and let $t_{12} = |t_1 - t_2|$. Use subscripts 1,2, or 12 to indicate partial derivatives:

$$f(0) = -\int_0^\infty ds(f_1(s,s,0) + f_2(s,s,0))$$

Apply the N = 1 formula to f_1, integrating wrt $t_2 - t_1 > 0$, $t_2 - t_1 = t_{12}$

And to f_2, integrating wrt $t_1 - t_2 > 0$, $t_1 - t_2 = t_{12}$

$$f(0) = \int_0^\infty dt_1 \int_0^\infty d(t_2 - t_1)(f_{1,2} + f_{1,12}) + (1 \longleftrightarrow 2)$$

since $\frac{dt_{12}}{dt_2} = 1$ for $t_2 > t_1$, and $\frac{dt_{12}}{dt_1} = 1$ for $t_1 > t_2$.

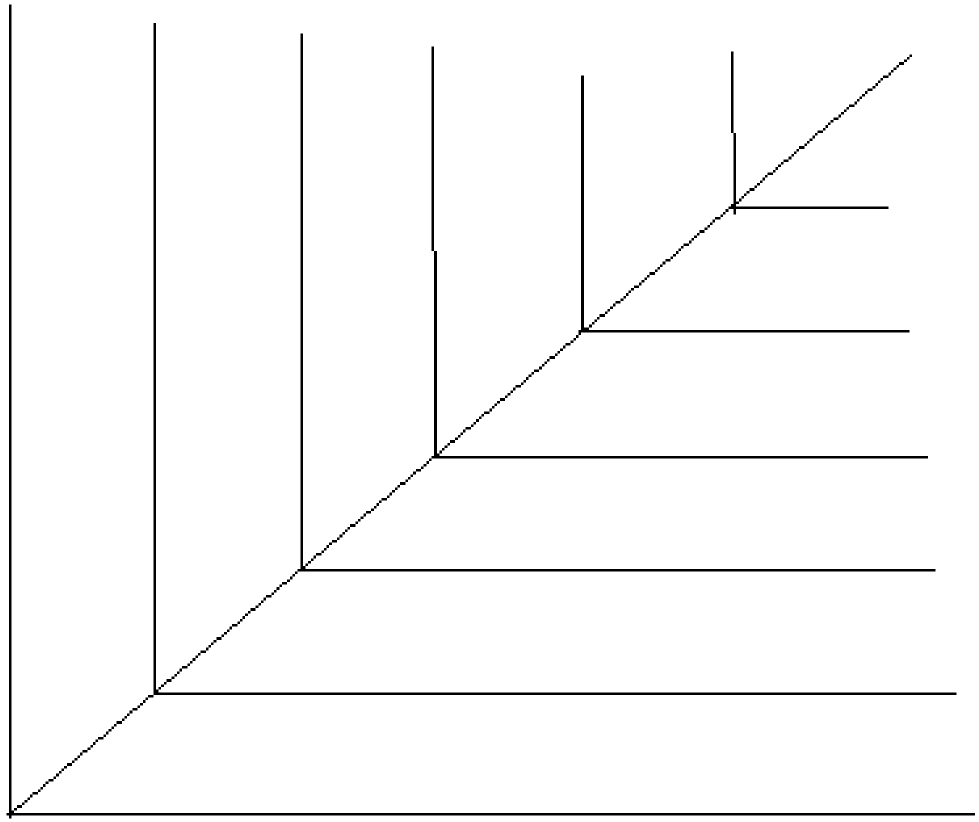
The two $f_{1,2}$ terms combine to form $\int_{\mathbb{R}_+^2} dt_1 dt_2 f_{1,2}$

Graphically, there are 3 terms (rooted forests):

$f_{1,2}$ o o

$f_{1,12}$ o------------------------x

$f_{2,12}$ x-----------------------o



General case

Let $f(\mathrm{t})$ be a smooth function of $\{t_i\}, \{t_{ij}\}$

which tends to zero when any of the t_i tends to infinity.

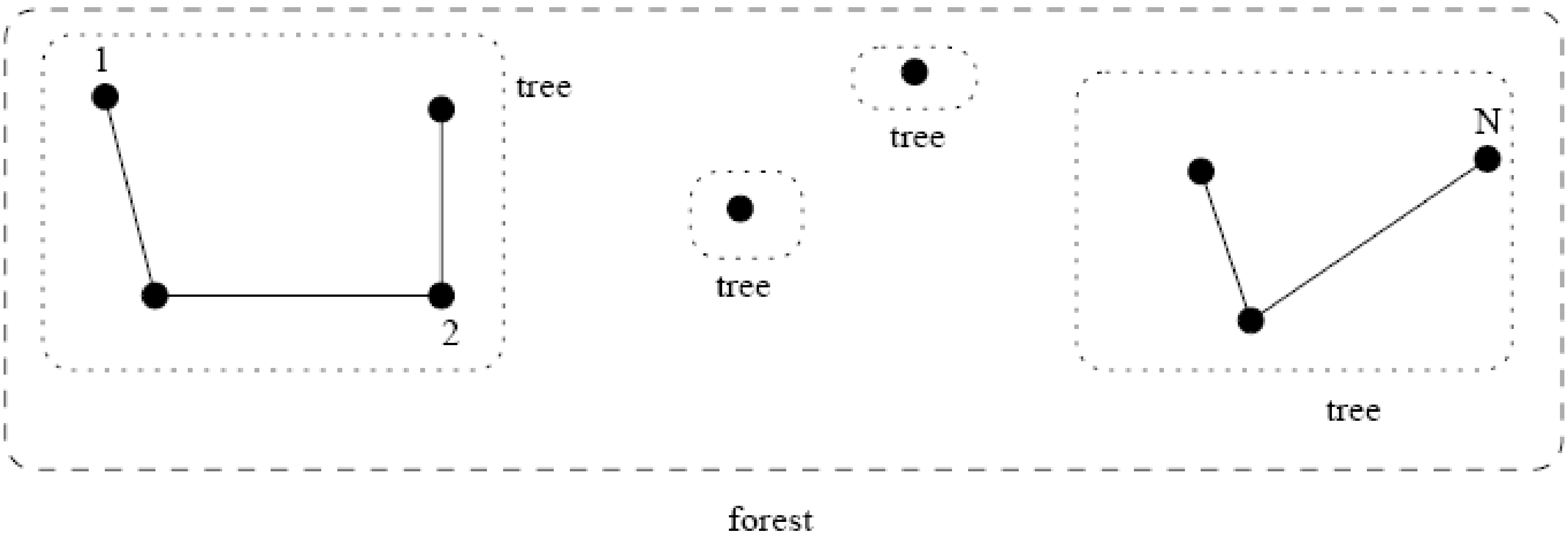
We allow “one-body” and “two-body” variables only.

Claim:

$$f(0) = \sum_{(F,R)} \int_{\mathbb{R}_+^N} \prod_{r \in R} [-dt_r] \prod_{ji \in F} [-d(t_j - t_i)] f^{(F,R)}(\mathrm{t})$$

Here F is a forest on {1,…,N}, each tree has a root.

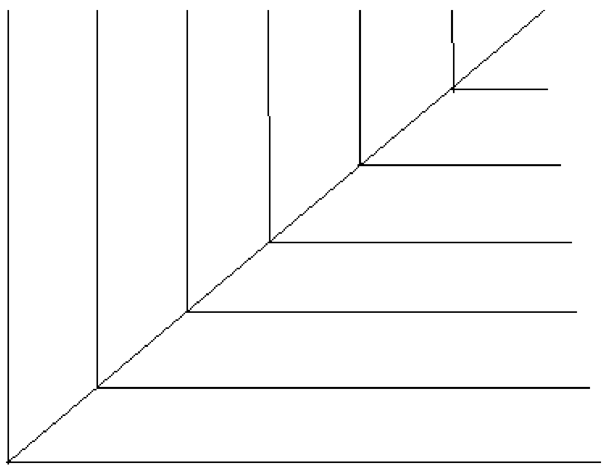
R is the set of roots. (F,R) denotes derivatives wrt edge variables t_{ij} with ij in F and root variables t_i with i in R.


1
tree
tree
N
2
tree
tree
forest

Inductive proof of Forest-Root formula

Begin with diagonal interpolation as before:

$$f(0) = -\int_0^\infty ds \sum_{k=1}^{N} f_k(s, \ldots, s, 0, \ldots, 0)$$



Proceed along the wings of the chevron, which now represent the N – 1 variables not yet differentiated.

Apply F-R formula, case N – 1, to each of the N terms

Each root derivative gives 2 terms as in previous example. Trees grow from below or sprout anew:

O becomes O----------------X + O X

Application to HC gases

Need 2-body interactions.

Full disclosure: AR 95 book has a formula which is related to our F-R formula but the margin is too small to demonstrate it.

Theorem II.2

$$\exp\Big(\sum_{l\in\mathcal{P}_n} u_l\Big) = \sum_{\substack{\mathfrak{F}=\{l_1,\dots,l_\tau\}\\ \text{u-forest}}} \Big(\prod_{\nu=1}^{\tau}\int_0^1 dw_{l_\nu}\Big)\Big(\prod_{\nu=1}^{\tau} u_{l_\nu}\Big)\exp\big(\sum_{l\in\mathcal{P}_n} w_l^{\mathfrak{F}}(\mathbf{w}).u_l\big)\ , \qquad \text{(II.2)}$$

where the summation extends over all possible lengths τ of $\mathfrak{F}$, including $\tau = 0$ hence the empty forest. To each link of $\mathfrak{F}$ is attached a variable of integration w_l. We define the $w_l^{\mathfrak{F}}$ as follows. $w_{\{ij\}}^{\mathfrak{F}}(\mathbf{w}) = 0$ if i and j are not connected by the $\mathfrak{F}$. If i and j fall in the support C of the same tree $\mathfrak{T}$ of $\mathfrak{F}$ then

$$w_{\{ij\}}^{\mathfrak{F}}(\mathbf{w}) = 0 \quad \text{if} \quad |l^{\mathfrak{T}}(i) - l^{\mathfrak{T}}(j)| \geq 2 \quad (i \text{ and } j \text{ in distant layers})$$

$$w_{\{ij\}}^{\mathfrak{F}}(\mathbf{w}) = 1 \quad \text{if} \quad l^{\mathfrak{T}}(i) = l^{\mathfrak{T}}(j) \quad (i \text{ and } j \text{ in the same layer})$$

$$w_{\{ij\}}^{\mathfrak{F}}(\mathbf{w}) = w_{\{ii'\}} \quad \text{if} \quad l^{\mathfrak{T}}(i) - 1 = l^{\mathfrak{T}}(j) = l^{\mathfrak{T}}(i'), \text{ and } \{ii'\} \in \mathfrak{T}.$$

(i and j in neighboring layers, i' is then unique). In particular, if $\{ij\} \in \mathfrak{F}$, then $w_{\{ij\}}^{\mathfrak{F}}(\mathbf{w}) = w_{\{ij\}}$.

HC gas partition function

$$Z_{\mathrm{HC}}(z) = \sum_{N=0}^{\infty} \frac{z^N}{N!} \int_{\Lambda^N} \prod_{i=1}^{N} dx_i \prod_{1 \le i < j \le N} U(0, x_{ij})$$

Here x_i are spatial variables in Z^D or R^D, $x_{ij} = x_i - x_j$.

The idea is to pick U(t,x) so that when all t's are zero we get a HC condition $\Pi_{ij}(1 - I(x_{ij}))$, where I(x) is the indicator function of a ball about 0. We take for example

$$U(t, x) = 1 - I(x)\vartheta(1 - t)$$

So the HC condition abruptly vanishes when t > 1.

Density of HC gas

$$\rho_{\mathrm{HC}}(z) = \lim_{\Lambda \nearrow S} \lim_{\epsilon \searrow 0} \frac{1}{Z_{\mathrm{HC}}(z)} \sum_{N=1}^{\infty} \frac{z^N}{N!} \int \prod_{i=1}^{N} dx_i f(\mathbf{0})$$

Where S = R^D or Z^D and

$$f(\mathbf{t}) = g(t_1/\epsilon) \prod_{i=2}^{N} g(\epsilon t_i) \prod_{1 \le i < j \le N} U(t_{ij}, x_{ij})$$

g is a smooth bump function, g(0) = 1. Apply F-R formula:

$$f(\mathbf{0}) = \sum_{(F,R)} \int_{\mathbb{R}_+^N} \prod_{r \in R} [-dt_r] \prod_{ji \in F} [-d(t_j - t_i)] f^{(F,R)}(\mathbf{t})$$

An Extra Dimension

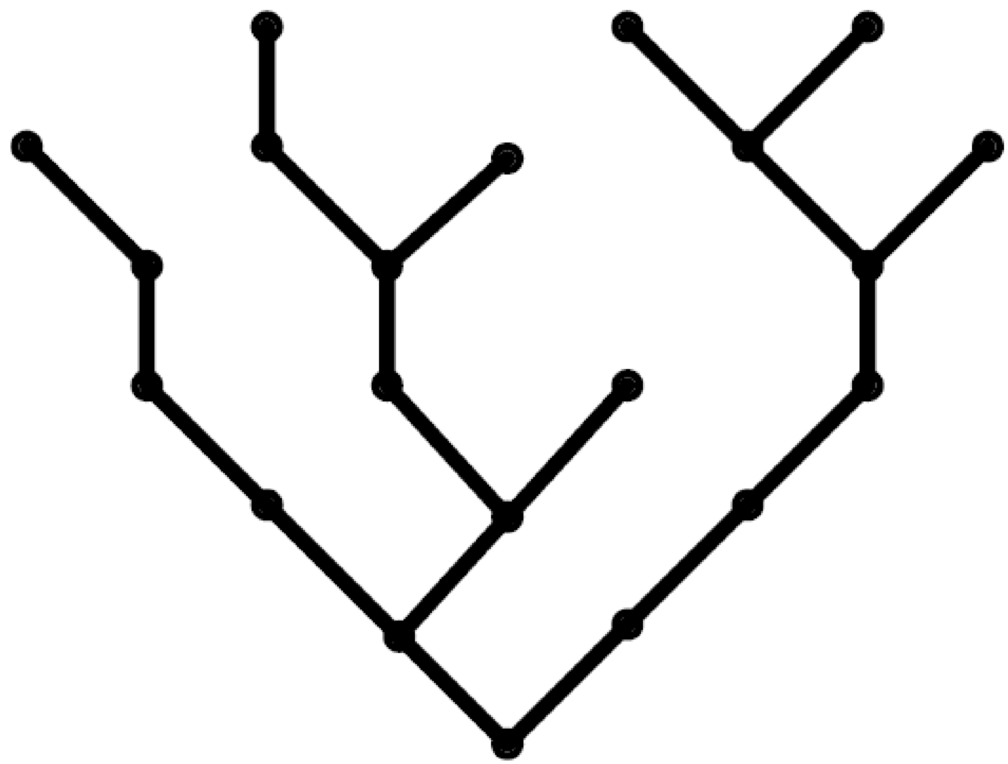
Apply the (F,R) derivatives to f. Each ji in F hits a U:

$$(d/dt)U(t,x) = V(t,x) = I(x)\delta(t-1)$$

Each i in R differentiates a g. For an n-vertex tree, $-(g(\varepsilon t)^n)'$ is a spread out probability measure. Free floating trees cancel the partition function. Only one tree remains, the one pinned at 0. The result is:

$$\sum_{N=1}^{\infty} (-1)^{N-1} \frac{z^N}{(N-1)!} \sum_T \int_{(\mathbb{R}_+ \times S)^{N-1}} \prod_{ji \in T} [dy_{ji} V(y_{ji})] \prod_{ji \notin T} U(y_{ji})$$

Note that x and t variables have been combined, y=(t,x) lives in R^D x R_+. The trees now live in an extra dimension!



Upward links denote factors of V which link the site below to an element of the ball about that site. Horizontal links not in the tree have hard core exclusion from factors of U.

Directed Branched Polymers

We have proven the following identity, which connects the density of the hard core gas in D dimensions with the generating function of directed branched polymers in D + 1 dimensions:

$$\rho_{\mathrm{HC}}(z) = -Z_{\mathrm{DBP}}(-z)$$

Critical Exponents

In D = 1, the nearest neighbor example is a dimer model which has a computable pressure:

$$p(z) = \ln\left(\tfrac{1}{2} + \tfrac{1}{2}\sqrt{1+4z}\right).$$

This has a square-root singularity at $z_c = -1/4$. The two-dimensional DBP generating function is thus

$$Z_{\mathrm{DBP}}(z) = -z\,\frac{d}{dz}\,p(-z) = \sum_{N=1}^{\infty} \frac{[2N-1]!!2^{N-1}z^N}{N!}$$

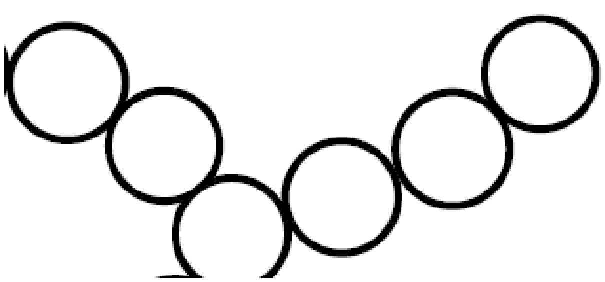
which has an inverse square-root singularity. The coefficient of z^N counts DBPs and it behaves like

$$d_N \sim z_c^{-N}\,N^{-\theta}$$ with $\theta = ½$.

Other examples

In D = 2 the density of the hard hexagon model behaves as $(z-z_c)^{1-\alpha}$ with α =7/6. This implies θ = 5/6 for a three-dimensional DBP model based on it.

Continuous examples have similar behavior.



Related Models

Directed Animals: There are exact results in two dimensions by Dhar, Sumedha, Bousquet-Melou, etc. coming from a representation as HC gas dynamics (80's). Results on exponents similar to those for DBP.

Di Francesco & Guitter 02: Lorentzian semi-random lattices (2d) are related to directed animals and also to D=1 HC gases.

A 2d Forest-Root Formula

As before we interpolate a function f(t) but now

$$t_{ij} = |w_i - w_j|^2,\ t_i = |w_i|^2 \text{ with } w_i \in \mathbb{C}.$$

w_i can be thought of as the position of a particle in the plane instead of the half-line. The new formula is

$$f(\mathbf{0}) = \sum_{(F,R)} \int_{\mathbb{C}^N} f^{(F,R)}(\mathbf{t}) \left(\frac{d^2 w}{-\pi}\right)^N$$

Case N = 1:

$$f(0) = \int_{\mathbb{C}} f'(t) \frac{d^2 w}{-\pi} = -\int_0^\infty f'(t) dt$$

Differential Forms

We need Grassman variables to get anywhere with this identity. It is natural to introduce them as differential forms as in Brydges's lecture.

$$\tau_i = w_i \bar{w}_i + \frac{dw_i \wedge d\bar{w}_i}{2\pi i}$$

$$\tau_{ij} = w_{ij} \bar{w}_{ij} + \frac{dw_{ij} \wedge d\bar{w}_{ij}}{2\pi i}$$

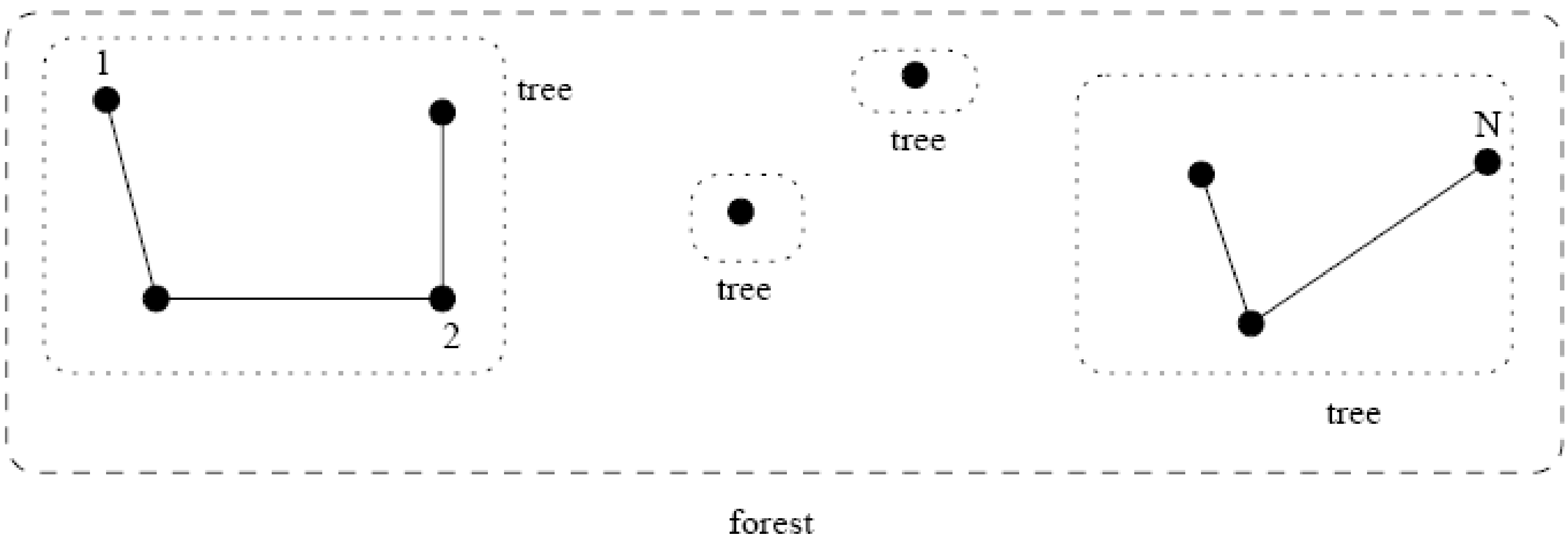
Then $f(\underline{\tau})$ is defined by its Taylor series.

Suppose we generate a loop of 2-forms on edges ij. Since $w_{ij} = w_i - w_j$, there is a relation and the product of 2-forms is 0. Therefore only forests appear in the Taylor series.

Each tree of the forest has a root which corresponds to a 2-form

$$\frac{dw_i \wedge d\bar{w}_i}{2\pi i}$$

This is needed to keep the total form degree equal to 2N and thereby allow the term to be nonvanishing.



F-R formula in form language

When expanded out, the equation

$$\int_{\mathbb{C}^N} f(\underline{\tau}) = f(\mathbf{0})$$

turns into the Forest-Root formula:

$$f(\mathbf{0}) = \sum_{(F,R)} \int_{\mathbb{C}^N} f^{(F,R)}(\mathbf{t}) \left(\frac{d^2 w}{-\pi} \right)^N$$

The constants are explained by the change of variable:

$$dw_i \wedge d\bar{w}_i = -2i dx_i \wedge dy_i$$

Feynman parameters

There is a "cosmological" proof of the F-R formula, using supersymmetry, but here I will give a more earthly argument which goes back to Brydges-Wright 88. Compute the Laplace transform of f:

$$\hat{f}(\mathbf{a}) = \int_0^\infty d\mathbf{t}\, f(\mathbf{t}) e^{\mathbf{a}\cdot\mathbf{t}}$$

Here $\mathbf{a} = (a_i), (a_{ij})$ is dual to $\mathbf{t}$, that is

$$\mathbf{a}\cdot\mathbf{t} = \Sigma_{ij} a_{ij} t_{ij} + \Sigma_i a_i t_i.$$

Note that $t_i = |x_i|^2$, $t_{ij} = |x_i - x_j|^2$. One could also use p's instead of x's which would make it a momentum space formula, and then the a's are Feynman parameters.

Linearity

Assume f decays exponentially in each ti. Then the a’s have positive real part in the inverse Laplace transform

$$f(\mathbf{t}) = \int \prod_i \frac{da_i}{2\pi i} \prod_{ij} \frac{da_{ij}}{2\pi i} \hat{f}(\mathbf{a}) e^{-\mathbf{a}\cdot\mathbf{t}}$$

By linearity, the F-R formula reduces to the case f(t) = $e^{-\mathbf{a}\cdot\mathbf{t}}$

Quadratic form

Note that $$\mathbf{a}\cdot\mathbf{t} = \langle w, A\bar{w}\rangle + \left\langle \frac{dw}{\sqrt{2\pi i}}, A\frac{d\bar{w}}{\sqrt{2\pi i}} \right\rangle$$

where
$$\begin{aligned} A_{ij} &= -a_{ij}, \qquad i \neq j, \\ A_{ii} &= a_i + \sum_{j\neq i} a_{ij}. \end{aligned}$$

Get this by expanding into four terms the two-form

$$a_{ij}(dw_i - dw_j) \wedge (d\overline{w}_i - d\overline{w}_j)$$

and combining coefficients for each monomial $dw_i \wedge d\overline{w}_j$

Determinants cancel

$$\int_{\mathbb{C}^N} e^{-\mathbf{a}\cdot\mathbf{t}} = \int_{\mathbb{C}^N} e^{-\langle w, A\bar{w}\rangle} \exp\left[-\left\langle \frac{dw}{\sqrt{2\pi i}}, A\frac{d\bar{w}}{\sqrt{2\pi i}} \right\rangle\right]$$

$$= \int_{\mathbb{C}^N} e^{-\langle w, A\bar{w}\rangle} \det A \prod_{i=1}^{N} \left[\frac{-dw_i \wedge d\bar{w}_i}{2\pi i}\right].$$

The “Fermionic” determinant is actually a Jacobian. It cancels the “Bosonic” determinant that arises from doing the Gaussian integral over w. This proves the F-R formula for exponentials.

$$\pi^{-N} \det A \int e^{-\langle w, A\bar{w}\rangle} d^N x \, d^N y = 1$$

Matrix-Tree theorem

We have learned that

$$1 = \int_{\mathbb{C}^N} e^{-\mathbf{a}\cdot\mathbf{t}} = \sum_{(F,R)} \int_{\mathbb{C}^N} e^{-\mathbf{a}\cdot\mathbf{t}\,(F,R)}(\mathbf{t}) \left(\frac{d^2 w}{-\pi}\right)^N$$

Perform the derivatives to obtain

$$1 = \sum_{(F,R)} \prod_{i\in R} a_i \prod_{ij\in F} a_{ij} \int_{\mathbb{C}^N} e^{-\langle w, A\bar{w}\rangle} \left(\frac{d^2 w}{-\pi}\right)^N \text{, so}$$

$$\det A = \sum_{(F,R)} \prod_{i\in R} a_i \prod_{ij\in F} a_{ij} \,,$$

and one can express the a's in terms of the matrix entries A_{ij}:

$$a_i = \sum_{j=1}^{N} A_{ij}, a_{ij} = -A_{ij}$$

which gives the usual form of the matrix tree theorem. (If one puts a_i = 0 one gets a sum over trees only.)

Grassman variable proofs of matrix-tree theorems appear in AA04 and CJSSS04.

More dimensional reduction

A new interpolation formula should lead to new results for the HC gas. We restrict attention to the continuum, so let x_i be in R^D.

Use the following HC weight for hard disks:

$$U(t_{ij}) = \theta(t_{ij} - 1)$$

Then

$$Z_{\mathrm{HC}}(z) = \sum_{N=0}^{\infty} \frac{z^N}{N!} \int_{\Lambda^N} dx_1 \cdots dx_N \prod_{1 \le i < j \le N} U(|x_i - x_j|^2)$$

Two extra dimensions

The integrand is

$$f(\mathbf{0}) = \prod_{1 \le i < j \le N} U(|x_{ij}|^2)$$

Extend to nonzero t:

$$f(\mathbf{t}) = \prod_{1 \le i < j \le N} U(|x_{ij}|^2 + t_{ij}) \times (\text{large } t \text{ cutoff})$$

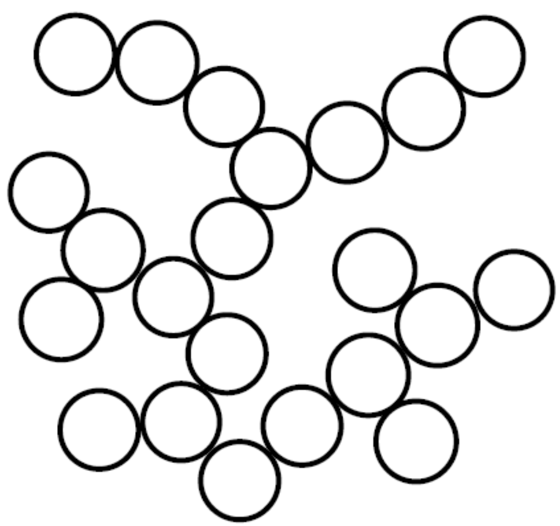
With $y_{ij} = (x_{ij}, w_{ij})$ in R^{D+2}, U now represents a hard core condition in D + 2 dimensions.

Branched Polymers in dimension D + 2

Apply the Forest-Root Formula:

$$f(\mathbf{0}) = \sum_{(F,R)} \int_{\mathbb{C}^N} f^{(F,R)}(\mathbf{t}) \left(\frac{d^2 w}{-\pi} \right)^N$$

Each d/dt_{ij}, when applied to U_{ij}, becomes ½ surface measure for the integration over $y_{ij} = (x_{ij}, w_{ij})$ in R^{D+2}. The spheres are stuck together according to the forest F.



Dimensional Reduction

Thinking of the trees as connected Mayer graphs, they become independent of each other as the large t cutoff is removed. Then we can compute the logarithm and the pressure as

$$\lim_{\Lambda \nearrow \mathbb{R}^D} \frac{1}{|\Lambda|} \log Z_{\mathrm{HC}}(z) = -2\pi Z_{\mathrm{BP}}\left(-\frac{z}{2\pi}\right)$$

where

$$Z_{\mathrm{BP}}(z) = \sum_{N=1}^{\infty} \frac{z^N}{N!} \sum_T \int dy_2 \cdots dy_N \prod_{ij \in T} [2U'_{ij}] \prod_{ij \notin T} U_{ij}$$

is the generating function for branched polymers in dim D + 2.
Here $2U'_{ij} = 2U'(|y_i - y_j|^2) = \delta(|y_i - y_j| - 1)$

Critical Exponents

The hard disk pressure is computable in D = 0 or 1, so we learn the exact form of the BP generating function in dimensions 2:

$$Z_{\mathrm{BP}}(z) = -\frac{1}{2\pi}\log(1-2\pi z)$$

and 3:

$$Z_{\mathrm{BP}}(z) = \frac{1}{2\pi}T(2\pi z) = \sum_{N=1}^{\infty}\frac{N^{N-1}}{2\pi N!}(2\pi z)^N$$

From this we obtain the volume exponents:

θ= 1 in D + 2 = 2

θ= 3/2 in D + 2 = 3

Remarks

Due to the alternating nature of the Mayer expansion, the first singularity of the pressure is at negative activity. It is one of several systems classified with the Lee-Yang edge singularity (Ising in imaginary field).

We confirm the Parisi-Sourlas predicted relation between θ and the Lee-Yang edge exponent.

Kenyon-Winkler 07: More invariances for the hard sphere BP model, allow varying radii in dim 2.

Thanks to my long time friend and collaborator David Brydges!