Stat mech diary

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Preface:

This is a diary containing worked-out problems in statistical mechanics. These problems are either elaborations on calculations in papers which I wanted to work out in detail, explanations of well-known facts that I wanted to remember, problems which arose when doing research, or problems assigned in grad classes. There are doubtless many typos, and I have not been very diligent about adding citations. Moreover, some entries were written near the beginning of grad school; I take no responsibility for any misguided beliefs that my younger self decided to write down.

Contents

Thermodynamics of the 1d Ising QCP

Today we are going to calculate various thermodynamic properties for the finite temperature quantum Ising model in 1d near its QCP. I'm sure this information is out in the literature somewhere, but I couldn't find it in Sachdev's book, so I thought it'd be worthwhile to just do myself.

We will write the Hamiltonian as

$$H = \sum_i \left(Z_i Z_{i+1} + (1-g) X_i \right), \tag{1}$$

so that the QCP is at $t = 0, g = 0$, where t is the dimensionless temperature.

The Hamiltonian is of course diagonalized in terms of Majoranas. In the usual way, this gives

$$H = \frac{1}{\pi} \int_0^\pi dk\, \varepsilon_k (\gamma_k^\dagger \gamma_k - 1/2), \qquad \varepsilon_k = \sqrt{g^2 + 2(1-g)(1 - \cos k)}. \tag{2}$$

Some straightforward algebra then leads to the free energy density

$$f = -t \left(\ln 2 + \frac{1}{\pi} \int_0^\pi dk\, \ln \cosh x \right), \qquad x \equiv \beta \varepsilon_k / 2. \tag{3}$$

Taking $-\partial_t$ we get the entropy density:

$$s = \ln 2 + \frac{1}{\pi} \int_0^\pi dk\, (\ln \cosh x - x \tanh x). \tag{4}$$

The $\ln 2$ is necessary to keep track of to be consistent with the third law of thermo since $\lim_{x \to \infty} (\ln \cosh x - x \tanh x) = -\ln 2$. Taking $\partial_{\ln t}$ of this expression, we get the specific heat

$$c = \frac{1}{\pi} \int_0^\pi dk\, x^2 \text{sech}^2 x. \tag{5}$$

We can also consider the g derivative of the entropy:

$$- \partial_g s = \frac{1}{2\pi} \int_0^\pi dk\, \frac{1 - g - \cos k}{t^2} \text{sech}^2 x, \tag{6}$$

where we used $\partial_g x = (t\varepsilon_k)^{-1}(g - 1 + \cos k)$.

While I don't know how to evaluate this expressions analytically at arbitrary points in the t-g plane, we can just go ahead and make some plots:[1] the entropy and specific heat

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[1] Note that the lack of symmetry about $g \to -g$ here at higher t is just because KW duality only does $g \to -g$ near the QCP. In general, the duality is

$$KW : (t, g) \mapsto (t/(1-g), g/(g-1)). \tag{7}$$

(divided by t since we expect them to go as t in the critical fan by hyperscaling; more on this in a sec) are

$$(8)$$
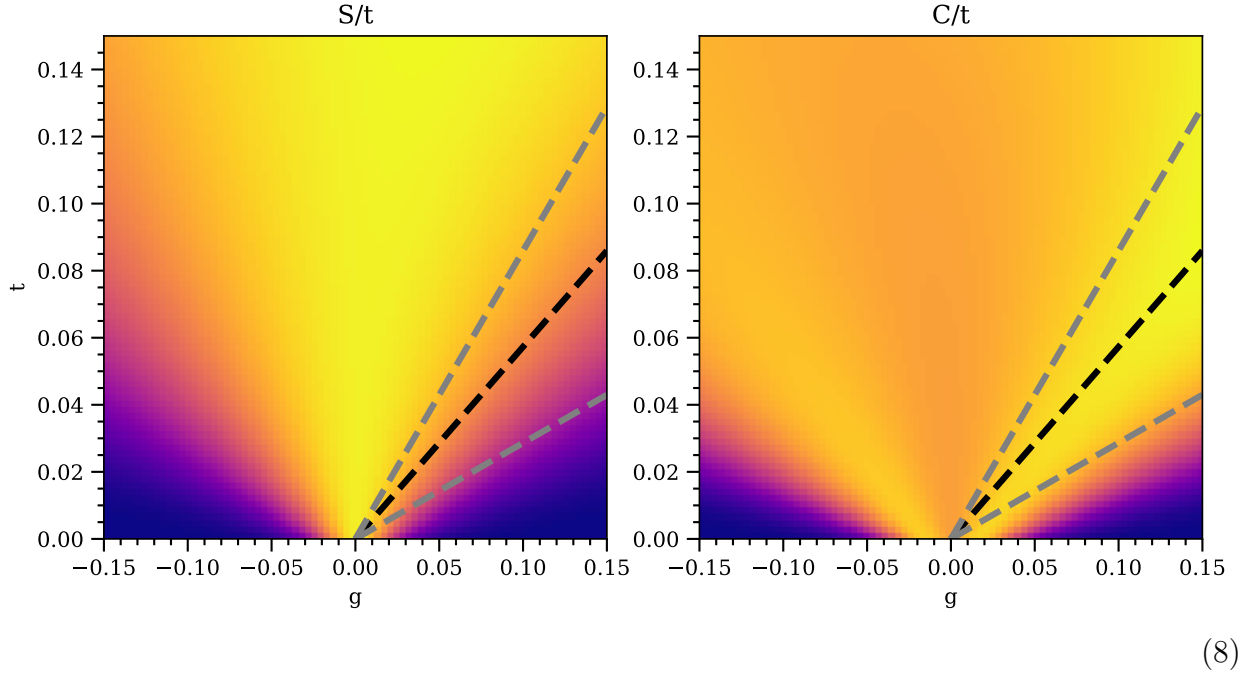
Here the dashed lines are a crude estimate of the extent of the crossover region. It can also help to look at cuts in different regions of the plane: for s/t we have

$$(9)$$

4
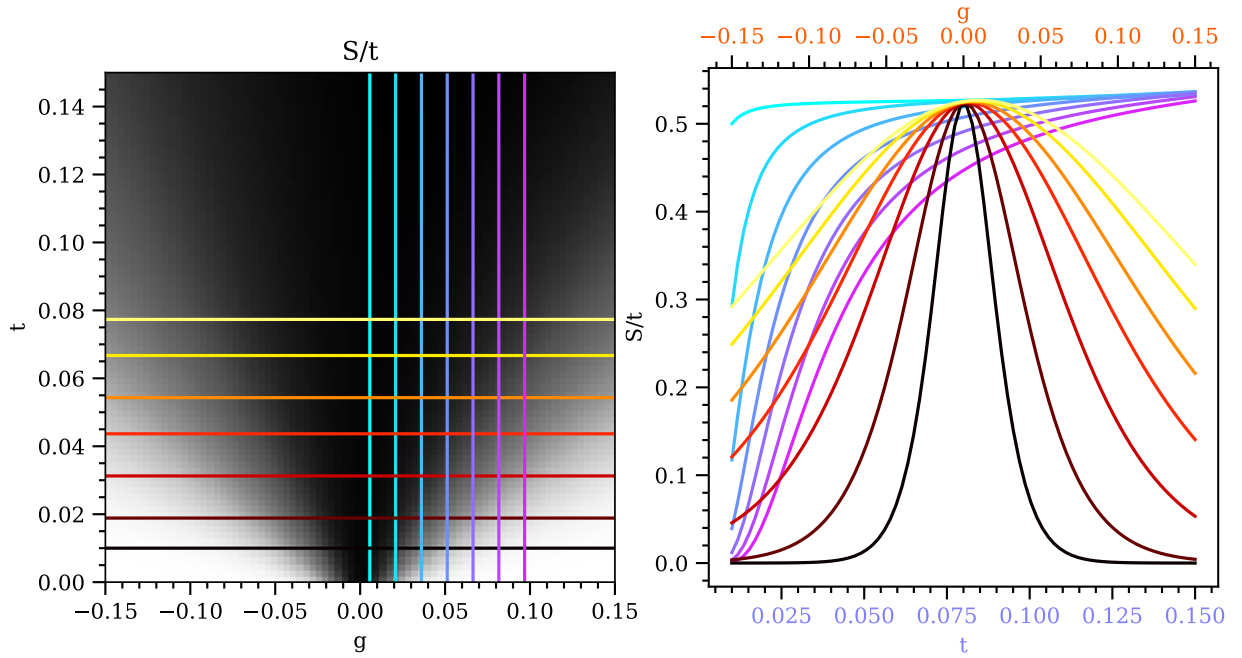
while for c/t we have

$$(10)$$
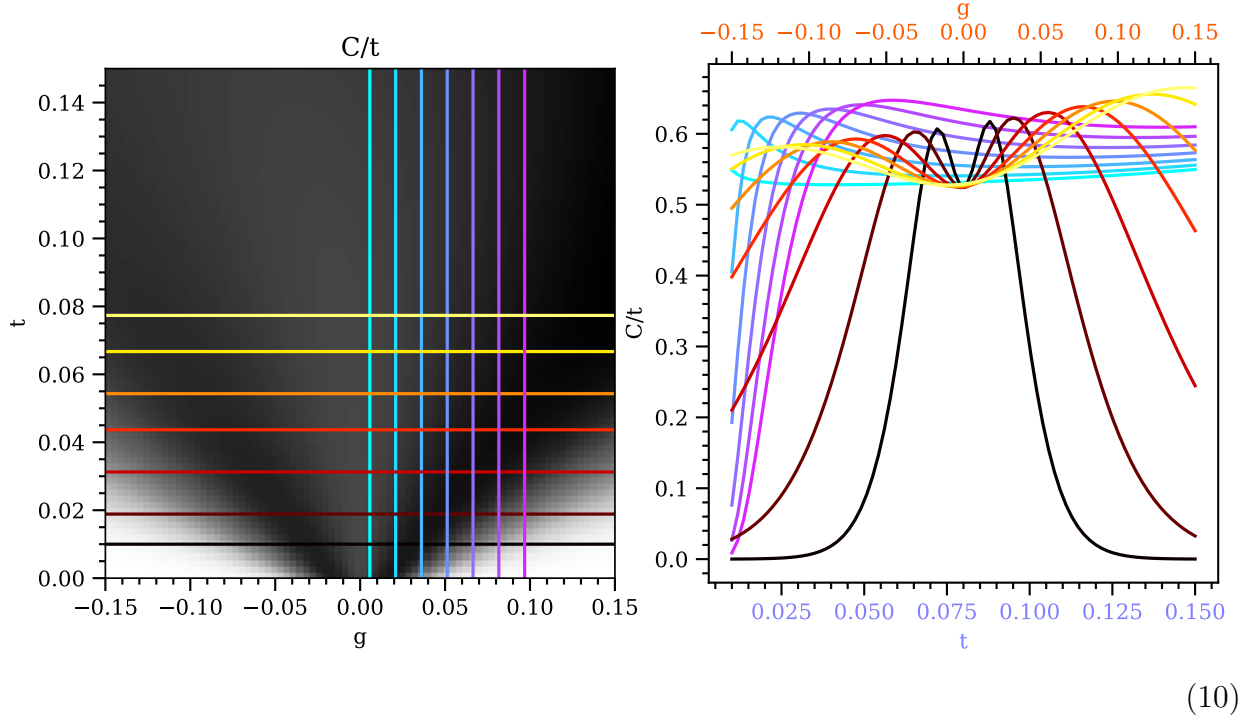
Just for completeness, we include the same plot but with c instead of c/t:

$$(11)$$
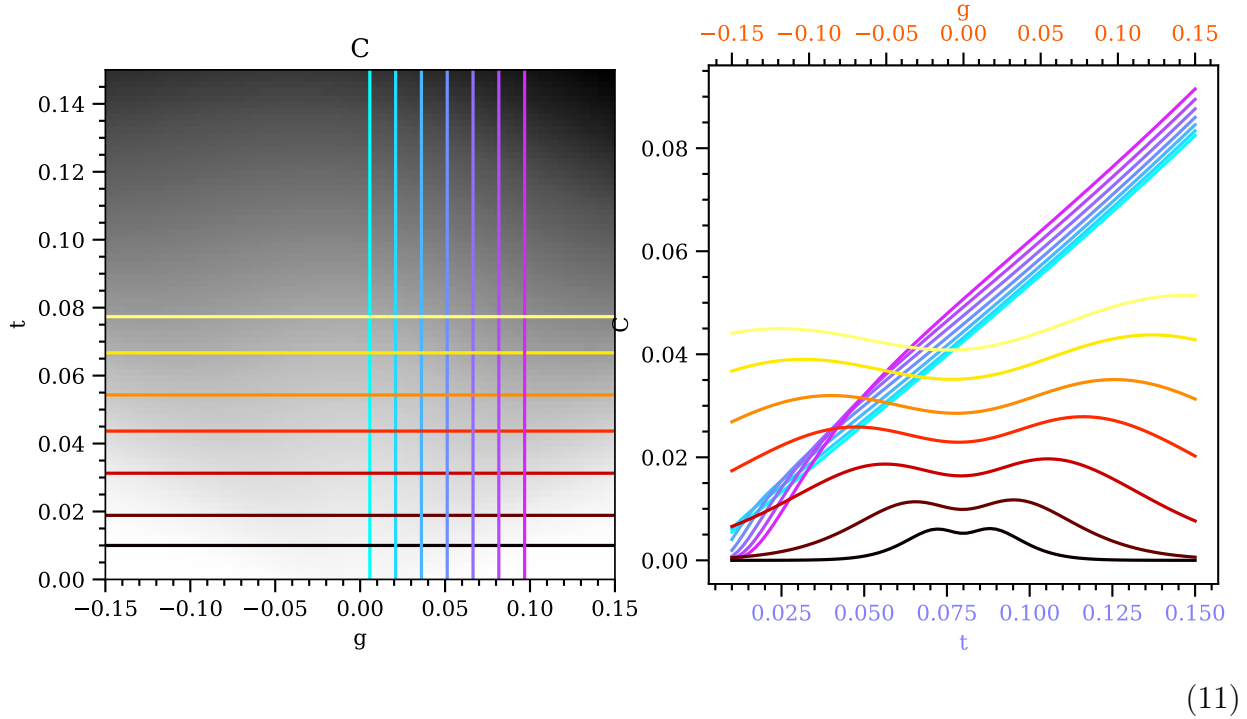
When we just plot c instead of c/t, we see that the maxima in c in the constant-g cuts disappear.

The constant-t slices are what we use to estimate the extent of the cross-over region: we know that $t_{cr}(g) \propto |g|$ since all the relevant exponents are unity, and we fix the slope by

looking at how the g-value of the maxima of constant-t cuts move with t. We then determine the width schematically by setting it equal to $t_{cr}(g)$.

Finally we can look at the g derivative of the entropy:

$$(12)$$

Let's check that these pictures make sense with what we'd expect from hyperscaling. Hyperscaling says that the free energy ought to scale as

$$f_s \sim g^{(d+z)\nu}\Phi_g(g^{-z\nu}t) \tag{13}$$

and

$$f_s \sim t^{d/z+1}\Phi_t(t^{-1/\nu z}g). \tag{14}$$

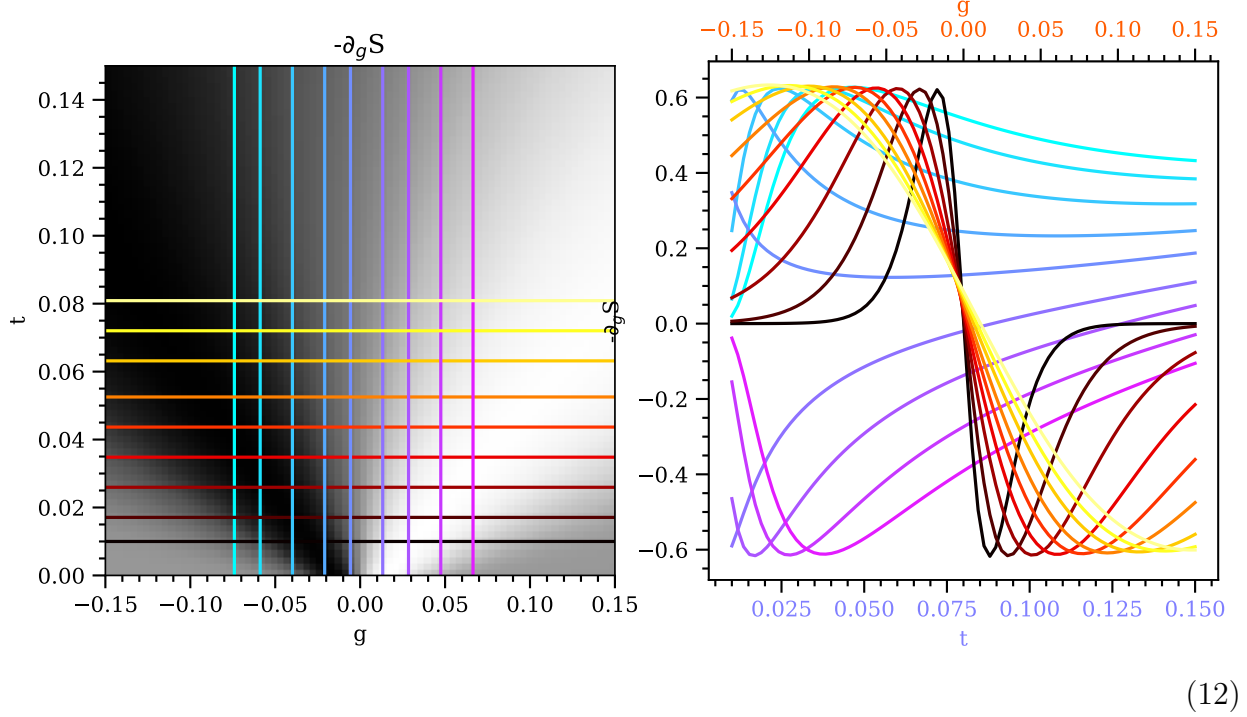Since the scaling functions $\Phi_{g/t}$ correspond to the free energy evaluated far from the critical point (where $|g| \sim 1$ or $t \sim 1$ respectively), and since both t and g are relevant, we expect both $\Phi_{g/t}(y)$ to be analytic in y. Therefore the former is useful when $t \ll g^{z\nu}$, while the latter is useful in the opposite limit. Actually this scaling form is not quite correct when either $(d+z)\nu$ or $d/z+1$ are integers: since the singular part of the free energy obeys scaling only up to analytic terms, if the $g^{(d+z)\nu}$ or $t^{d/z+1}$ are analytic then f_s can contain logarithmic terms of the form $g^{(d+z)\nu}\ln 1/|g|$ or $t^{d/z+1}\ln 1/t$, respectively (and we will indeed see such an example in what follows).

Of course from the fermion representation we know d, z, ν are all equal to unity, and we can see that this is indeed the case by the linear shape of the crossover region. Hyperscaling predicts $s, c \propto t$ in both scaling regimes; from the figure above we see that this indeed holds.

We can confirm the scaling forms by expanding the above expressions for the thermodynamic functions in the appropriate regimes. In the critical $t \gg |g|$ regime, we have (not

writing constants)

$$f \sim -t \int dk \, \ln \cosh \left[\frac{\sqrt{g^2 + 4\sin^2(k/2)}}{2t} \right]. \tag{15}$$

The integral can be roughly split into parts at the momentum $k_* \sim t(1 - g^2/t^2)$, which is where the argument of the cosh becomes of order 1. The low-momenta part is the one which dominates the thermodynamics, and can be written schematically as

$$f \sim -t \int_0^{k_*} dk \, \ln(1 - k^2/t^2). \tag{16}$$

The integral can be done in terms of a $\tanh^{-1}$ and a log, and when the $|g|/t \ll 1$ limit is taken we get

$$f \sim t^2 \Phi_t(|g|/t), \qquad \Phi_t(y) = a + by^2, \tag{17}$$

where a, b are numerical constants. The high-momentum part of the integral just modifies a, and is not important. Note that the absence of a linear term here is not due to the fact that we need $s(t = 0, g) = 0$,[2] but rather because of the KW duality that acts as $g \leftrightarrow -g$ in this regime.

In the disordered regime $|g| \gg t$ (where x is always large), the free energy is approximated by

$$f \sim t \int dk \, \ln[e^{\varepsilon/2t}(1 + e^{-\varepsilon/t})] \sim \int dk \, \varepsilon + t \int dk \, e^{-\varepsilon/t}. \tag{18}$$

The first integral (total energy) is independent of t and gives a logarithmic contribution:

$$\int dk \, \varepsilon \sim \int dk \, \sqrt{k^2 + g^2} \sim g^2 \ln(\Lambda/|g|), \tag{19}$$

where we have dropped constants and regulated the momentum integral at the scale Λ. The second integral gives us the t dependence, and looks like

$$t \int_0^\infty dk \, e^{-|g|/t - k^2/(2|g|t)} \sim t^{3/2} |g|^{1/2} e^{-|g|/t}. \tag{20}$$

Putting these together, we see that the singular part has the scaling form (no one ever said Φ_g had to be a polynomial or had to have nonzero derivatives at $y = 0$!)

$$f(|g| \gg t) \sim g^2(\Phi_g(t/|g|) - \ln|g|), \qquad \Phi_g(y) = y^{3/2} e^{-1/y}. \tag{21}$$

We will now look at derivatives of the entropy. In the critical regime where $|g| \ll t$, we have a nearly massless linearly dispersing fermion at low k; hence we expect a constant c/t. This agrees with hyperscaling, since in this regime we expect $f_s \sim t^{d/z+1} = t^2 \implies c \propto t$. Looking at the plot (blue curve), this is indeed what is observed. This also follows from the function form of c above: again not writing constants, the leading behavior as $g \to 0$ is

$$c(g \ll t) \sim \int_0^\infty dk \, t^{-2} k^2 e^{-k/t} \propto t, \tag{22}$$

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[2] Since we need $g \ll t$ for this expansion to be valid and a linear term would give $f \supset tg \implies s \sim g$, which in the current regime vanishes at $t = 0$.

as expected. The g derivative of the entropy is similar. We notice that the expression reduces to the same one above for c: proportional to t and to zeroth order independent of g. This is confirmed by looking at the cuts in the plot for $-\partial_g s$, which all towards the same linear slope once then get into the $t \gg |g|$ regime.

Likewise in the paramagnetic regime where $t \ll |g|$, we have a massive fermion, and so we expect a specific heat given by a power law times an exponential suppression in the dimensionless ratio $|g|/t$, since $|g| \sim m/2$ controls the mass of the fermion. Indeed, this is what happens:

$$c(t \ll |g|) \sim \int dk \, e^{-(m/t+k^2/(2mt))} t^{-2}(m^2 + \cdots) \sim \sqrt{t|g|}(g/t)^2 e^{-2|g|/t}. \tag{23}$$

This is in agreement with hyperscaling (the Φ functions don't have to be simple polynomials!), and fits the above numerical result well. For the g derivative of s, we have

$$-\partial_g s(t \ll |g|) \sim \int_0^\infty dk \, t^{-2} g e^{-(g/t+k^2/(2gt))} \sim \sqrt{t|g|} g t^{-2} e^{-2|g|/t}. \tag{24}$$

That this functional form works can be seen from a plot:

$$\tag{25}$$
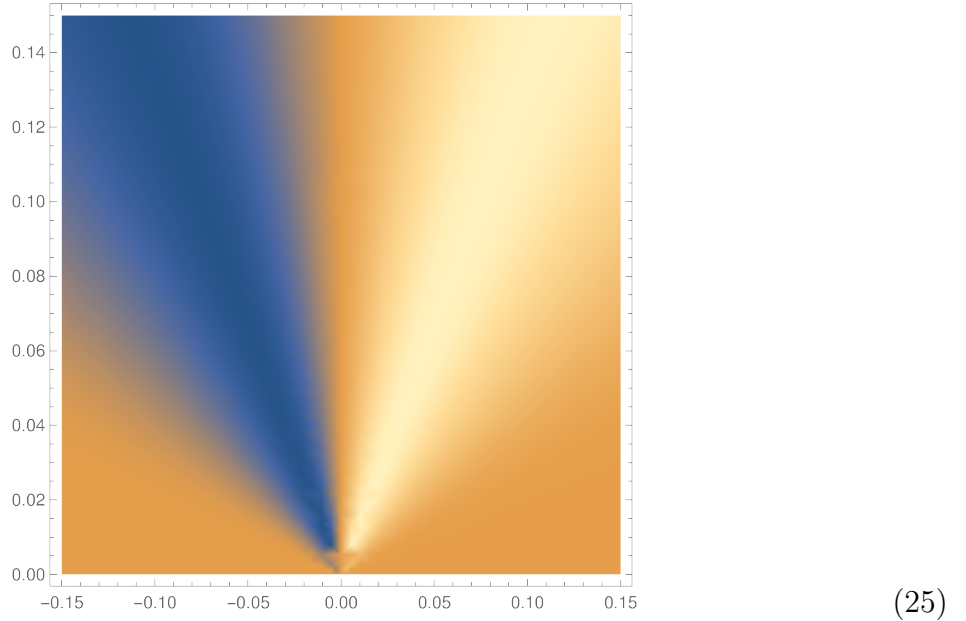
which agrees well with the exact numerical result above (the only thing it misses is the linear increase in t in the critical region).

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Practice with transfer matrices

This is a quasi-trivial brain-warmer. Consider a "spin chain" in one dimension with nearest neighbor interactions of the form

$$H = \sum_i |q_i - q_{i+1}|, \tag{26}$$

where $q_i \in [-1, 1]$ are the "spins". Find the spectrum of the transfer matrix and the correlation length in the limit of $T \to 0$.

Recall that $\mathbb{T}(q, q')$ is basically the part of the action that connects q and q'. It acts on vectors by integration against the kernel provided by the interaction, and so its eigenvectors ψ with eigenvalue λ will satisfy

$$[\mathbb{T}\psi](q) = \int_{-1}^{1} dq' \mathbb{T}(q, q')\psi(q') = \int_{-1}^{1} dq' e^{-|q-q'|/T}\psi(q') = \lambda\psi(q). \tag{27}$$

Differentiating this once gives

$$\lambda\partial_q\psi(q) = -\frac{1}{T}\int_{-1}^{1} dq' \mathrm{sgn}(q - q')e^{-|q-q'|/T}\psi(q'). \tag{28}$$

Differentiating again and using $\partial_q\mathrm{sgn}(q - q') = 2\delta(q - q')$ gives

$$\lambda\partial_q^2\psi(q) = -\frac{2}{T}\psi(q) + \frac{1}{T^2}\int_{-1}^{1} dq' e^{-|q-q'|/T}\psi(q'), \tag{29}$$

and so we have the DE

$$T^2\lambda\psi''(q) = -2T\psi(q) + \lambda\psi(q). \tag{30}$$

Let

$$\omega^2 = \frac{2T - \lambda}{T^2\lambda}, \tag{31}$$

so that the solutions are

$$\psi(q) = A\cos(\omega q) + B\sin(\omega q). \tag{32}$$

We can get boundary conditions relating ψ and ψ' by using the expression for ψ'. This gives

$$T\lambda\partial_q\psi(1) = -\lambda\psi(1) \tag{33}$$

and so, applying this to $\psi(q)$ and equating terms in A and B,

$$\cos(\omega) = T\omega\sin(\omega), \qquad \sin(\omega) = -T\omega\cos(\omega), \tag{34}$$

so that

$$\tan(\omega) = \frac{1}{T\omega}, \qquad \text{or} \qquad \tan(\omega) = -T\omega. \tag{35}$$

Let us choose e.g. the sin solution. Writing $\omega = n\pi + xT$ for $n \in \mathbb{Z}$, we have

$$xT \approx -Tn\pi - xT^2 \implies \omega \approx n\pi(1 - T). \tag{36}$$

From the definition of ω then, we get

$$\lambda_n = \frac{2T}{1 + n^2\pi^2T^2}. \tag{37}$$

Now we want to get the correlation length. For a generic two point function $\langle q_0 q_l \rangle$, we expect $|\langle q_0 q_l \rangle_c| \sim \exp(-|l|/\xi)$, and so we define the correlation length by

$$\xi = -\lim_{l\to\infty} \frac{|l|}{\ln\left(|\langle q_0 q_l \rangle_c|\right)}. \tag{38}$$

We now want to write this in terms of the spectrum of the transfer matrix. In the thermodynamic limit the expression $Z = \mathrm{Tr}\mathbb{T}^n$ collapses onto the largest eigenvalue λ_0, so that for n sites it goes to λ_0^n. Let Q be the position operator, so that $Q(q, q') = q\delta(q - q')$. Then the two point function is (projecting onto the ground state wavefunction ψ_0 and assuming PBC on a chain of total length L)

$$\begin{aligned}
\langle q_0 q_l \rangle &= \frac{1}{\lambda_0^L} \int dq_0 dq_l \ \psi_0(q_0) \mathrm{Tr}\left(\mathbb{T}^{L-l}Q\mathbb{T}^l Q\right)\psi_0(q_l) \\
&= \frac{1}{\lambda_0^l} \int dq_0 dq_l \ \psi_0(q_0)q_0[\mathbb{T}^l](q_0, q_l)q_l\psi_0(q_l) \\
&= \frac{1}{\lambda_0^l} \int dq_0 dq_l \ \sum_n \psi_0(q_0)q_0\lambda_n^l\psi_n(q_0)\psi_n(q_l)q_l\psi_0(q_l) \\
&\approx \frac{1}{\lambda_0^l} \int dq_0 dq_l \ q_0 q_l \left(\lambda_0^l\psi_0^2(q_0)\psi_0^2(q_l) + \lambda_1^l\psi_0(q_0)\psi_1(q_0)\psi_0(q_l)\psi_1(q_l)\right),
\end{aligned} \tag{39}$$

where we've kept only the two leading terms in the spectral decomposition of $\mathbb{T}$. Subtracting off $\langle q^2 \rangle$ to get the connected piece, we have

$$\langle q_0 q_l \rangle_c = \left(\frac{\lambda_1}{\lambda_0}\right)^l \Gamma^2, \qquad \Gamma = \int dq \ q\psi_0(q)\psi_1(q). \tag{40}$$

Taking $l \to \infty$ and taking the log, we get

$$\xi = \frac{1}{\ln(\lambda_0/\lambda_1)}. \tag{41}$$

For us, this means that the correlation length at $T \to 0$ is

$$\xi \approx \frac{1}{\pi^2 T^2}. \tag{42}$$

Since this diverges, the continuum limit can be taken safely.

Specific heats for fermions and bosons

Today's diary entry is super simple, and also comes from a problem in Ashvin's class. Calculate the specific heat for free Dirac fermions in 1+1D, as well as for free relativistic massless bosons. Now do the same in 2+1D — what does the result mean for bosonization?

First we get C for the Dirac fermions in two dimensions. The L and R components of a massless Dirac fermion are decoupled, and so we can just calculate C for a single component and then multiply the result by 2. The energy of excitations with respect to the Dirac sea where all negative energy states are filled is $v_F|k|$, and so we have, for a single component,

$$
\langle E \rangle = -\partial_\beta \ln Z = -\partial_\beta \ln \left[\sum_{n_k=0,1} e^{-\beta v_F \sum_k |k| n_k} \right] = -\partial_\beta \int_{\mathbb{R}} \frac{dk}{2\pi} \ln \left[1 + e^{-\beta v_F |k|} \right] = \frac{v_F}{\pi} \int_0^\infty dk \frac{k}{e^{\beta v_F k} + 1}
$$

$$
= \frac{T^2}{\pi v_F} \int_0^\infty dl \frac{l}{e^l + 1} = \frac{\pi T^2}{12 v_F}.
$$

(43)

Thus the heat capacity for a single component is $\pi T/(6v_F)$, and so we have

$$
C_{Dirac}^{1+1} = \frac{\pi T}{3 v_F}.
$$

(44)

Now for the bosons. The calculation is almost the same:

$$
\langle E \rangle = -\partial_\beta \ln \left[\sum_{n_k \in \mathbb{Z}^{\geq 0}} \prod_k e^{-\beta |k| v_F} \right] = -\partial_\beta \int_0^\infty \frac{dk}{\pi} \ln \left[\frac{1}{1 - e^{-\beta k v_F}} \right] = \frac{v_F}{\pi} \int_0^\infty dk \frac{k}{e^{\beta k v_F} - 1}
$$

$$
= \frac{\beta^2}{\pi v_F} \int_0^\infty dx \frac{x}{e^x - 1} = \frac{\pi T^2}{6 v_F},
$$

(45)

and so we get

$$
C_{boson}^{1+1} = \frac{\pi T}{3 v_F} = C_{Dirac}^{1+1}.
$$

(46)

Thus bosonization in two dimensions has a chance of relating a relativistic scalar with a Dirac fermion.

Alternatively, we could get this from our knowledge that in a CFT on a cylinder of circumference L, the vev of the holomorphic stress-energy tensor is (using the conventions in the Big Yellow Book and setting the "speed of light" to 1):

$$
\langle T \rangle = -\left(\frac{2\pi}{L} \right)^2 \frac{c}{24} \implies \langle T_{00} \rangle = \langle T_{zz} \rangle + \langle T_{\bar{z}\bar{z}} \rangle = -\frac{2}{2\pi} \langle T \rangle = \frac{\pi c}{6 L^2}.
$$

(47)

Thus since a cylinder of circumference L maps to a one-dimensional quantum system at temperature $T = 1/L$, (the units are right since we're taking the derivative of the energy *density*, not the energy)

$$C = \partial_T \langle T_{00} \rangle = \frac{\pi c T}{3}. \tag{48}$$

Since the bosons and fermions both have $c = 1$ (the ψ_L, ψ_R are decoupled and each have central charge $1/2$), we recover $C = \pi T/3$ for both systems.

Now we go to $2 + 1$ dimensions. The only things that change are the numbers, basically. For the fermions, since the Eigenvalues of H are $\pm v_F |k|$, we have

$$\langle E \rangle = -\partial_\beta \int_0^\infty \frac{dk}{2\pi} k \ln\left[1 + e^{-\beta v_F k}\right] = \frac{v_F}{2\pi} \int_0^\infty dk \frac{k^2}{e^{\beta v_F k} + 1} = \frac{T^3}{2\pi v_F^2} \int_0^\infty dx \frac{x^2}{e^x + 1} = \frac{3\zeta(3) T^3}{4\pi v_F^2}, \tag{49}$$

and so

$$C_{Dirac}^{2+1} = \frac{9\zeta(3) T^2}{4\pi v_F^2}. \tag{50}$$

For the bosons, we have

$$\langle E \rangle = -\partial_\beta \int_0^\infty \frac{dk}{2\pi} k \ln\left[\frac{1}{1 - d^{-\beta k v_F}}\right] = \frac{T^3}{2\pi v_F^2} \int_0^\infty dx \frac{x^2}{e^x - 1} = \frac{\zeta(3) T^3}{\pi v_F^2}, \tag{51}$$

and so

$$C_{bosons}^{2+1} = \frac{3\zeta(3) T^2}{\pi v_F^2}. \tag{52}$$

This is not equal to the specific heat of the Dirac fermions, unless we let the fermions and bosons have different v_F (we can set $v_F = 1$ for one system or the other, but need to remember to re-instate v_F when comparing the two). If they have different v_F they definitely can't be related by bosonization in the same manner as in 1+1D since the two theories have different causal structures, and so we can conclude that in three dimensions more ingredients (e.g. gauge fields) are needed to make bosonization work. This isn't surprising since in contrast to the two-dimensional case where particle statistics aren't really meaningful, in three dimensions braiding statistics is well-defined, and bosons at fermions are different statistically.

A QFT-flavored view of thermodynamic potentials

In my opinion discussions of the various thermodynamic[3] "potentials" (free energy, Gibbs free energy, Helmholtz, enthalpy, ad nauseum) are usually much more confused that they need

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[3]Even the name of the field sucks! Why thermo*dynamics*, when the whole point is that the theory can only answer questions about static stuff that's in equilibrium?

to be. For some reason most textbooks assume that defining a jillion different functions and then calculating partial derivatives in a jillion different ways will teach people something—didn't work for me, in any case. Today we'll try to explain a common framework for thinking about these different functions.

To derive thermodynamics, we need to start with an axiom regarding entropy / Boltzmann weights / etc. in order to get going. I can think of two reasonably good choices. One is a "bath-centric" point of view. Here we imagine our system X as being in contact with a bath B, such that the full system $X \cup B$ is closed. The full system can then be treated micro-canonically, with an entropy that is simply $S = \ln \Omega$, with Ω the number of microstates.[4] Since we are working in a closed system, there is no real notion of an interesting probability distribution here—we are assuming the ergodic hypothesis holds so that each mircostate makes an equal contribution to S. Thermodynamics is then done on X by e.g. maximizing S subject to the constraint that e.g. the energy of the subsystem X has a certain value, with equilibrium being defined through $\partial_{E_X} S_X = \partial_{E_B} S_B$. After tracing out the bath, one can then do thermodynamics in X. The point of this approach is that one is always secretly working in a closed system, with entropy always being calculated by $\ln \Omega$.

The second point of view, which we will adopt, basically never deals explicitly with a bath per se. Instead, the starting point is to declare that the right thing to do is to maximize the shannon entropy (here we will be using classical language)

$$S = \langle I \rangle = - \sum_k p_k \ln p_k, \tag{53}$$

where I is the information. Recall why this function is singled out as the right function to use: it is positive, maximal on uniform distributions, doesn't count states with $p_k = 0$, vanishes if the state of the system is certain with some $p_k = 1$, behaves correctly under super-imposing two systems ($\{p_k\} \to \{p_k q_l\}$ gives $S(\{p_k, q_l\}) = S(\{p_k\}) + S(\{q_l\})$), and so on.

The variables that act as input to a thermodynamic theory in this philosophy are the conserved quantities that we use to label the equilibrium states: U, V, N, M, etc. These extensive variables are all expectation values of operators that to each state k assign quantities U_k, V_k, etc, so that e.g. $U = \sum_k p_k U_k$.

These conserved quantities are what make thermodynamics, the study of the maximization of (53), nontrivial. They act as constraints on the optimization of (53), which if unconstrained would be maximized by all of the p_k being constant.

The problem is then to maximize (53) subject to fixed values of $\sum_k p_k \mathcal{O}_k^i$ for each conserved quantity $\mathcal{O}^i$. There are two paths forward. One is to solve the constraints first, i.e. to solve for the p_k as a function of the $\mathcal{O}^i = \sum_k p_k \mathcal{O}_k^i$, and then try to maximize S with respect to these expectation values. This is basically impossible, though. Instead, it is better to use Lagrange multipliers. This way we can first do an *unconstrained* minimization (which

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[4]We will always be setting $k = 1$.

in contrast is easy—just take derivatives and set them equal to 0), and then later solve the constraint. Therefore we want to instead maximize

$$\mathcal{S} = -\sum_k p_k \ln p_k + \sum_i \lambda_i \left(\sum_k p_k \mathcal{O}_k^i - \mathcal{O}^i \right) + \alpha \left(\sum_k p_k - 1 \right), \tag{54}$$

where the (unconstrained) maximization is carried out with respect to the p_ks and the λ_is as well as the last Lagrange multiplier α, which lets the p_k be fully unconstrained by being a Lagrange multiplier for the normalization of the p_ks.

The extremization is now easy to do (we get a maximum by convexity); we get

$$p_k = \frac{1}{Z} \exp\left(-\sum_i \lambda_i \mathcal{O}_k^i \right). \tag{55}$$

Therefore we have derived Boltzmann weights, rather than starting for them as an axiom. The point then is that as long as we write the probabilities in the above Boltzmann weight form, *we have already maximized the entropy*—there is no further extremization to be done in order to find equilibrium. The (maximized) entropy is evidently

$$S = -\sum_k \frac{e^{-\sum_i \lambda_i \mathcal{O}_k^i}}{Z} \left(-\sum_i \lambda_i \mathcal{O}_k^i - \ln Z \right) = \sum_i \lambda_i \mathcal{O}^i + \ln Z. \tag{56}$$

To make contact with conventional notation, we call the Lagrange multiplier for energy β, and the Lagrange multipliers for the other variables things like $p\beta, \mu\beta, H\beta$, and so on.[5] If we then define a free energy $\mathcal{F} \equiv -\beta^{-1} \ln Z$, we have

$$\mathcal{F} = U - \beta^{-1} S + \sum_i (\lambda_i \beta^{-1}) \mathcal{O}^i, \tag{57}$$

where we've separated out the energy U from the list of Lagrange multipliers due to the special role played by temperature and energy (of course, the terms in the sum would typically be written $-pV + \mu N - MH + \dots$). The fact that we've singled out U here is because in what follows we will always invert $S(U, V, N, \dots)$ and think about S, and not U, as an extensive variable, so that $U = U(S, V, N, \dots)$. This inversion can be done since we expect S to be monotonically increasing as a function of U, and is done because U is a more readily measurable quantity than S.

Now we're not really done, because a full solution to the problem would be to write the Lagrange multipliers λ_i in terms of the expectation values $\mathcal{O}^i$, which we took as inputs to the theory. However, doing this would require exactly computing the partition function and then doing some seriously heinous algebra to invert the resulting mess and get expressions for the λ_i.

However, now we can change our viewpoint a little, and regard the Lagrange multipliers as the independent variables. From the definition of $\mathcal{F}$, we see that functionally differentiating

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[5] Another complaint: who decided that β should multiply all the terms in the exponential of the Boltzmann weight? It'd seem to be much better if it only appeared in front of the energy.

$\mathcal{F}$ with respect to these Lagrange multipliers (since I think like a QFTheorist, I'm imagining that the sum over all states k has a product over e.g. all spatial points, so that we get statistical weights like $e^{-\beta \int d^d x\, U - MH + \cdots}$; hence functional differentiation is meaningful, and we can take the Lagrange multipliers / expectation values to be non-uniform in space) generates correlation functions of their associated conserved quantities. Therefore we see that the "intensive" variables $\beta, p, H, \ldots$ are nothing more than background fields—a background β field generates correlation functions of energy, a background H field generates correlation functions of magnetization, and so on.

These background fields / Lagrange multipliers are the way in which the "bath" manifests itself in this way of thinking about things. This is just as in regular QFT, where coupling the theory to background fields can be thought of as coupling the theory to a bath which can act as a source for particles, currents, etc.

The process of switching from using a background field (Lagrange multiplier) as an independent variable to using its corresponding intensive variable (expectation value of a conserved quantity) is done via a Legendre transform.

One particular Legendre transform is the one that swaps out all of the background fields as independent variables for all of the expectation values of conserved quantities. This is the Legendre transformation that relates U and F. For economy of notation, consider the case when energy is the only conserved quantity. Then we will have $\mathcal{F} = \mathcal{F}(\beta)$ and $U = U(S) = U[S(\beta)]$. We calculate

$$
\begin{aligned}
\partial_\beta \mathcal{F} &= \beta^{-2} \ln Z - \beta^{-1} \frac{\partial_\beta Z}{Z} = \sum_k \left(\beta^{-2} p_k \ln Z + \beta^{-1} \frac{p_k U_k}{Z} \right) \\
&= -\sum_k \beta^{-2} \left(-p_k \ln Z + p_k \ln(p_k Z) \right) = \beta^{-2} S.
\end{aligned}
\tag{58}
$$

Therefore

$$
\partial_T \mathcal{F} = -S.
\tag{59}
$$

Then applying this to $\mathcal{F} = U - TS$,

$$
-S = \partial_T S \partial_S U - S - T \partial_T S \implies \partial_S U = T.
\tag{60}
$$

So we see that $\mathcal{F}$ and U are not just any two functions satisfying $\mathcal{F} = U - TS$; rather they are constrained by the relations

$$
\partial_T \mathcal{F} = -S, \qquad \partial_S U = T.
\tag{61}
$$

The relation between the potentials $\mathcal{F}$ and U is therefore better expressed by writing

$$
\mathcal{F} = \min_S [U - TS], \qquad U = \min_T [F + TS],
\tag{62}
$$

which explicitly shows that U and $\mathcal{F}$ are Legendre transform pairs with respect to the conjugate variables S and T.[6] When there are more conserved quantities beyond just energy, there

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[6]Again, this whole rather arbitrary procedure of working with T instead of the Lagrange multiplier β, and attaching β's to all the conserved quantities in the Boltzmann weight rather than just the energy, is done so that we end up getting equations with dependent variables such that it is U, and not S, which appears as a thermodynamic potential with a free energy Legendre transform partner.

are accordingly more variables appearing, and more ways of taking Legendre transforms—but the basic game is still the same.[7]

Let's now briefly recall why Legendre transforms come up when solving constrained optimization problems. We will use the example of L and H, for simplicity. The problem is to extremize

$$\min_{x,v} \int dt \, L(x,v)|_{v=\partial_t x}, \tag{63}$$

where we need to put in the constraint that $v = \partial_t x$. If we directly solve the constraint first and then optimize we get the Euler-Lagrange equations, which are second order and sometimes hard to solve. In the Hamiltonian approach, we first optimize over an unconstrained system with a Lagrange multiplier p, and solve the constraint at the end: therefore the problem is to minimize

$$\min_{p,x,v} \int dt \, (L(x,v) + p(\partial_t x - v)) = \min_{p,x} \int dt \, (p\partial_t x - H(x,p)), \tag{64}$$

where we have defined

$$H(p,x) = \min_v (vp - L). \tag{65}$$

Notice that the minimization over p and x in (64) is unconstrained—this is the primary advantage of the Hamiltonian approach.

Maybe it helps to make explicit the analogies between Lagrangian mechanics, thermodynamics, and effective actions (as usual, the ϕ in the effective actions column denotes an expectation value in the presence of a current). The analogies in the first two columns are helpful for thinking about things physically since they give a nice field theory-flavored way of looking at thermodynamics, while the last column on mechanics is just included for building mathematical familiarity of what sorts of objects go where in Legendre transforms.

Thermo	Effective actions	Mechanics	
T	J	p	
S	$-\phi$	v	
$\mathcal{F}(T)$	$W[J]$	$H(x,p)$	
$U(S)$	$\Gamma[\phi]$	$L(x,v)$	(66)
$\mathcal{F} = \min_S[U - TS]$	$W = \min_\phi[\Gamma + \int J\phi]$	$H = \min_v[vp - L]$	
$U = \min_T[\mathcal{F} + TS]$	$\Gamma = \min_J[W - \int J\phi]$	$L = \min_p[\partial_t xp - H]$	
$\partial_T \mathcal{F} = -S$	$\delta_J W = \phi$	$\partial_p H = v$	
$\partial_S U = T$	$\delta_\phi \Gamma = -J$	$\partial_v L = p$	

The most interesting things to compute here are usually second derivatives of the generating functionals $\mathcal{F}, U, W, \Gamma$. By the Legendre transform pairing, the first derivative of a

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[7]Here we have defined "the" free energy to be a function only of the Lagrange multiplier background fields, but we could instead do some Legendre transformations and write it as a function of extensive quantities. For example, the Helmholtz free energy is normally $F = U - TS$, which is a function of extensive variables like $V, N, \dots$ but differs from U by the fact that it depends on T, and not S. When we say "free energy" in the text, we will generally one which is the "full" Legendre transform of U, which only depends on intensive quantities.

functional of the background fields / intensive variables (like $\mathcal{F}$) will be an argument of its Legendre pair (like U), i.e. it will be an expectation value / extensive variable. Therefore for any thermodynamic potential $F[X]$ which is "dual" to a potential $\widetilde{F}[\widetilde{X}]$, we will have

$$\partial_X^2 F[X] = \partial_X \widetilde{X}. \tag{67}$$

Therefore second derivatives of thermodynamic potentials are response functions.[8]

Anyway, the point to keep in mind is that *all of physics essentially reduces to computing path integrals with background fields.* Thermodynamics is basically the simplest manifestation of this, and the panoply of thermodynamic potentials that appear in textbooks are there just because in different situations one has different conserved quantities and different background fields to which they can couple. Even given a fixed set of conserved quantities, we can still choose to solve the constraints and write our thermodynamic potentials in terms of the expectation values of the extensive quantities rather than the background fields, with the process of switching out the independent variables being given by the Legendre transform.

Specific heats of stuff

Today we're going to derive specific heats for a few simple systems that come up often in stat-mech.

We are interested in calculating the specific heat at constant density, and so particle number and volume will be held fixed, which means that μ will *not* be an independent variable when taking derivatives, but rather will be a function of N and T and so on, complicating things. First we'll do stuff without chemical potentials.

Free classical stuff

We start with the most trivial example: non-interacting classical systems. Here we assume a Hamiltonian like $H = \sum_i p_i^2/2m + \sum_{i,j} u_{i-j} r_i r_j$, so that if we are working in the canonical

---

[8]Recall that response functions appear as the kernels that determine the expectation value of a variable X in the presence of its Legendre-dual source field $\widetilde{X}$ as (schematically) $\langle X \rangle = \int \chi \widetilde{X}$. χ is then $\partial_{\widetilde{X}} \langle X \rangle = \partial_{\widetilde{X}}^2 F$, so that response functions always come from second derivatives of thermodynamic potentials (of course we don't need to take both derivatives with respect to the same variable, we can also consider how $\langle X \rangle$ changes under the variation of background fields other than $\widetilde{X}$).

ensemble,

$$\ln Z = \ln \left[\frac{1}{N!} \left(\int d^d r d^d p \, e^{-\beta H} \right)^N \right] \tag{68}$$

We then re-scale the dof by $p' = \sqrt{\beta} p$, $r' = \sqrt{\beta} r$, which makes the T-dependence of $\ln Z$ manifest:

$$\ln Z = -Nd \ln \beta + \dots, \tag{69}$$

where ... is T-independent. Therefore in such systems U always has a T-dependence of dNT, meaning that

$$C = dN, \tag{70}$$

which is precisely the equipartition theorem. In fact we can make a slightly more general statement: if the single-particle partition function goes as T^α, then we will have $\ln Z \sim N\alpha \ln T$ and hence $U \sim N\alpha \implies C = N\alpha$. Therefore all such classical systems have a constant heat capacity. We get around this in e.g. quantum mechanics since the single-particle partition function $\sum_{n=0}^{\infty} e^{-\beta \hbar \omega n} = (1 - e^{-\beta \hbar \omega})^{-1}$ doesn't scale as a power of T.

Heisenberg and Ising models

We'll do the high T limit first. For the Ising model, we expand the energy U as a series in $\beta J \ll 1$,

$$U = \frac{1}{Z} \sum_{\{s_i\}} \sum_{\langle ij \rangle} J s_i s_j \left(1 - \beta J \sum_{\langle ij \rangle} s_i s_j + \frac{\beta^2 J^2}{2} \sum_{\langle ij \rangle \langle kl \rangle} s_i s_j s_k s_l + \dots \right). \tag{71}$$

The first contribution is the one where $s_i s_j$s from the first sum multiply the same pair of spins in the sum proportional to β. Therefore to lowest order,

$$U \approx -\frac{J^2 \beta}{Z} \sum_{\{s_i\}} \sum_{\langle ij \rangle}. \tag{72}$$

When we differentiate this wrt T the term with a derivative of Z^{-1} will die by oddness of the sum, and so the derivative just hits the β. Therefore

$$C(T) \approx 2^N (N/2)(J/T)^2, \tag{73}$$

where N is the number of sites. Therefore we get a decaying power law with exponent 2.[9]

The exact same story goes through for the Heisenberg model: there we're taking a trace, and the trace (to lowest order in β) projects onto the same product of spins on identical links as before (the structure only becomes different when you go to higher powers in the expansion, since then you can have e.g. $XYZ \propto \mathbf{1}$, which is traceful). Therefore we again get $C(T) \sim T^{-2}$ at large T.

---

[9]This makes sense cause in the Ising model the energy starts to saturate at high temperatures, in contrast to e.g. harmonic oscillators, where the energy can be made arbitrarily big by heating the system sufficiently.

Free things without chemical potentials

Let the things be described by a distribution function $\rho(\beta\varepsilon)$ (the absence of a chemical potential means that the things are not conserved), and let the dynamical exponent z be such that $\varepsilon = \alpha k^z$. Then

$$U = \int d^d k\, \rho(\beta k^z \alpha)\alpha k^z. \tag{74}$$

Then letting $x \equiv \beta k^z \alpha$, we have

$$U \sim \int_0^\infty dx\, \rho(x) \left(\frac{x}{\beta\alpha}\right)^{d/z+1}, \tag{75}$$

where we've ignored factors relating to volumes of spheres. Since x is dimensionless, we get

$$U \sim (\beta\alpha)^{-1-d/z} \implies C(T) \sim \alpha^{-1-d/z} T^{d/z}. \tag{76}$$

When talking about e.g. phonons, this T dependence is appropriate at low temperatures, with $T/\omega_D \ll 1$ where ω_D is the Debeye frequency, set by the finite size of the BZ. As T approaches ω_D $C(T)$ will start to freeze out (as with any system where the energies of the modes are bounded from above), eventually reaching the constant $C \sim N$ at $T \gtrsim \omega_D$ in accordance with equipartition. This is checked just by fixing ω_D as the upper bound on the integral, but needs to be done numerically to get the full profile.

Free fermions with a chemical potential

This is actually a surprisingly hard example to do in full generality! The presence of the chemical potential actually complicates our ability to solve things exactly.

One limit where we can of course solve things exactly is when $\mu\beta \gg 1$—in this case, only states with energies close to μ contribute, and we can essentially take $\mu(T) = \mu(0)$.[10] The classic example is that of the Fermi liquid at $T \ll T_F$. Intuitively, U (relative to the ground state) will be given by the number of particles excited to deviate from the $T = 0$ distribution times their average energies. Now a typical thermally excited fermion comes from within a distance β^{-1} of $\mu \approx \varepsilon_F$, and acquires a typical energy of β^{-1}; hence $U \propto \beta^{-2} \implies C(T) \propto T$. Of course this can be checked by doing

$$U \sim \int_0^\infty d\varepsilon\, N(0)\frac{\varepsilon}{1 + e^{\beta(\varepsilon-\mu)}} \sim \int_{-\infty}^\infty dx\, N(0)T^2 \frac{x}{1 + e^x} \implies C(T) \sim N(0)T. \tag{78}$$

---

[10]I think one thing that is easy to forget after just reading cond-mat stuff is that the chemical potential in this setting is not the Fermi energy, nor is it T-independent. Indeed, we have

$$N \approx \int d^d\mathbf{k}\, \rho[\beta(\varepsilon_\mathbf{k} - \mu)] \tag{77}$$

for some distribution ρ. When we change β but hold N fixed, μ must evidently also change to keep the LHS invariant. This is basically another way of saying that when we write the distribution function in terms of μ, μ is a Lagrange multiplier that we haven't yet solved the constraint to determine—it will generally be a function of all the expectation values of the conserved quantities in the system.

The simplifications coming from $\mu\beta \gg 1$ were that we could approximate the density of states by the constant $N(0)$, and that we could take $\mu \to \varepsilon_F$ to be T-independent and big enough to extend the integral over $\beta(\varepsilon - \mu)$ to be over the whole $\mathbb{R}$ line.[11]

Now in the low density limit we know that we need to get $C \sim T^{d/z}$, and so evidently there must be some rather complicated crossover as T changes form between the small $\mu\beta$ and large $\mu\beta$ regimes. Basically, the complications stem from doing an integral from $-\beta\mu$ to ∞, and expanding the result in terms of powers of $\beta\mu$. Since the analysis looks rather involved, we'll leave it at that.

Gasses with internal degrees of freedom

Let the typical energy spacing between the levels coming from the internal dof be Δ. If $\beta\Delta \gg 1$ or $\beta\Delta \ll 1$, the internal levels makes no contribution to the specific heat. Intuitively this is clear since for $\beta\Delta \gg 1$ the internal dof are frozen out, while for $\beta\Delta \ll 1$ their energies are completely saturated, so that U no longer changes with T. More precisely, if $\beta\Delta \ll 1$ then the internal dof contribute to the partition function a factor

$$Z_I \approx N_{dof}, \tag{79}$$

which affects things like the entropy and chemical potential, but not the specific heat due to the trivial T-dependence. For $\beta\Delta \gg 1$, we can project onto the internal energy level of lowest energy—since the internal dofs are then frozen out, we should get $C_I = 0$. Indeed,

$$C = -\partial_T\partial_\beta \ln Z = \beta^{-2}\partial_\beta^2 \ln Z \implies C_I = \partial_T\partial_\beta(\beta\Delta) = 0. \tag{80}$$

Therefore the contribution to C from the internal dof will have some nontrivial behavior as a function of T, with a local maximum near the order of $T \sim \Delta$ and dying back down to zero at $T = 0$ and $T \to \infty$.

A simple example is a two-level system with a gap Δ. Since $e^{-\varepsilon\beta}$ factors don't contribute to the specific heat, we may take the lower level to have energy 0 and the upper level to have energy Δ. Therefore the internal dof partition function is

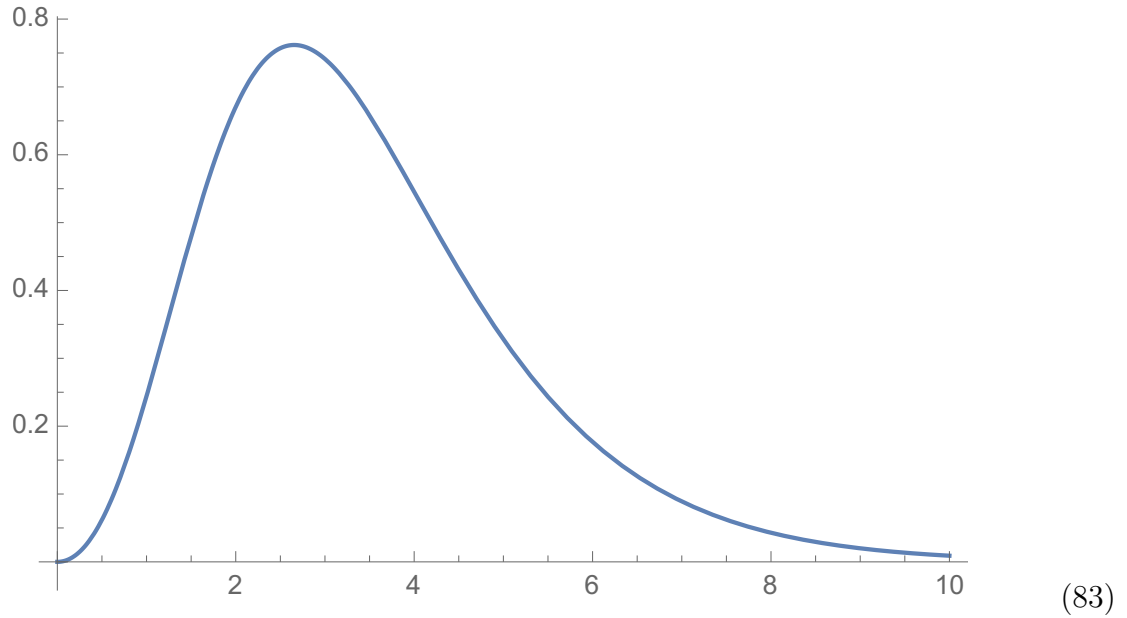$$Z_I = g_0 + g_1 e^{-\beta\Delta}. \tag{81}$$

The specific heat is then easy to calculate—some algebra gives

$$C(T) = \frac{(\beta\Delta)^2}{2 + (g_0/g_1)e^{-\beta\Delta} + (g_1/g_0)e^{\beta\Delta}}. \tag{82}$$

---

[11]This is of course a good assumption in most metals, since the corrections to μ from ε_F are of order T^2/ε_F^2, which is $O(10^{-4})$ in most metals.

This looks like (shown is $C(\beta\Delta)$ against $\beta\Delta$).

$$(83)$$

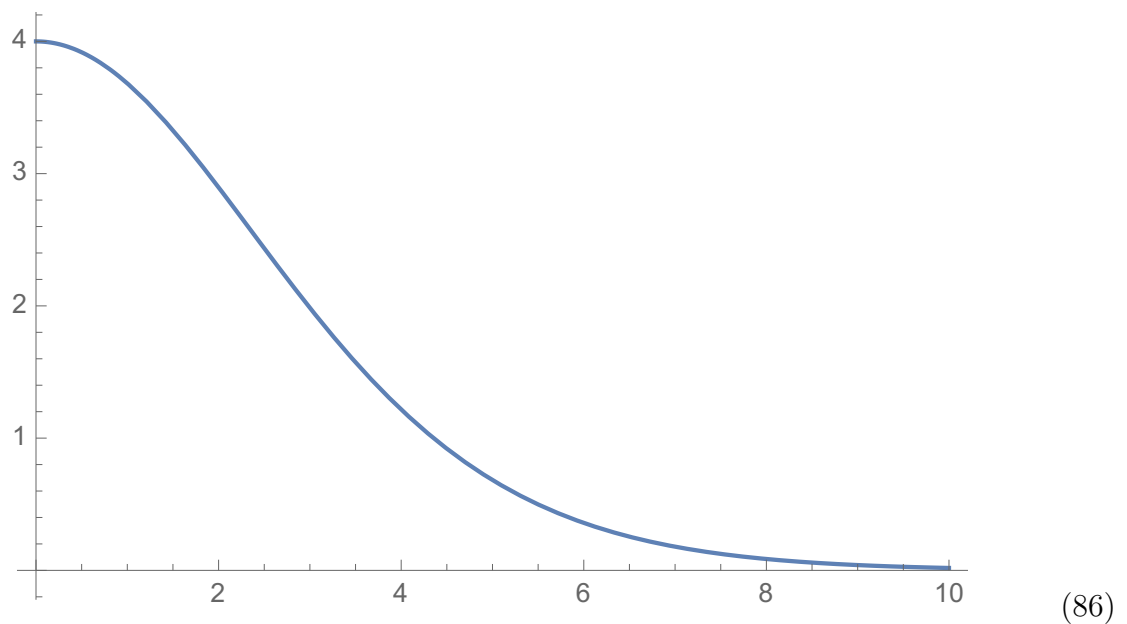which is the shape we expect.

Another example is the specific heat coming from internal vibrational modes, which we treat as harmonic oscillators. The internal partition function is then

$$Z_I = \frac{2}{\sinh(\omega\beta/2)}. \tag{84}$$

After some algebra, we get

$$C = (\beta\omega)^2 \sinh^{-2}(\omega\beta/2). \tag{85}$$

Again, plotted as a function of $\beta\omega$, this looks like

$$(86)$$

The important thing here is that at high T, we get a non-zero constant, in accordance with the equipartition theorem. As T drops below ω, $C \to 0$ as expected from freezeout.

Yet another example is rigid rotors coming from rotational dof. The parition function is

$$Z_I = \sum_{l \in \mathbb{N}} (2l+1)e^{-\beta l(l+1)J}, \tag{87}$$

with $J = 1/2I$. When $\beta J \ll 1$, we can turn this into an integral. This yields

$$\begin{aligned}
Z_I &\approx \int dl\,(2l+1)e^{-\beta J l(l+1)} \\
&= \int_{1/2}^{\infty} dl\,2l e^{-(l^2-1/4)\beta J} \\
&= \int_{\beta J/4}^{\infty} du\,\frac{1}{\beta J}e^{\beta J/4}e^{-u} \\
&= (\beta J)^{-1}.
\end{aligned} \tag{88}$$

Anytime we get a partition function that's linear in T, we get a specific heat capacity that's constant—again, this is in accordance with the equipartition theorem. On the other hand, when $\beta J \gg 1$, we can keep only the first two terms, which are all that's needed to get a nontrivial T dependence:

$$Z_I \approx 1 + 3e^{-2\beta J}, \tag{89}$$

which is in the same form as that of the two-level system we considered earlier, and gives

$$C \approx 12(\beta J)^2 e^{-2\beta J}, \tag{90}$$

where we have expanded the sinh at large βJ.

Clarification of chemical potential confusions

When reviewing stat mech for the oral exam, I got a little confused about a few things relating to the definition of μ. What follows is a slightly rambling attempt to resolve these confusions.

Let F be the free energy at constant particle number N. To realize the constraint on particle number statistically, we do the usual Legendre transform by defining

$$\mathcal{F} = \min_{N}[F - \mu N] \tag{91}$$

This just means that $\mathcal{F} = F - \mu N$, subject to the constraint that $\partial_N F = \mu$. This consequently ensures that

$$\partial_\mu \mathcal{F} = \partial_N F \partial_\mu N - N - \mu \partial_\mu N = -N, \tag{92}$$

as desired. Of course, the explicit formula for $\mathcal{F}$ is

$$\mathcal{F} = -\beta^{-1} \ln \mathcal{Z}, \tag{93}$$

where

$$\mathcal{Z} = \prod_\alpha \sum_{\{n_\alpha\}} e^{-n_\alpha \beta (\varepsilon_\alpha - \mu)}, \tag{94}$$

where the product is over all energy levels. One way to see why this prescription gives $\mathcal{F} = F - \mu N$ is to calculate $\partial_\mu \mathcal{F}$ and check that it gives N:

$$\partial_\mu \mathcal{F} = -\frac{1}{\beta} \partial_\mu \sum_\alpha \ln \left[\sum_{\{n_\alpha\}} e^{-n_\alpha \beta (\varepsilon_\alpha - \mu)} \right] = \sum_\alpha \frac{\sum_{\{n_\alpha\}} n_\alpha e^{-\beta n_\alpha (\varepsilon_\alpha - \mu)}}{\sum_{\{n_\alpha\}} e^{-\beta n_\alpha (\varepsilon_\alpha - \mu)}} = N, \tag{95}$$

and therefore $\mathcal{F} = F - \mu N + C$, where C is a constant.

Some books make a point of only discussing the fugacity $z = e^{\beta \mu}$. This is a good idea, since dealing with the chemical potential directly is cumbersome on account of the fact that the Lagrange multiplier fixing the expectation value of N is *not* μ, but rather z (or $\beta \mu$ if you prefer). The reason for often focusing on μ is because of the β^{-1} in the definition of the free energy, which means that the free energies are more naturally thought of as functions of μ than z. But really we'd all probably be better off just working with $-\ln Z$ all of the time, at least from the point of view of computing things.

An example of why z is the more natural variable comes from trying to compute the expectation value of the energy, U, in the GCE. Here the log of the partition function is

$$\ln \mathcal{Z} = -\zeta \sum_\varepsilon \ln[1 - \zeta z e^{-\beta \varepsilon}], \tag{96}$$

where $\zeta = \pm 1$ according to statistics. Obviously, taking $\partial_\beta \ln \mathcal{Z}$ at fixed μ does not give U—rather, we need to take the derivative wrt β at fixed z, not fixed μ. This means that the more natural variables to work with are the real Lagrange multipliers, namely β and z.

Physical meaning of μ, and its sign

Recall that the chemical potentials for classical gases and bosons are negative, i.e. always less that the lowest energy level of the system—this is just to ensure that e.g. the Boltzmann weights $e^{-\beta \xi} = e^{-\beta \varepsilon} z$ are less than 1 and that occupation numbers $(e^{\beta \xi} - 1)^{-1} = (z^{-1} e^{\beta \varepsilon} - 1)^{-1}$ are positive. Therefore μ is *not* a measure of the amount of energy that it costs to add a particle to the system, which is never negative.

Instead, μ is the *free* energy that it costs to add a particle to the system (or rather, to change the expectation value of the particle number by 1). Adding a particle to the system in question will increase the energy, but it will also generically increase S at fixed T, since heuristically the system now has more ways to occupy its energy levels. Note that μ can also

be defined as the energy cost of a particle while working at fixed S (since then $dF = dU$). But for S to be fixed upon adding a particle to the system that particle must (according to the previous heuristic) have negative energy. This argument then says that $\mu < 0$.

The situation for fermions can be different because of Pauli exclusion. Adding a particle to a Fermi gas with relatively high density at low T will cost a large energy $\sim \varepsilon_F$. However, it will not come with a correspondingly large change in entropy, since Pauli exclusion means that the number of additional ways you have to arrange your occupation numbers doesn't become much greater—you still just have to fill up the FSea. Therefore for fermions the change in energy can be larger than the change in TS, meaning that low T fermions can have $\mu > 0$. Since turning up T decreases the free energy cost for added particles, we will have $\mu(T) < \mu(0)$ for all T, with μ being expanded like $\mu(T)/\mu(0) = 1 - a(T/T_F)^2 - b(T/T_F)^4 - \ldots$, with $a, b, \cdots > 0$. Eventually at high enough T_*, for which

$$E_F^{3/2} \sim \int_0^\infty d\varepsilon \frac{\sqrt{\varepsilon}}{e^{\varepsilon/T_*} + 1}, \tag{97}$$

we'll get $\mu < 0$; this happens at around $T_* = T_F$.

Classical limit

What is the classical limit? It is not $\beta \to 0$, but rather $\beta\mu \to -\infty$, i.e. $z \to 0$.[12] Actually more precisely, it is $\beta(\varepsilon - \mu) \to \infty$—the important thing here is that $\langle n_\varepsilon \rangle \to 0$.

One can see this rather explicitly in the case of the regular classical ideal gas. When we deal with the partition function we break up phase space into volume elements of size $2\pi\hbar$, which is introduced to make Z properly dimensionless. In three dimensions then, we need

$$N = \frac{V}{(2\pi\hbar)^3} \int d^3p\, e^{-\beta(p^2/2m - \mu)} \implies e^{-\beta\mu} = \frac{v}{(2\pi\hbar)^3}(2\pi m\beta^{-1})^{3/2}, \tag{98}$$

where $v = V/N$ is the specific volume. Therefore

$$\beta\mu = \frac{3}{2} \ln\left[\frac{2\pi\hbar^2}{v^{2/3}mT}\right]. \tag{99}$$

Therefore in the dilute limit $v \to \infty$, or in the high-T limit, or in the small phase-space-cell limit $\hbar \to 0$, we always get $\mu \to \infty$; since all of these limits are ones in which we expect to recover classical behavior, we see that indeed $\mu\beta \to -\infty$. This is another reason why BECs and metals are very much not classical.

As another check that the appropriate limit is $\mu\beta \to -\infty$, we can require that the partition functions of FD and BE gasses reduce to the Boltzmann gas partition function in the limit. Recall that

$$\ln Z_\zeta = -\zeta \sum_\varepsilon \ln[1 - \zeta e^{-\beta(\varepsilon - \mu)}], \tag{100}$$

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[12]Thinking of it as $T \to \infty$ isn't good—T isn't dimensionless, and we are totally within our rights to consider low T classical systems. Plus just sending $T \to \infty$ would mean $\beta\mu \to 0$, which as we will see is definitely not the right classical limit.

where ζ is $+1$ for bosons and -1 for fermions. On the other hand, a classical gas is

$$\ln Z_{MB} = \ln \left[\sum_N \frac{1}{N!} e^{\beta \mu N} \left(\sum_\varepsilon e^{-\beta \varepsilon} \right)^N \right] = \sum_\varepsilon e^{-\beta(\varepsilon - \mu)}. \tag{101}$$

We see that $\ln Z_\zeta \to \ln Z_{MB}$ when we take $\beta \mu \to -\infty$, but that e.g. setting $\beta(\varepsilon - \mu) \to 0$, which would be the $(T \to \infty \implies$ classical$)$ thing to do, doesn't give the right answer.

What makes quantum gasses quantum

The difference between a quantum bose gas and a gas of classical particles lies in the indistinguishability of the particles in the quantum case. Today we will review how this effect is responsible for what one might call "statistical interactions": effects which in a classical system would come from interactions, but which arise even in non-interacting quantum systems. This counts as stat-mech 101 but is still very cool.

First, we will look at things in the canonical ensemble, where seeing the effects of the state counting are clearer. We would like to calculate the coordinate-space matrix elements of the density matrix for a free gas of n quantum particles. Since the density matrix is diagonal in momentum space, we have

$$\langle r_1, \ldots, r_n | \rho | r_1', \ldots, r_n' \rangle = \sum_{\mathbf{K}} \langle r_1, \ldots, r_n | \Psi_{\mathbf{K}} \rangle \exp \left(-\sum_i \frac{\beta k_i^2}{2m} \right) \langle \Psi_{\mathbf{K}} | r_1', \ldots, r_n' \rangle. \tag{102}$$

Here $\mathbf{K}$ is a composite label which sums over all distinct vectors $\mathbf{K} = (\mathbf{k}_1, \ldots, \mathbf{k}_n)$. By distinct, we mean that we regard e.g. $\mathbf{K} = (\mathbf{p}, \mathbf{q}) \sim (\mathbf{q}, \mathbf{p})$; since the particles are indistinguishable we shouldn't distinguish eigenstates based on which particle gets which momentum, but rather just on the un-ordered set $\mathbf{K}$ (this is just the same as counting states in the harmonic oscillator—there is only one state for a given occupation number of the levels).

The many-body[13] wavefunctions $\Psi_{\mathbf{K}}$ are given as appropriately (anti)symmetrized products of free plane waves: letting $\zeta = \pm 1$ depending on the statistics of the particles in

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[13]It may seem weird to use the adjective "many-body" when we're talking about a free system, but in fact it is entirely appropriate—the whole point of quantum statistical mechanics is that the effect of the statistics of the particles depends on how many particles there are, so that having many free bodies is not equivalent to the problem of just one (the partition function does *not* factor as a product of single-particle partition functions, even in the free case).

question, we have

$$\Psi_{\mathbf{K}} = \frac{1}{\sqrt{n!}} \sum_{\sigma \in S_n} \zeta^\sigma \bigotimes_i \psi(\mathbf{k}_{\sigma(i)}),$$ (103)

where $\langle \mathbf{r} | \psi(\mathbf{k}_{\sigma(i)}) \rangle = e^{i\mathbf{k}\cdot\mathbf{r}}$ and ζ^σ means $\zeta^{(1-\mathrm{sgn}(\sigma))/2}$. The $1/\sqrt{n!}$ ensures normalization (the combinatorics doesn't quite work when some of the k_i's are equal, but these choices of $\mathbf{K}$ contribute a set of measure zero to the integral over $\mathbf{K}$ and so we will ignore this subtlety). Putting this in,

$$\langle r_1, \ldots, r_n | \rho | r_1', \ldots, r_n' \rangle = \frac{1}{n!} \sum_{\mathbf{K}} \sum_{\sigma,\omega \in S_n} \zeta^{\sigma+\omega} \exp\left(i \sum_i [\mathbf{r}_i \cdot \mathbf{k}_{\sigma(i)} - \mathbf{r}_i' \cdot \mathbf{k}_{\omega(i)}] - \beta \sum_i \frac{k_i^2}{2m} \right)$$ (104)

Now instead of summing over all distinct $\mathbf{K}$, we can instead sum over all of the $\mathbf{k}_i$ independently (i.e. counting both $(\mathbf{p}, \mathbf{q})$ and $(\mathbf{q}, \mathbf{p})$). Since we are already (anti)symmetrizing over the $\mathbf{k}_i$, the only thing that this will do is to give us an answer which is too big by a factor of $n!$. So then

$$\langle r_1, \ldots, r_n | \rho | r_1', \ldots, r_n' \rangle = \frac{1}{n!^2} \int \prod_i \frac{d^d k_i}{(2\pi)^d} \sum_{\sigma,\omega \in S_n} \zeta^{\sigma+\omega} \exp\left(i \sum_i [\mathbf{r}_i \cdot \mathbf{k}_{\sigma(i)} - \mathbf{r}_i' \cdot \mathbf{k}_{\omega(i)}] - \beta \sum_i \frac{k_i^2}{2m} \right)$$ (105)

Now the only thing that matters for this integral is the relative difference between $\sigma(i)$ and $\omega(i)$. Therefore we may fix $\omega = \mathbf{1}$ and multiply by $n!$. We may further transfer the permutation onto the $\mathbf{r}_i$ index, so that the exponent looks like $\mathbf{k}_i \cdot (\mathbf{r}_{\sigma(i)} - \mathbf{r}_i') - \ldots$. We can then do the integrals over k_i, and get

$$\langle r_1, \ldots, r_n | \rho | r_1', \ldots, r_n' \rangle = \frac{1}{n!} \lambda^{-dn} \sum_{\sigma \in S_n} \zeta^\sigma \exp\left(-\pi \sum_i \frac{|\mathbf{r}_i - \mathbf{r}_{\sigma(i)}'|^2}{\lambda^2} \right),$$ (106)

where the thermal length is

$$\lambda \equiv \sqrt{\frac{h^2}{2\pi m T}}.$$ (107)

When $h \to 0$ only the trivial permutation in S_n contributes, and we get the correct classical partition function (with the correct Gibbs $1/n!$ factor—recall that the h surviving in the thermal length also appears in classical stat mech in order to make Z dimensionless).

To understand the effects of the permutations, consider the two-pody density matrix $\rho(0, x)$ for a one-dimensional system. This matrix element is plotted below for the case of

the three different statistics ($\zeta = \pm 1$ and then the $h \to 0$ limit)

$$(108)$$
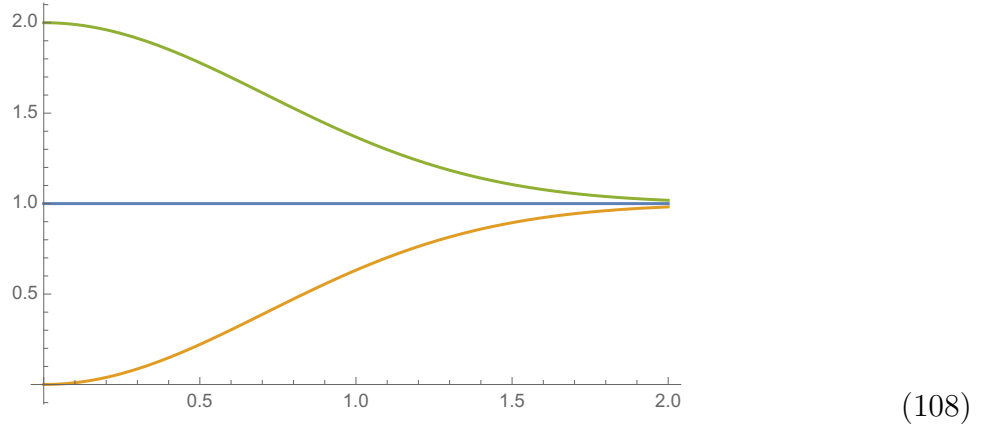
We see that even though they are non-interacting, bose particles tend to clump together more than expected classically, while fermions tend to avoid each other.

This result is perhaps best understood within the framework of the path integral. We know that we can represent the $\mathbb{R}$-space matrix elements density matrix as a path integral over a strip of length β, with fixed ∂ conditions. In quantum mechanics, loosely speaking the uncertainty principle means that we can't track the trajectories of each of the particles along the strip exactly, and indistinguishability means our boundary conditions can't distinguish between trajectories which differ by particles braiding past each other and swapping endpoints at the boundary. Therefore we must sum over all possible worldline topologies for the particles, keeping the endpoints fixed. The amplitude for a particle to propagate from r to r' along a time interval of length β is precisely[14]

$$Z(r, r'; \beta) = \sqrt{\frac{2\pi m}{h^2 \beta}} e^{-\pi(r-r')^2/\lambda^2}. \tag{110}$$

Summing this over worldline topologies then reproduces the expression derived above.

Ginzburg criterion for fluctuations at second-order phase transitions

Today we are writing down some stuff that will help us remember the Ginzburg criterion, which is a way of estimating how close one has to get to a second-order phase transition

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[14]This can be derived by doing the trace over momentum states as we have done, or by solving the appropriate diffusion equation

$$\partial_\beta Z(r, r'; \beta) = D\partial_r^2 Z(r, r'; \beta), \tag{109}$$

which just comes from writing the density matrix as $e^{-\beta H}$.

in order for fluctuations[15] of the order parameter to be "important", done from within the purview of GL theory. This is the same thing as determining in what circumstances we expect mean field theory to be valid.

The tl;dr argument is as follows. Fluctuations in the order parameter field ϕ will become important when the condensation free energy within a correlation length becomes less than the fluctuation / thermal free energy within a correlation length (with the former determined through mean field theory). The fluctuation / thermal free energy density within a correlation length is independent of the dimensionless distance from the critical point t. In the context of thermal phase transitions this free energy is just $k_B T$; in the context of $T = 0$ Euclidean field theory it is

$$F_{fluc} \sim \xi(t)^d \int d^d k \, \ln\left(\xi_0^2(k^2 + \xi(t)^{-2})\right) \sim 1. \tag{111}$$

Here ξ_0 is a microscopic length scale needed for dimensionality reasons; we will work in $\xi_0 = 1$ units from here out.

Unlike F_{fluc}, the condensation free energy within a correlation length F_c depends on t. On one hand, the condensation free energy density gets smaller as the critical point is approached from the ordered phase. On the other hand, the correlation length gets larger. The size of F_c then depends on the competition between these two effects, with

$$F_c \sim \xi(t)^d f_c \sim \xi(t)^d \frac{t^2}{u} \sim \frac{t^{2-d/2}}{u}, \tag{112}$$

where we have written the condensation free energy density as $t\langle\phi^2\rangle \sim t^2/u$. Therefore fluctuations will be important (and mean field will fail) provided that

$$F_c/F_{fluc} \lesssim 1 \implies t \lesssim u^{2/(4-d)}. \tag{113}$$

Since we usually want $u \ll 1$, smaller d for $d < 4$ means that the exponent of u is smaller, so that fluctuations will be important at a larger distance from the critical point in lower dimensions. When $d > 4$ we will need to discuss the meaning of the fluctuation contribution more carefully; of course we know that mean field works in $d > 4$ and so we should only interpret the above equation as holding for $d < 4$.

⋄ ⋄ ⋄

Now for a more detailed argument. We will be taking the archetypal n-component ϕ^4 theory as an example, for which the starting point is of course

$$H = \int \left(\frac{K}{2}|\nabla\phi|^2 + \frac{t}{2}|\phi|^2 + u|\phi|^4\right) \tag{114}$$

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[15]The word 'fluctuations' here refers just to ordinary free Gaussian fluctuations about the mean-field value, and not to e.g. any sort of fluctuations coming from loop diagrams involving interactions.

where ϕ is some *dimensionless n*-component field (always broken up into real parts; the $||^2$s mean dot products). Approaching the phase transition from the ordered side, we can split up the field into a longitudinal part φ along the ordering direction $\hat{\mathbf{x}}_1$ and transverse components ζ_i as

$$\phi = (v + \varphi)\hat{\mathbf{x}}_1 + \sum_{i>1}^{n} \zeta_i \hat{\mathbf{x}}_i, \tag{115}$$

with v the magnitude of the vev of ϕ. We then put this expression into H, and expand to quadratic order in all of the fluctuations. This gives

$$H \approx H_0 + \frac{K}{2} \int \left(\varphi[-\nabla^2 + \xi_l^{-2}]\varphi + \zeta_i[-\nabla^2 + \xi_t^{-2}]\zeta^i \right), \tag{116}$$

where $H_0 = H|_{\phi = v\hat{\mathbf{x}}_1}$ and we have defined the two parameters

$$\xi_t^{-2} \equiv \frac{t + 4uv^2}{K}, \qquad \xi_l^{-2} \equiv \frac{t + 12uv^2}{K}, \tag{117}$$

which set the masses for the two types of fluctuations in the theory. Note that the value of v is $v = \sqrt{-t/(4u)}$ for $t < 0$ and $v = 0$ for $t > 0$, and hence the longitudinal modes are massless below the phase transition as expected, with $\xi_l(t < 0) = \infty$, and are massive above the transition, with $\xi_l(t > 0) = \sqrt{K/t}$. In contrast, the longitudinal mode has $\xi_l(t < 0) = \sqrt{-K/2t}$[16] and $\xi_l(t > 0) = \xi_t(t > 0)$ (since there is no difference between longitudinal and transverse in the absence of ordering).

Doing the field integral over the fluctuations gives the free energy

$$F = -\frac{t^2}{16u}\theta(-t) + \frac{1}{2} \int_{\mathbf{q}} \left(\ln[K(q^2 + \xi_l^{-2})] + (n-1)\ln[K(q^2 + \xi_t^{-2})] \right). \tag{118}$$

To diagnose the relative importance of the fluctuations, we will look at their affect on thermodynamical variables. Actually we will just look at the (singular part of the) specific heat, since it gives us an idea of what degrees of freedom are getting turned on as we pass through the critical point. We then just have to take the above and differentiate twice with respect to t. The only t-dependence is in the lengths ξ_i, and the first F_0 term in the front, provided that $t < 0$. We then find the singular contribution to C to be

$$C = -\partial_t^2 F = \begin{cases} 0 + \dfrac{n}{2K^2} \displaystyle\int_{\mathbf{q}} \dfrac{1}{(|\mathbf{q}|^2 + \xi_l^{-2})^2} & t > 0 \\[3mm] \dfrac{1}{8u} + \dfrac{2}{K^2} \displaystyle\int_{\mathbf{q}} \dfrac{1}{(|\mathbf{q}|^2 + \xi_l^{-2})^2} & t < 0 \end{cases} \tag{119}$$

We just care about how this scales with the correlation length, and so we don't need to do the integral very carefully. When $d > 4$ the integral is UV divergent and diverges in the usual MF way. When $d < 4$, dimensional analysis tells us that the integrals are ξ_l^{4-d}. We

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[16]Note that this is precisely the same as the coherence length in LG theory (the typical length scale of fluctuations in the magnitude of the order parameter).

can then separate the contribution to the change in C across the transition into two parts: one from the ordering,

$$\delta C_0 \sim 1/u, \tag{120}$$

and one from the fluctuations,

$$C_{fluct} \sim K^{-2}\xi_l^{4-d}. \tag{121}$$

In the above we have restricted to $d < 4$, since when $d > 4$ the fluctuation contribution gives us a UV divergent term that is just a constant across the transition, and so the form of the discontinuity across the transition is unchanged by fluctuations in $d > 4$ dimensions.

The "importance" (in the thermodynamic sense) of fluctuations for $d < 4$ can be diagnosed by comparing the two specific heat discontinuities; fluctuations will become strong when $C_{fluct} \gtrsim C_0$. Since $\xi_l \sim \sqrt{-K/t}$, fluctuations will be important provided that

$$\delta C_0 \lesssim C_{fluct} \implies t \lesssim \frac{u^{2/(4-d)}}{K^{d/(4-d)}}, \tag{122}$$

which is the Ginzburg criterion. The parameters K and u will of course depend on the microscopics, and the message here is that even below the upper critical dimension where MFT should fail, it may happen that fluctuations are sufficiently weak due to the values of K, u that it is experimentally infeasible to tune t close enough to 0 to be able to see their effects. This is what happens for many type I superconductors, where for $d = 3$ we would need to tune t to something like $t < (T_c/E_F)^4 \sim 10^{-16}$, which is out of the question. A sanity check is that the better the SC, the smaller we have to tune t to see fluctuations, since stronger order implies larger K.[17] The fact that t needs to be so small in order to see the thermodynamic effects of fluctuations is why type I superconductors are so well described

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[17]e.g. in three dimensions $K \sim 1/\xi_0$, with ξ_0 the $(T = 0)$ microscopic coherence length of the SC, which serves as the UV cutoff for the continuum theory and which is smaller for better superconductors, with

$$\xi_0 \sim \hbar v_F/kT_c. \tag{123}$$

Let's derive this. Deep inside the SCing phase, one estimates the size of the smallest wavepackets the Cooper pairs as follows: the zero-T gap, or kT_c (they are proportional in BCS) sets the energies of the electrons involved in forming the SCing condensate. Since these electrons live near the FS, the corresponding range of momenta involved is

$$\delta p \approx kT_c/v_F \approx \Delta(0)/v_F. \tag{124}$$

Then through the uncertainty principle, the minimal-sized wavepackets are of a scale

$$\xi \approx \frac{\hbar v_F}{kT_c}. \tag{125}$$

This acts as the UV cutoff in the GL theory. Sanity check: when T_c gets smaller the SC gets weaker, giving a larger UV cutoff, as expected. Likewise when v_F gets larger it should be "harder to form pairs", and hence the UV cutoff length gets larger.

The coherence length at non-zero temperatures is defined in LG theory as the length appearing as the scale in the equation minimizing the free energy: it is

$$\xi_{LG}(T) = \frac{\hbar}{|2m^*\alpha(T)|^{1/2}}. \tag{126}$$

At low temperatures, this becomes equalish to the ξ defined above.

by mean field theory: we can essentially always set $|\phi| = v$ to be a constant, except when t is (prohibitively) small.

The Harris criterion

In this diary entry, we will review the derivation of the Harris criterion for a few different types of disorder.

Heuristics

The Harris criterion is a simple heuristic for determining when disorder is relevant, in the sense of inducing an RG flow away from a disorder-free fixed point.

The basic idea is to ask whether disorder ruins one's ability to measure scaling relations as the critical point is approached. Let g be a parameter parameterizing the distance from the clean critical point at $g_* = 0$. Introducing disorder will have the effect of displacing g_* from zero.

Consider a correlation volume of size ξ^d. By assumption, this is the volume within which the degrees of freedom which go critical at the transition can affect each other. Within ξ^d the system is effectively critical, and we ask what the effective value of g_* is in this volume, after disorder has been accounted for.

Now any calculation of g_* will come from averaging over the disorder. If we assume that the disorder is parametrized by independent Gaussian variables on each site, then the CLT[18] can be used to address the standard deviation of the distribution over the correlation volume: $g_* \propto 1/\sqrt{(\xi/a)^d}$ where $(\xi/a)^d$ measures the number of indpendent random variables in the correlation volume. Using the critical exponent ν defined via $\xi \sim g^{-\nu}$, the spread of g_*'s is

$$\sigma_{g_*} \sim g^{\nu d/2}. \tag{128}$$

If $\sigma_{g_*} > g$, then we can't do scaling, since we have no way of controlling a precise distance with resect to the critical point—our use of g as a knob to probe the critical dof has been

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[18]If we have N random variables with given moments $\langle x^n \rangle$, then the distribution for their average is

$$P(A \equiv N^{-1} \sum_{i=1}^{N} x_i) \propto \exp\left(-\frac{(A - \langle x \rangle)^2}{2\sigma_A^2}\right), \qquad \sigma_A \sim \sqrt{\frac{\langle x^2 \rangle}{N}}. \tag{127}$$

washed out by the disorder. Therefore the criterion for disorder to be irrelevant (and not affect the existence of the critical point) is that $\nu > 2/d$. Note that this inequality becomes easier to saturate for a given ν if d is larger; this makes sense due to the less important role of randomness in systems of larger dimensionality (think random walks). Also note that the $\nu = 1/2$ of MFT saturates the inequality in the usual critical dimension of $d = 4$, telling us that disorder behaves as an effective ϕ^4 term.

Slightly more formal heuristics; disorder with long-range correlations

Let us first imagine that the disorder couples to the energy operator ε, viz. the relevant operator which drives the transition we're interested in. We will write this as

$$\delta S = \int d^d x \, \varepsilon \, D, \tag{129}$$

where $D(x)$ is a scalar representing the disorder, assumed for now to follow a white noise Gaussian (the standard deviation won't be important; we will be dropping constants anyway). This is the situation of the previous section, since we assumed that the effect of the disorder was to lead to random values of g_*, i.e. random values of T_c.

The disorder is treated as quenched disorder as usual, with the disordered free energy being obtained by averaging the free energy in a specific disorder configuration, evaluated via the replica trick. The replica action thus contains the term

$$S \supset \int d^d x \left(\sum_a \varepsilon_a D + \frac{1}{2\sigma_D^2} D^2 \right). \tag{130}$$

When D is integrated out, we generate a replica-diagonal action, plus a term coupling the replicas:

$$\delta S = C \sum_{a,b} \int d^d x \, \varepsilon_a \varepsilon_b, \tag{131}$$

where C is some dimensionful constant (this is local since the disorder was taken to be δ function correlated).

Now from the definition $\xi \sim g^{-\nu}$ (with again g the coefficient of the $\int \varepsilon$ term in S), we see that the energy operator has dimension $\Delta_\varepsilon = d - 1/\nu$. Therefore since there are no other terms coupling the replica in the action, the perturbation δS has dimension $2(d - 1/\nu)$, i.e. $C \propto \Lambda^{d+2/\nu}$. Assuming that all the RG technology works despite the implicit replica limit that needs to be taken, we thus conclude that the disorder is irrelevant if

$$2(d - 1/\nu) > d \implies d\nu > 2, \tag{132}$$

which is what we found in the previous section. Using this formalism one can then use the known OPE of the energy operator at the clean fixed point to search for disordered fixed points via conformal perturbation theory.

Now it does not always need to be the case that disorder couples to the energy operator— it needn't always just change T_c. A more severe type of disorder is when the disorder couples

to the order parameter, that is, when it acts as a random magnetic field. In this case the replica non-diagonal part of the action is

$$\delta S \propto \sum_{a,b} \int d^d x \, \phi_a \phi_b, \tag{133}$$

with ϕ_a the order parameter. This is always relevant, and therefore local disorder that couples to the order parameter always destroys the clean fixed point (this is not to say that it destroys the existence of a fixed point; the RG flow under the above δS can have a nontrivial fixed point distinct from the disorder-free one).

One generalization is to consider disorder that has a distribution other than white noise. For example, consider the case where the field D is power-law correlated (and go back to the case where we couple D to the energy operator):

$$\langle D(x)D(y) \rangle \sim \frac{1}{|x-y|^{d+\alpha_D}}, \tag{134}$$

where α_D can be negative. The replica off-diagonal term generated is then

$$\delta S \propto \int d^d x \, d^d y \, \frac{\varepsilon_a(x)\varepsilon_b(y)}{|x-y|^{d+\alpha_D}}. \tag{135}$$

The dimension of this operator is then increased by α_D relative to the δ function white noise case. The appropriate Harris criterion is then that disorder is irrelevant provided that

$$\nu > \frac{2}{d+\alpha_D}. \tag{136}$$

As expected, shorter-ranged correlations for the disorder (larger α_D) make the disorder less relevant.

Equivalence between the $\mathbb{Z}_4$ clock model and two decoupled Ising models

Today's diary entry is simple — we will be showing that the quantum $\mathbb{Z}_4$ clock model is equivalent to two decoupled Ising models. We will use notation such that $\mathcal{Z}, \mathcal{X}$ are $\mathbb{Z}_4$ clock and shift matrices, while Z, X are the usual Pauli matrices.

The Hamiltonian for the $\mathbb{Z}_4$ clock model is

$$H = g \sum_i (\mathcal{X}_i + \mathcal{X}_i^\dagger) + h \sum_{\langle ij \rangle} (\mathcal{Z}_i^\dagger \mathcal{Z}_j + \mathcal{Z}_j^\dagger \mathcal{Z}_i). \tag{137}$$

We can relate this to two decoupled Ising models as follows. The basic idea is to separate the fourth roots of unity into two pairs which are orthogonal on the complex plane, viz. $(1, -1)$ and $(i, -i)$. The variables for these pairs will then roughly constitute the degrees of freedom in two Ising models.

To proceed it is helpful to work in rotated coordinates, by rotating the fourth roots of unity through an angle of $\pi/4$. The rotated positions on the unit circle correspond to the points $(\pm 1, \pm i)$. Thus any forth root of unity can be equivalently specified by a pair of $\pm$ signs. Writing these $\pm$ signs as $Z_1 \equiv Z \otimes \mathbf{1}$ and $Z_2 \equiv \mathbf{1} \otimes Z$, we then write

$$\mathcal{Z} = \frac{1}{2} \left(Z_1 + Z_2 + i(Z_1 - Z_2) \right) = \frac{1}{\sqrt{2}} \left(\zeta_8 Z_1 + \zeta_8^* Z_2 \right) \tag{138}$$

Note that this actually gives $\mathcal{Z} = \mathrm{diag}(1, i, -i, -1)$, which is not the standard order on the diagonal. This is however just a matter of a change of basis via the matrix $\mathbf{1} \oplus X$, and we will work in this basis for now. Note that we can also invert this via

$$Z_1 = \frac{1}{\sqrt{2}}(\zeta_8 \mathcal{Z} + \zeta_8^* \mathcal{Z}^\dagger), \qquad Z_2 = \frac{1}{\sqrt{2}}(\zeta_8^* \mathcal{Z} + \zeta_8 \mathcal{Z}^\dagger). \tag{139}$$

$\mathcal{X}$ generates the $\mathbb{Z}_4$ symmetry, which here is acted by interchanging the eigenvalues of Z_1 and Z_2, and then multiplying the eigenvalue of Z_2 by -1. We cannot find a similar $\otimes$ representation of the $\mathcal{X}$ operator in terms of X_1, X_2, since its action includes a swap of the two $\otimes$ factors (one can show that using linear combinations of X_1 and X_2, its impossible to get $\mathcal{Z}\mathcal{X} = i\mathcal{X}\mathcal{Z}$). We can however find a $\otimes$ representation for the real operator $\mathcal{X} + \mathcal{X}^\dagger$, which is what appears in the Hamiltonian. Indeed, in our present nonstandard basis we have

$$\mathcal{X} = \begin{pmatrix} & & 1 & \\ 1 & & & \\ & & & 1 \\ & 1 & & \end{pmatrix} \tag{140}$$

so that we have the very simple

$$\mathcal{X} + \mathcal{X}^\dagger = \begin{pmatrix} & 1 & 1 & \\ 1 & & & 1 \\ 1 & & & 1 \\ & 1 & 1 & \end{pmatrix} = X_1 + X_2. \tag{141}$$

We can now plug this $\otimes$ representation into the Hamiltonian. The transverse field term is already taken care of, while the nearest neighbor term gives

$$\begin{aligned} \mathcal{Z}_i^\dagger \mathcal{Z}_j + h.c. &= \frac{1}{2}(Z_{1i}Z_{1j} + Z_{2i}Z_{2j} + i(Z_{2i}Z_{1j} - Z_{1i}Z_{2j})) + c.c. \\ &= Z_{1i}Z_{1j} + Z_{2i}Z_{2j} \end{aligned} \tag{142}$$

Therefore we have

$$H = H_1 + H_2, \tag{143}$$

where

$$H_a = g \sum_i X_{ai} + h \sum_{\langle ij \rangle} Z_{ai} Z_{aj} \tag{144}$$

is an Ising Hamiltonian for flavor a. Thus the $\mathbb{Z}_4$ clock model is indeed a direct sum of two Ising models, so long that we remember that the $\mathbb{Z}_4$ symmetry acts non-diagonally on the flavor index (it acts as KW duality on one of the two Ising models, which corresponds to T duality at the critical point when things are written in the compact boson formulation).

Inverted XY transitions

Today's entry is trivial and has no equations — we will just be explaining what is meant by an "inverted" XY transition.

The most common place one runs into inverted transitions seems to be in the context of the 2+1D XY model, and so for concreteness we will focus on this case. While both sides of the transition are related by particle-vortex duality, the way in which the transition is approached is different on both sides. In the standard XY transition, one condenses particles upon going from the disordered high-T phase to the ordered spin-wave phase, and condenses vortices on going in the reverse direction. While particle worldlines look like vortices, they are energetically different: in the disordered phase where the particles are massive, the action of a given particle worldline is perimeter law, and comes only from the rest energy needed to create the particle. On the other hand, the action of a vortex worldline is a logarithmically marginal type of area law.

In an inverted XY transition, the situation is (duh) inverted: here the strings which condense to pass from the ordered to the disordered phase have perimeter law, while the strings one condenses to pass from the disordered phase to the ordered phase have a logarithmically marginal area law. The canonical example of an inverted XY transition is the transition that occurs in superconductors (i.e. in the Abelian Higgs model). Here the long-range Coulomb interaction (which appropriately gives a logarithmic potential in 2+1D) means that the particles one condenses to transition into the ordered (superconducting) phase have worldlines with a logarithmic area law, while the vortices one condenses to transition into the disordered phase follow a perimeter law (due to the screening of the gradient energy by the gauge field).

Langevin dynamics from the Caldeira-Leggett model

This diary entry was written when preparing to teach a class on Brownian motion and the FDT. In the course of preparing I came accross some subtleties relating to sum rules and the Langevin equation, and thus decided to write up the lecture notes for posterity's sake.

Spectral functions

Standard cond-mat textbooks are rife with confusion surrounding the objects that come up when studying linear response. The notation is often abstruse and misleading (especially when it involves things like χ' and χ''), and sometimes simplifications are made which obfuscate important results. A common example of this arises in discussions of the conductivity, whose *real* part controls dissipation, despite us often being told that spectral functions are defined by the imaginary parts of susceptibilities.

In this section we will try to set some of this confusion straight. We define the spectral function

$$A_{XY}(t - t') \equiv \frac{1}{2}\langle[X(t), Y(t')]\rangle, \tag{145}$$

with the factor of $1/2$ chosen so that

$$A_{XY}(\omega) = \pi \sum_{n,m}(\pi_n - \pi_m)X_{nm}Y_{mn}\delta(E_{mn} - \omega), \tag{146}$$

where π_n is the equilibrium occupation of the eigenstate $|n\rangle$. $A_{XY}(t)$ looks almost like the susceptibility, but in real time it differs by a $\Theta(t)$ and a factor of $2i$:

$$\chi_{XY}(t) = 2i\Theta(t)A_{XY}(t). \tag{147}$$

In frequency space, it is *not* always true that $A_{XY}(\omega)$ is the imaginary part of $\chi_{XY}(\omega)$. The correct relation (as follows from the spectral representation) is

$$A_{XY}(\omega) = \frac{1}{2i}(\chi_{XY}(\omega) - \chi_{Y^\dagger X^\dagger}(\omega)^*), \tag{148}$$

which gives the imaginary part only when $\chi_{XY}(\omega) = \chi_{Y^\dagger X^\dagger}(\omega)$.

The operators we are interested in are usually either even or odd under time reversal. Let t_X denote the $\mathcal{T}$-parity of X. Then it is easy to check that

$$\chi_{XY}(\omega) = t_X t_Y \chi_{YX}(\omega). \tag{149}$$

Thus, letting X, Y be Hermitian for simplicity, we have

$$A_{XY}(\omega) = \frac{1}{2i}(\chi_{XY}(\omega) - t_X t_Y \chi_{XY}(\omega)^*) = \begin{cases} \operatorname{Im}\chi_{XY}(\omega) & t_X = t_Y \\ -i\operatorname{Re}\chi_{XY}(\omega) & t_X = -t_Y \end{cases}. \tag{150}$$

The second line on the RHS is relevant when we are computing the conductivity, for which $X = J$ is the current and $Y = D$ is the dipole operator (since D is what the electric field couples to). This explains why the real part of σ is what controls dissipation, since $t_J = -1$ while $t_D = +1$.

Sum rules

The simplest sum rule comes from realizing that the equal-time spectral function $A_{XY}(0)$ is just

$$\int_\omega A_{XY}(\omega) = \frac{1}{2}\langle [X(0), Y(0)]\rangle. \tag{151}$$

In particular, the RHS is *independent* of the Hamiltonian, requiring that the integrated spectral weight be a function only of the operators under consideration, and not on the nature of the dynamics (it also vanishes when $X = Y$ which is why the sum rule is often not discussed in this way). For the conductivity, it is easy to see that $[J, D]$ gives the expected ne^2/m.[19] For a fixed choice of X, Y we can generate other sum rules by differentiating (145) with respect to both t and t' before setting $t = t' = 0$, giving constraints on all moments of $A_{XY}(\omega)$:

$$\int_\omega \omega^{n+m} A_{XY}(\omega) = \frac{i^{m-n}}{2}\langle[\frac{d^m X}{dt^m}, \frac{d^n Y}{dt'^n}]|_{t=t'=0}\rangle \tag{152}$$
$$= \frac{(-1)^m}{2}\langle[\operatorname{Ad}_H^m(X(0)), \operatorname{Ad}_H^n(Y(0))]\rangle.$$

The RHS usually easy (in principle) to compute for any m, n, and is usually constant. We will now explain why the $m, n > 0$ versions of this equation will force us to critically re-examine the Langevin equation.

Langevin dynamics and the problem with Lorentzians

The canonical Langevin equation is[20]

$$\ddot{x} + \Omega x + \gamma\dot{x} = \frac{1}{m}\xi, \tag{153}$$

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[19]One could argue that this actually does depend on the Hamiltonian since J is determined by the commutator of H with the charge density — but you get the point.

[20]We are somewhat abusing notation here by letting x denote $\langle\hat{x}\rangle$ in the quantum case.

where ξ has zero mean and a variance fixed by γ, T, m via the FDT. Consider for illustration the simple case of $\Omega = 0$. The above equation then only involves the velocity $v \equiv \dot{x}$, and so

$$v = \frac{1}{m(-i\omega + \gamma)}\xi. \tag{154}$$

Since the field ξ acts as a random force which couples to the position x, we have

$$\chi_{vx}(\omega) = \frac{1}{m(-i\omega + \gamma)}. \tag{155}$$

Since v and x have opposite transformations under time reversal (recall our discussion of the conductivity), the spectral function is a Lorentizian:

$$A_{vx}(\omega) = -i\,\mathrm{Re}\,\chi_{vx}(\omega) = -i\frac{\gamma}{m(\omega^2 + \gamma^2)}. \tag{156}$$

The dangerous thing about Lorentzians is that all of their moments (beyond the zeroth) are infinite! Thus while $A_{vx}(\omega)$ can (and does) fulfill the sum rule $\int A_{vx}(\omega) = -i/(2m)$, it violates all of the higher sum rules where at least one of m, n is nonzero. We will eventually see that the problem lies in the assumption that the drag force $-v\gamma$ is local in time — this is a good enough assumption when one only cares about long times, but is problematic at short times and leads to bad behavior at large ω which produces the diverging higher moments.[21]

The Caldeira-Leggett model

We can understand how to fix the above issue with the naive Langevin equation (the one with constant γ) by considering a model in which the emergence of Langevin behavior from the underlying microscopic dynamics can be explicitly calculated. This is what Calderia and Leggett did in their paper (they were mostly interested in how decoherence — viz. the coupling of a quantum system to a bath — modifies the probability of objects to tunnel through barriers; we will not have anything to say about this problem here).

The model is the simplest system one could imagine using to study thermalzation and Brownian motion from a microscopic perspective. It consists of $N \gg 1$ "bath oscillators" (with phase space coordinates (q_i, p_i), fundamental frequencies ω_i, and masses m_i) coupled to one "big" oscillator (with coordinates (x, p), mass M, and fundamental frequency Ω). The coupling between the "system" (just a single oscillator!) and the bath is linear and parametrized by constants C_i, with total Hamiltonian

$$H = \frac{1}{2}M\Omega^2 x^2 + \frac{p^2}{2M} + \sum_i \frac{p_i^2}{2m_i} + \frac{1}{2}\sum_i m_i\omega_i^2\left(q_i - x\frac{C_i}{m_i\omega_i^2}\right)^2. \tag{157}$$

Our strategy in what follows will be to integrate out the bath oscillators and arrive at a Langevin-esque equation for the system oscillator. We start by writing down Newton's law for the system oscillator, which is

$$\ddot{x} = \frac{-i}{M}[p, H] = -x\left(\Omega^2 + \frac{1}{M}\sum_i \frac{C_i^2}{m_i\omega_i^2}\right) + \frac{1}{M}\sum_i C_i q_i. \tag{158}$$

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[21]This can be seen by noting that the Greens function for the velocity is $\mathcal{G}_{vv}(t) = e^{-\gamma t}\Theta(t)$. The instantaneous response at $t = 0^+$ is the source of the problem.

Defining an effective frequency

$$\widetilde{\Omega} \equiv \sqrt{\Omega^2 + M^{-1} \sum_i C_i^2/(m_i\omega_i^2)} \tag{159}$$

and an effective "noise field"

$$\xi_q(t) \equiv \sum_i C_i q_i(t), \tag{160}$$

we can write this in the more suggestive form

$$\ddot{x} + x\widetilde{\Omega}^2 = \xi_q(t). \tag{161}$$

So far it is not entirely obvious how the noise field $\xi_q(t)$ will end up producing a viscous term like $-\gamma\dot{x}$. We can investigate this by simply solving for the full evolution of each of the $q_i(t)$. Their EOM is simply

$$\partial_t^2 q_i + \omega_i^2 q_i = \frac{C_i}{m_i}x. \tag{162}$$

This EOM is solved by $q_i(t) = q_i^h(t) + q_i^p(t)$, where $q_i^{h,p}$ are homogenous and particular solutions, respectively. The homogenous solution is

$$q_i^h(t) = q_i(0)\cos(\omega_i t) + \dot{q}_i(0)\frac{\sin(\omega_i t)}{\omega_i}. \tag{163}$$

The particular solution is

$$q_i^p(t) = \frac{C_i}{m_i}\int_0^\infty dt'\,\mathcal{G}_i(t-t')x(t') \tag{164}$$

where the ith oscillator Greens function satisfies $(\partial_t^2 + \omega_i^2)\mathcal{G}_i(t-t') = \delta(t-t')$ and is consequently

$$\mathcal{G}_i(t) = \Theta(t)\frac{\sin(\omega_i t)}{\omega_i}. \tag{165}$$

Since we want to write $\xi_q(t)$ in terms of $\dot{x}$, we will choose to integrate by parts and write

$$\begin{aligned}
q_i^p(t) &= \frac{C_i}{m_i}\int_0^\infty dt'\,\Theta(t-t')\frac{\sin(\omega_i(t-t'))}{\omega_i}x(t) \\
&= \frac{C_i}{m_i\omega_i^2}\left(-\int_0^t dt'\,\cos(\omega_i(t-t'))\partial_t x(t') + (x(t) - x(0)\cos(\omega_i t))\right).
\end{aligned} \tag{166}$$

We now substitute this expression for $q_i(t)$ into the $\xi_q(t)$ appearing in the EOM for x. Some algebra yields

$$\ddot{x} + \Omega^2 x + \int_0^t dt'\,\gamma(t-t')\dot{x}(t') = \frac{1}{M}\xi(t), \tag{167}$$

where we have defined the relaxation kernel

$$\gamma(t) \equiv \frac{1}{M}\sum_i \frac{C_i^2}{m_i\omega_i^2}\cos(\omega_i t) \tag{168}$$

and the effective noise field

$$\xi(t) \equiv \sum_i C_i \left(\cos(\omega_i t)\delta q_i(0) + \frac{p_i(0)}{m_i \omega_i}\sin(\omega_i t) \right) \tag{169}$$

with $\delta q_i(0) \equiv q_i(0) - \frac{C_i}{m_i \omega_i^2}x(0)$. The retarded nature of the relaxation kernel cures the sharp short-time jump in Langevin Greens function $\Theta(t)e^{-\gamma t}$, and renders higher moments of the spectral function finite.

Note that the effective noise field is completely deterministic, depending as it does solely on the initial conditions $q_i(0), p_i(0), x(0)$. Of course in reality ξ effectively becomes a random variable in the $N \to \infty$ limit, which we deal with by averaging over the initial coordinates of the bath oscillators. Writing this average with angle brackets, we have $\langle \xi \rangle = 0$ if the initial conditions are random across the different oscilators (just having N be large isn't enough — if e.g. for some reason all of the initial momenta where colinear, ξ could potentially not behave as a random variable, and the motion of the system oscillator would not be of the Brownian form we expect).

Now we check the noise correlation function. Is it in accordance with the FDT? To compute the noise power spectrum we need

$$\langle \delta q_i(0)\delta q_j(0) \rangle = \frac{1}{2m_i \omega_i}\delta_{i,j}(2n_B(\omega_i) + 1)$$
$$\langle p_i(0)\delta q_j(0) \rangle = -\frac{i}{2}\delta_{i,j}. \tag{170}$$

Therefore

$$\langle \xi(t)\xi(0) \rangle = \sum_i \frac{C_i^2}{2m_i \omega_i} \left(\cos(\omega_i t)(2n_B(\omega_i) + 1) - i\sin(\omega_i t) \right)$$
$$= \sum_i \frac{C_i^2}{2m_i \omega_i} \left(n_B(\omega_i)e^{i\omega_i t} + (n_B(\omega_i) + 1)e^{-i\omega_i t} \right). \tag{171}$$

Fourier transforming,

$$\langle |\xi(\omega)|^2 \rangle = \sum_i \frac{C_i^2}{2m_i \omega_i} \left(n_B(\omega_i)\delta(\omega + \omega_i) + (n_B(\omega_i) + 1)\delta(\omega - \omega_i) \right)$$
$$\equiv \int_0^\infty d\omega' \, A^B(\omega') \left(n_B(\omega')\delta(\omega + \omega') + (n_B(\omega') + 1)\delta(\omega - \omega') \right), \tag{172}$$

where we defined the bath spectral density

$$A^B(\omega) \equiv \sum_i \frac{C_i^2}{2m_i \omega_i}\delta(\omega - \omega_i), \tag{173}$$

with the integral over ω' going from 0 to ∞ just because all the $\omega_i \geq 0$.

Note that the bath spectral density also determines the relaxation kernel, since we may write

$$\gamma(t) = \frac{2}{M} \int_0^\infty d\omega' \, \frac{A^B(\omega')}{\omega'} \cos(\omega' t). \tag{174}$$

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The naive Langevin equation corresponds to taking $\gamma(t) = \gamma\delta(t-t')$, which can be engineered via the choice

$$A^B_{naive}(\omega) = \frac{\omega M \gamma}{2\pi}. \tag{175}$$

This choice gives a large number of oscillators with large frequencies, leading to the unphysical behavior of the vx spectral function at short times, but of course correctly captures long-time physics. Note that regardless, for Langevin-esque behavior to emerge, it is essential for $A^B(\omega)$ to be a rather *broad* function of frequency. If we happened to find ourselves in a situation where e.g. $A^B(\omega) = \delta(\omega - \omega_0)$, with all of the bath oscillators at the same frequency, we would most certainly not thermalize, as the "damping" term would be purely oscillatory and long-ranged in time. Thus for the oscillators to act as an effective thermal bath, it is essential that they contain a relatively diverse range of fundamental frequencies.

We also expect that the choice $A^B_{naive}(\omega)$ should lead to an Einstein relation between γ and T, M, at least in the limit where we expect such a relation to hold. This is the high-temperature limit, where we set $\omega_i/T \ll 1 \forall i$, so that $n_B(\omega) \approx T/\omega_i$ (of course since $A^B_{naive}(\omega)$ is not damped at large ω this is not true for the whole integration domain, but we will not go through the hassle of introducing a soft cutoff). Indeed, it is easy to see that in this limit the noise power spectrum is simply
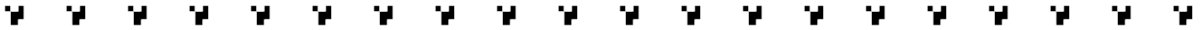
$$\langle |\xi(\omega)|^2 \rangle \to 2M\gamma T, \tag{176}$$

in agreement with FDT.

Ising model on a tree

In the following we will discuss some aspects of the Ising model on a $k > 2$-regular tree $\mathbb{T}_k$. Doing so was partly inspired by an educational email exchange with Andy Lucas, who wrote a problem exploring some aspects of this model available here.

The zeroth order thing to note about $\mathbb{T}_k$ is that a) the bounddary $\partial\mathbb{T}_k$ contains a constant fraction of the total number of sites N, and b) in addition to this, the number of sites further than a distance of $\sim \log\log(N)$ from the boundary consitute an exponentially small fraction of all sites. This makes the Ising model on $\mathbb{T}_k$ slightly sick: in Euclidean space, where the fraction of boundary sites vanishes in the TDL, the divergent susceptibility that accompanies SSB can be diagnosed by looking at how the fixed but few-in-number boundary sites exert

influence on the rest of the system; on the tree, having everything so close to the boundary gives a slightly strange TDL,[22] and as we shall see gives the free energy some unusual properties.

No magnetic field, free boundary conditions

Things are simplest with free boundary conditions and in the absence of a magnetic field, although as we will see the result obtained in this limit is slightly misleading. Here the free energy can be computed exactly, by integrating out the spins from the outside in, starting with those at the boundary. For a fixed configuration $\{s_{i\in\text{bulk}}\}$ of bulk spins, we may redefine each boundary spin as $s_i \to s_i s_{\text{parent}(i)}$, where i is a boundary vertex and $\text{parent}(i)$ is its parent vertex. This decouples the boundary spins completely, and gives

$$Z_d = Z_{d-1}(2\cosh(\beta))^{k(k-1)^{d-1}} \tag{177}$$

where Z_d is the partition function on the depth d tree and $k(k-1)^{d-1}$ is the number of leaves at depth d. Letting the total number of nodes be $N \sim (k-1)^d$, the free energy density F/N is accordingly

$$\frac{F}{\beta N} = -\ln[2\cosh(\beta)], \tag{178}$$

which is analytic at all β—there is thus apparently *no* phase transition at any finite temperature, and the system is always in the disordered phase.

This result can be understood in two ways. First, from the above strategy, we see that one can perform a change of variables which turns the model into N decoupled spins. This change of variables proceeds by taking products of spins from the outside of the tree along paths proceeding to the tree center, and will of course fail if loops were to be introduced. The thermodynamic triviality inferred from this reasoning also occurs in various glassy models, like the Newmann-Moore model, or Hamiltonians obtained from LDPC codes (see e.g. Hong, Guo, Lucas 24 or Mezard + Montanari for a contemporary discussion). Alternatively, one could decude the above result by thinking about the energy landscape on the tree. Unlike in Euclidean space, on the tree there are an extensive number of low-lying states with extensive Hamming distance from the two ground states. For example, there are $N-1$ states of energy 1, obtained by flipping all of the spins in a given subtree. This profusion of near-minima smoothen out the energy landscape and produce a thermodynamically trivial system. Both of these explanations could also be given to explain why the Ising model on a line ($\mathbb{T}_2 = \mathbb{Z}$) lacks a phase transition (although the types of barriers present in the energy landscape are very different on $\mathbb{T}_{k>2}$ and $\mathbb{Z}$).

The conclusion that there is no phase transition on $\mathbb{T}_{k>2}$ is however slightly hasty: in spite of the trivial-looking expression for F, we will momentarily see that the magnetic susceptibility diverges at a finite β, producing a non-analyticity in F in the standard limit where $N \to \infty$ before the field $h \to 0$. Thus the free energy $F(\beta, h)$ is an analytic function

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[22]This "problem" can be partially mitigated by working on a 2d hyperbolic manifold with periodic boundary conditions (obtained by tesselating a genus $g \gg 1$ surface M_g). However in this case g diverges in the TDL, and there exist a continuum of different length scales set by the sizes of the generators of $H_1(M_g; \mathbb{Z})$. These models are presumably much harder to analyze analytically however, so we will stick to $\mathbb{T}_k$ for now.

of β at $h = 0$, but is a non-analytic function of h at $h = 0$ for $\beta > \beta_c$. I am unaware of any other models producing a phase transition like this (which e.g. does not show up in the specific heat at all). This fact also demonstrates that despite mean field approximations working well on trees, the present model definitely yields a free energy distinct from the mean field expression.

Nonzero field / fixed boundary conditions

The near-degeneracy of the aforementioned energy landscape is lifted in the presence of a nonzero magnetic field h, or in the presence of non-free uniform boundary conditions. Consider then taking

$$H = -\sum_{\langle i,j \rangle} s_i s_j - bh \sum_{i \in \text{bulk}} s_i - h \sum_{i \in \text{boundary}} s_i, \qquad (179)$$

where $b = 0$ if the field is only at the boundary and $b = 1$ if the field is uniform throughout the system. Fixing the boundary conditions to be $s_{i \in \text{boundary}} = +1$ corresponds simply to setting $b = 0, h = 1$.

After integrating out the boundary spins, we have

$$Z_d = \sum_{\{s_{\text{bulk}}\}} e^{-\beta H(\{s_{\text{bulk}}\})} \prod_{i \in S_{d-1}} [2\cosh(\beta(s_i + h))]^{k-1}, \qquad (180)$$

where S_{d-1} is the set of vertices at depth $d - 1$. We claim that the effect of integrating out the boundary spins can be captured entirely by renormalizing the field experienced by the spins in S_{d-1} and adjusting the partition function by an overall constant. This is true provided that we can write

$$[2\cosh(\beta(s_i + h_n))]^{k-1} e^{(k-1)f_n} = e^{\beta(h_{n-1} - bh)s_i + f_{n-1}} \qquad (181)$$

for some constants f_n (with $f_d = 0$); here the $-bh$ on the RHS is included so that a spin at depth n feels an effective field of h_n. Indeed, since $s_i \in \{\pm 1\}$ we may write $e^{\beta(h_{n-1} - bh)s_i/(k-1)} = \cosh(\beta(h_{n-1} - bh)/(k-1)) + s_i \sinh(\beta(h_{n-1} - bh)/(k-1))$, while on the LHS we may use $\cosh(x + s_i y) = \cosh(x)\cosh(y) + s_i \sinh(x)\sinh(y)$. Matching the s_i on both sides gives the recursion relation (which will be familar to those who know about belief propagation—see e.g. Mezard and Montanari)

$$\tanh(\beta)\tanh(\beta h_n) = \tanh\left(\frac{\beta(h_{n-1} - bh)}{k-1}\right) \qquad (182)$$

with $h_d \equiv h$, from which the f_n are determined via

$$f_{n-1} = (k-1)\left(f_n + \ln\left[\frac{2\cosh(\beta)\cosh(\beta h_n)}{\cosh(\beta(h_{n-1} - bh))}\right]\right). \qquad (183)$$

From the recursion relation for Z_d we see that the free energy density on a tree with N spins is

$$F/N = -\beta^{-1} f_0/N + \cdots, \qquad (184)$$

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where the $\cdots$ vanish as $N \to \infty$. As a sanity check, note that when $h = b = 0$ we get $f_n/N = \ln(2\cosh(\beta)) + O(1/N)$, which agrees with the zero-field result.

The phase of the system is—at least if one defines things by associating order to bulk sensitivity to boundary fields—determined by the effective field $h_{n\to 0}$ produced deep in the bulk. Consider first the high temperature limit $\beta \ll 1$. Then

$$h_{n-1} = \beta(k-1)h_n + bh, \tag{185}$$

which is solved as

$$h_n = h\left(b\frac{1 - \widetilde{\beta}^{d-n}}{1 - \widetilde{\beta}} + \widetilde{\beta}^{d-n}\right), \qquad \widetilde{\beta} \equiv (k-1)\beta. \tag{186}$$

Thus as long as $\widetilde{\beta} \ll 1$, the effective field seen in the bulk is finite, and approaches either 0 (if $b = 0$, viz. if the field is only at the boundary), or a renormalized value of $h/(1 - \widetilde{\beta})$ (if $b = 1$, viz. if the field is everywhere).[23]

On the other hand, when $\beta \gg 1$ it is easy to see that $h_d = \varepsilon \ll 1$ does not give an h_n that converges to 0 as $n \to 0$. To find the location of the transition where the behavior switches, we can look at the stability of the recursion relation for h_n. Consider for simplicity the case with no bulk field ($b = 0$). Then expanding the recursion relation in small h_n, h_{n-1}, we have

$$\frac{h_{n-1}}{h_n} = (k-1)\tanh(\beta), \tag{187}$$

and so the critical inverse temperature β_* satisfies $\tanh(\beta_*) = 1/(k-1)$. This can be re-written by taking $\beta_* = \ln(\lambda)$ and using $\tanh(\log(\lambda)) = (\lambda^2 - 1)/(\lambda^2 + 1)$ and then solving for λ; doing so gives

$$\beta_* = \frac{1}{2}\ln\frac{k}{k-2}. \tag{188}$$

Note as sanity checks that a) $\beta_* = \infty$ when $k = 2$, recovering the absence of a transition on the line, and b) $\beta_* \to 0$ when $k \to \infty$, since the number of nearest neighbors of each spin becomes infinite in this limit. Furthermore, if we restore the Ising coupling J and take the limit $k \to \infty$ with $J\beta$ fixed, we get

$$\beta_*|_{k\to\infty} = \frac{1}{Jk}. \tag{189}$$

This limit is the one we would take when doing mean field,[24] and indeed $T_* = Jk$ matches exactly the expected mean field critical temperature (in which the magnetization m as a function of field h is $m = \tanh[\beta(kJm + h)]$). This is one sense in which mean field "works" on the tree (although there are of course distinct differences, as was seen in the behavior of $F(\beta, h = 0)$).

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[23]In both cases, the approach to this value is exponentially fast in distance from the tree boundary.

[24]Here by "mean field" we mean taking the coupling to be all-to-all and sufficiently weak to produce a well-defined TDL. It appears that sometimes people mean "infinite spatial dimension with local couplings", viz. working on $\mathbb{T}_k$, precisely what we are doing here.

The above result highlights why the previous conclusion about the absence of a phase transition in the zero-field case is (in some sense) too hasty: while the free energy is that of a trivial paramagnet in the absence of a field, when $\beta > \beta_*$ any nonzero boundary field will grow to a nonzero value as spins near the boundary are integrated out, leading to ordering in the center of the tree. I believe the reason the "phase transition" at β_* does not show up in e.g. the specific heat (so that the system in some respects is still thermodynamically trivial at $\beta > \beta_*$) is that it is only the susceptibility at vertices very near the center of $\mathbb{T}_k$ that diverge. Indeed, while h_n approaches h_0 exponentially fast in distance from the boundary, almost all sites are close to the bounadry, where they see a non-divergent h_n, so that $(\partial_h \langle s_i \rangle_h)|_{h=0} \to 0$ for most sites at all β.

Phase diagram

We now briefly discuss the "phase" diagram in the (β, h) plane. For us the ordered phase will be defined purely by the region in which the Gibbs measure is not unique (irrespectivity of the triviality [or not] of $F(\beta, h)$).

Consider first $\beta = \infty$. The ordered phase here in fact has a finite critical h_c, equal to

$$h_c|_{\beta=\infty} = k - 2. \tag{190}$$

I believe this follows by realizing that at $h = k-2$, the energy change of flipping a line of spins (beginning and ending on $\partial \mathbb{T}_k$) vanishes when starting from a ferromagnetic state aligned against h (provided the boundary conditions at the path ends are chosen appropriately). As a partial sanity check, $h_c|_{\beta=\infty} = 0$ on the line ($k = 2$). As β is decreased, we expect h_c to decrease as well, until it vanishes at β_*.

The fact that at $\beta = \infty$ the different Gibbs measures at $h = k - 2 - \varepsilon$ are obtained by flipping spins along lines means that the number of symmetry broken minima (extremal points of the convex set of Gibbs states) is larger than two (and in fact infinite) in this regime. This comes from the fact that in this regime, the magnetization of spins in the bulk can be affected when only a vanishing fraction of the boundary spins are changed (something which is easily checked to *not* happen at $\beta = \beta_* + \varepsilon, h = 0$). Thus there must be a further transition between a doubly degenerate ferromagnetic phase—where $\langle s_{\text{center}} \rangle$ is sensitive only to the net magnetization of spins on $\partial \mathbb{T}_k$—and an extensively-degenerate phase, where $\langle s_{\text{center}} \rangle$ is sensitive to the full details of the boundary conditions.

The value of $\beta'_*(h)$ above which the system enters the extensively-degenerate phase should in fact be equal to the $\pm J$ spin glass transition temperature at bond probability $p = 1/2$ (again, at least at $h = 0$). From some results quoted in Martinelli, Sinclair and Weitz 03, at $h = 0$ this temperature is apparently

$$\beta'_*(0) = \frac{1}{2} \ln \frac{\sqrt{k+1}+1}{\sqrt{k+1}-1}. \tag{191}$$

The connection between these temperatures (at least at $h = 0$) follows from realizing that the disorder in the $\pm J$ spin glass can be completely pushed off to the boundary: the change of variables discussed above renders all couplings ferromagnetic since $\mathbb{T}_k$ has no loops, and modifies only the boundary conditions (and thus the glass problem is trivial with free boundaries), and hence it is non-homogenous boundary conditions which produce frustration (since

$|\partial \mathbb{T}_k|/|\mathbb{T}_k|$ is constant, one pays a constant energy density penalty if one ignores the boundary and satisfies only the bulk interaction terms). Thus the EA order parameter at the center of $\mathbb{T}_k$, viz. $\mathbb{E}_{\text{disorder}}\langle s_{\text{center}}\rangle^2_{\text{glass}} = \mathbb{E}_{\partial \text{ conds}}\langle s_{\text{center}}\rangle^2_{\text{clean}}$, directly measures the influence of typical boundary conditions on the tree center, thereby identifying the spin glass temperature with β'_*.

Mixing times

We now briefly comment on the mixing times t_{mix} of Glauber dynamics in the scenarios discussed above.[25] This discussion is done purely because I wanted to remember the results, and comes mostly by pulling results from the aforementioned paper by Martinelli et al.

Recall first the story in Euclidean space: for Glauber dynamics on $\mathbb{Z}^d$ with PBC, $t_{\text{mix}} = O(\log(N))$ at $\beta < \beta_*$ and $t_{\text{mix}} = \exp(\Omega(N^{1/d}))$ at $\beta > \beta_*$. The former is the smallest t_{mix} can be ($t_{\text{rel}} = O(1)$ since the spectral gap is $1/L$, and the $\log(N)$ factor comes from the fact that independently relaxing spins take $\log(N)$ to relax essentially because of rare-region effects). With fixed ferromagnetic boundary conditions, we expect $t_{\text{mix}} = O(\text{poly}(N))$ for all T, although apparently this has not actually been proven.

Things change on $\mathbb{T}_{k>2}$. For arbitrary boundary conditions, $t_{\text{mix}} = O(\log(N))$ when $\beta < \beta'_*$ or when $h > h_c(\beta)$, while for $\beta > \beta'_*$ and $h = 0$ one has[26]

$$t_{\text{mix}} = O(N^{c\beta}) \tag{192}$$

where c is an $O(1)$ constant. With ferromagnetic boundary conditions, $t_{\text{mix}} = O(\log(N))$ for all β, h; this is unsurprising since with ferromagnetic boundary conditions the mixing time on a graph G in the ordered phase should be $O(\text{poly}(\text{diam}(G)))$. I am at present not actually sure if the mixing time remains slow in the presence of a nonzero field. While the Gibbs measure is indeed not unique until a finite critical h, note that in the zero field case, it is $\beta'_*(h)$—and not $\beta_*(h)$—which is relevant for determining the regime in which mixing is slow, so that there exists a regime in the "ordered phase" (according to our definition) where mixing is nevertheless *fast* with free boundary conditions. Therefore a priori the mixing in the ordered phase at finite-field may also be fast; in fact basic reasoning about spin flips starting from the boundary make a $\text{poly}(N)$ mixing time seem unlikely.

For this reason we will attempt to update our prior for t_{mix} by running some low-effore

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[25]Our definition of t_{mix} will be the "physicist's" definition, counting the number of time steps for Glauber dynamics to mix, with each time step involving $\Theta(N)$ updates, one applied at each site. Thus t_{mix} is shorter than its definition in the math literature by $\sim N$.

[26]The fact that $t_{\text{mix}} = o(\exp(N^\alpha))$ for all α is immediately clear due to the fact that the energy barriers on the tree are exponential in the *log* of $|\mathbb{T}_k|$ (this is to be contrasted e.g. with the Ising model on a ER graph past the percolation threshold or on the tanner graph of a good LDPC code, which has linear confinement [barriers going as $\sim N$ rather than $\sim \log(N)$], giving gives an exponential lifetime).

numerics. At zero field, we get

$$(193)$$
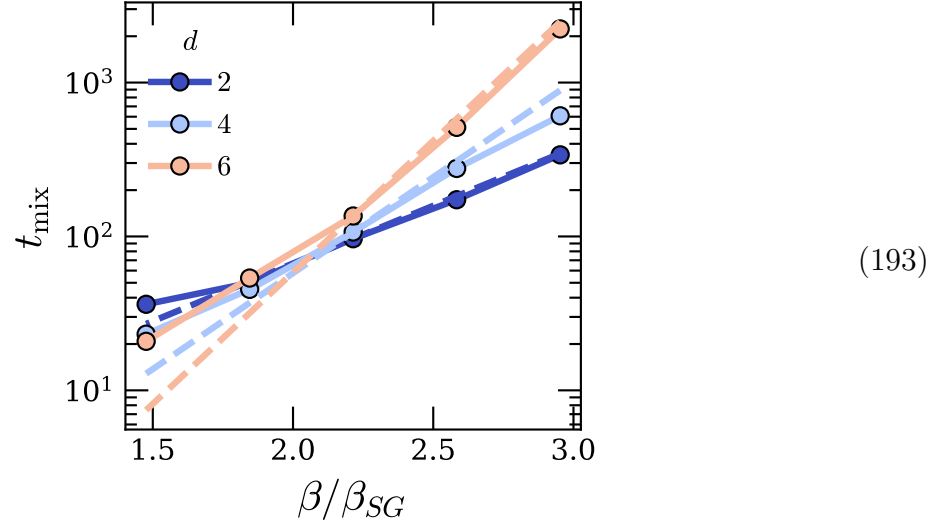
where the fits are to $t_{\mathrm{mix}} \sim N^{c\beta}$ for $c = 0.75/\beta_{SG}$ (β_{SG} is what we have been calling β'_* above). I am not sure why the transition appears to happen at $\beta = 2\beta_{SG}$ as I do not appear to be missing any obvious factors of 2.

At a finite but small magnetic field of $h = h_c(\beta = 0)/10$, and at moderately large values of β, we find

$$(194)$$
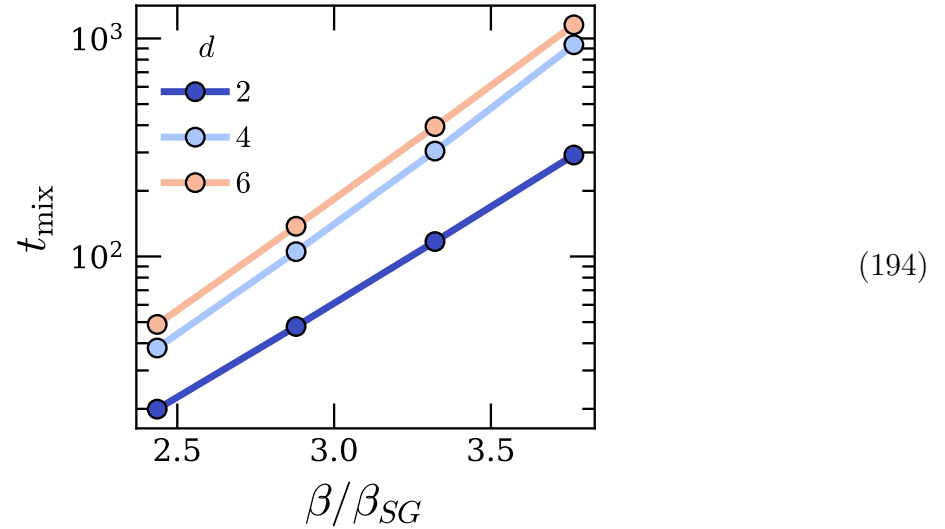
giving a mixing time which appears to be $t_{\mathrm{mix}} \sim \mathrm{poly}(L)e^{c\beta}$ wth c independent of L. Either the critical field for slow dynamics is extremely small or the dynamics is in fact fast at all non-zero fields (which seems more likely to me at present).

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Multipole-constrained diffusion

This entries contains some calculations relating to kinetically constrained diffusion processes. Thanks to Sunghan Ro and Jung Hoon Han for patient tutelage regarding the generating functional formalism.

Generalities

First let us understand what types of "diffusive" behavior we expect to find in lattice gases whose dynamics is multipole moment conserving. The setting we have in mind is a lattice gas where particles hop in a multipole-conserving way, with the probability of a given hopping event occuring being proportional to the total number of distinct groups of particles[27] that can be selected to hop. For example with only charge (0-pole) conservation, a hopping process which moves a particle on site i to a site $j \neq i$ will have a probability of occuring proportional simply to the number of particles on site i, ρ_i. A dipole-conserving hopping process which moves a pair of particles at sites (i, j) to sites $(i + \delta, j - \delta)$ has an occurance probability proportional to the number of pairs that can be selected to hop, viz.

$$P_{(i,j)\to(i+\delta,j-\delta)} \propto \rho_i \rho_j. \tag{195}$$

Higher multipole moments are similar.

The above rule for the hopping probabilities amounts to taking a "mean-field" limit, with the probability for a multipole-conserving hop factorizing in terms of a product of the densities ρ_i at the sites where the hopping occurs. While this factorization is not generic per se, note that *any* possible hopping probability must vanish if any of the ρ_i do, thus e.g. the dipole hopping probability $P_{(i,j)\to(i+\delta,j-\delta)}$ must vanish when either ρ_i or ρ_j do. The product form above is the simplest rule compatible with this constraint.

For simplicity we will mostly restrict ourselves to the multipole group of degree n in 1d, with the dynamics conserving

$$Q^{(m)} \equiv \int_x x^m \rho_x \qquad \forall \, m \leq n. \tag{196}$$

Note that translation invariance plus conservation of $Q^{(n)}$ automatically imply conservation of all $Q^{(m)}$ for $m \leq n$. In this case, while the value of $Q^{(m)}$ is only independent of the choice of origin if $Q^{(o<m)} = 0$ for all o, the conservation of $Q^{(m)}$ is true independently of the choice of origin.

Generalizing to higher dimensions can be done easily if we generalize to the *maximal* multipole group, i.e. if the dynamics conserves $\int_{\mathbf{r}} p_n(r_a) \rho_{\mathbf{r}}$ for *all* degree-n polynomials of

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[27]viewing the particles as being distinguishable.

the coordinates r_a. Non-maximal multipole groups (where e.g. one has a conservation law for $p_n(r_a) = x^2, y^2$ but not xy) are more complicated and will only be briefly touched on.

Translation invariance and conservation of the n-pole moment requires the continuity equation to look like

$$\partial_t \rho = \partial_{I_n} J^{I_n}, \tag{197}$$

where $I_n = \{i_1, \ldots, i_n\}$ is a composite index. The most natural thing to write—and indeed what most people in the literature seem to do—is to take

$$J^{I_n} \overset{?!}{=} D\partial^{I_n}\rho. \tag{198}$$

This however gives a *linear* (sub)diffusion equation, which cannot be right in our model, since the kinetic constraints force the dynamics to freeze out when $\rho \to 0$. Another way of saying this is that since the probabilities for a given hopping event are nonlinear in ρ (as long as $n > 0$), the constitutive relation for the current must also be nonlinear in ρ. One guess of how to fix this would be to let D simply be proportional to ρ raised to an appropriate power, capturing the fact that diffusion becomes frozen out at low densities. Luckily, this (rather boring) solution also turns out to be incorrect.

equilibrium

A slightly hacky[28] way of seeing this is to find the steady states of the density that arise when we maximize the entropy—which in the current context is just $S = -\int_x \rho_x \ln \rho_x$—subject to the constraints of having fixed multipole moments. Doing this gives

$$\rho_x^{eq} = \exp\left(\sum_{m=0}^{n} \lambda_m x^m\right), \tag{199}$$

where the Lagrange multipliers λ_m are determined from the values of the multipolar charges by $\int_x x^m \rho_x = Q^{(m)}$. The fact that we get *exponential* functions as *steady-state* solutions to our multipolar diffusion processes guarantees that we cannot simply take the multipolar current J to be linear in ρ, as we need J to vanish on solutions of the form (199).

For illustration consider the $n = 1$ case of dipole conservation, and let the system live in a box with $x \in [-L/2, L/2]$. Then the equilibirum distribution is

$$\rho_{\text{eq}}(x) = e^{-\beta(x-\mu)}, \qquad \mu = \frac{1}{\beta}\ln\left(\frac{N}{2\beta\sinh(L/2\beta)}\right), \tag{200}$$

where β solves the equation

$$x_{\text{cm}} \equiv \frac{Q^{(1)}}{L} = \frac{1}{\beta} - \frac{L}{2}\coth(L\beta/2). \tag{201}$$

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[28]I describe this argument as being "hacky" since it relies on entropy maximization, while the systems we are considering are not ergodic for any strictly local implementation of dipole-conserving dynamics. Complaining about ergodicity is rather legalistic though, as we will always be interested in the dynamics that occurs in sectors that occupy "very big" subsets of configuration space, and here the dynamics will be ergodic enough that the microcanonical and grand canonical approaches will agree.

Note that we are at "infinite temperature" $\beta = 0$ (giving a uniform density distribution) when $x_{\mathrm{cm}} = 0$ (or if $L \to \infty$ and x_{cm} is finite); in all other cases we obtain an exponentially concetrated steady-state profile which hugs one of the edges of the box. In particular, when $x_{\mathrm{cm}} = -L/2$ we obtain a $T = 0^+$ "zero temperature" state with all of the particles on the left boundary, while when $x_{\mathrm{cm}} = L/2$ we obtain a $T = 0^-$ "barely negative temperature" state with all of the particles on the right boundary.

When we think from the perspective of the dynamics, the fact that the particles end up localizing themselves despite the "infinite temperature" (rejection-free) nature of the dynamics may seem surprising, but in the interpretation above it is not surprising at all: as far as the equilibrium state is concerned, we are simply studying the statistical physics of particles in a linear potential, with the steady-state of course being one in which the particles are clumped at one end of the system or another.

minimal nonlinearities of the consitutive relation

To determine the kinds of multipolar diffusion equations that have (199) as solutions, we start by lower-bounding the number of powers of ρ that must enter into the constitutive relation. To this end, in this subsection we prove the following proposition:

Proposition 1. *For dynamics that conserves the n-pole moment of the charge, the constitutive relation expressing the current in terms of the density must involve at least $n+1$ powers of ρ and $n+1$ spatial derivatives. This lower bound can be saturated for at least all $n \leq 10$.*

Proof. Let us first determine the minimal number of powers of ρ that must appear in the constitutive relation for the current. This number is determined by finding the smallest number of particles that can participate in an n-pole preserving particle hopping process. For a process involving m particles, let $\mathbf{a}, \mathbf{b} \in \mathbb{Z}^m$ denote the initial and final positions of the particles, respectively. Note that if $a_i = b_j$ for any $i, j \in 1, \ldots, m$, then at least one particle does not actually move during the hopping process; thus wolog we may restrict to $\{a_i\} \cap \{b_i\} = \emptyset$. If the process $\mathbf{a} \mapsto \mathbf{b}$ is to preserve all multipole moments up to n, we require that

$$\sum_i a_i^p = \sum_i b_i^p \ \forall \ p \in \{0, \ldots, n\}. \tag{202}$$

The goal is thus to find the smallest-length pair of disjoint integer-valued sets such that the above equation is satisfied.

We now show that (202) can be satisfied only when $m > n$. Indeed, suppose that $m = n$. It is a well-known fact [2] that the set of "power-sum polynomials"

$$P_q(\mathbf{a}) \equiv \sum_{i=1}^m a_i^q \tag{203}$$

for $q \in \{0, \ldots, m\}$ generate all symmetric polynomials in m variables (not over $\mathbb{Z}$, but over $\mathbb{Q}$, although this doesn't matter for us). This means that the symmetric polynomials $\prod_{i=1}^m a_i, \prod_{i=1}^m b_i$ can be expressed as $\mathbb{Q}$-valued linear combinations of the $P_q(\mathbf{a}), P_q(\mathbf{b})$, respectively. But since we have assumed that all $o \leq m$ multipole moments are conserved, we

have

$$P_q(\mathbf{a}) = P_q(\mathbf{b}) \; \forall \; q \in \{0, \ldots, m\} \implies \prod_{i=1}^{m} a_i = \prod_{i=1}^{m} b_i. \tag{204}$$

Now we use the fact that (202) is invariant under translations, in that (202) implies

$$P_q(\mathbf{a} - x) = P_q(\mathbf{b} - x) \tag{205}$$

for any constant vector x (this follows from the fact that $P_q(\mathbf{a} - x)$ is also a symmetric polynomial). In particular, we may choose $x = a_1$ to effectively set $a_1 = 0$ wolog. But then from the above we see that since $\prod_i a_i = 0$, we must also have $\prod_i b_i = 0$. In particular, one of the b_i must equal zero, which contradicts our assumption about the disjointness of $\{a_i\}, \{b_i\}$.

This shows that any n-pole conserving hopping process must involve at least $n + 1$ particles, so that the constitutive relation must involve at least $n + 1$ powers of the density. This also implies that the current must involve at least $n + 1$ derivatives; if it involved fewer than $n + 1$ derivatives then it would be proportional to an overall power of the density $J = \rho^k(\cdots)$ (where $\cdots$ involves derivatives of ρ), and the ρ^k in front could be stripped away without affecting the nature of the zero-current solutions.

$\square$

We have shown that $n + 1$-body terms are necessary, but not that they are sufficient. Showing this would amount to proving that one can always find two mutually disjoint size-$n + 1$ sets of integers satisfying (202). Such solutions are known to exist for $n \leq 10$ and $n = 12$, but for other values of n the answer is unknown, and the full resolution of this question is in fact a famous open problem in number theory [1] known as the Prouhet-Tarry-Escott problem.

The explicit solutions of (202) quickly get rather complicated for large n, meaning that they involve very long-range hopping processes. For example, when $n = 7$ the simplest solution has an eight-body hopping process with

$$\begin{aligned} a &= [1, 5, 10, 24, 28, 42, 47, 51] \\ b &= [2, 3, 12, 21, 31, 40, 49, 50] \end{aligned} \tag{206}$$

meaning that the minimal-body hopping process extends over 50 lattice sites.

Depending on the physical context it may be unreasonable to consider such long-range hopping terms, instead considering shorter-range but higher-body hopping processes. The minimal-range hopping processes involve a number of particles that scales exponentially in n but has range equal to $n + 2$, which can be constructed by letting

$$\mathbf{a} = \bigoplus_{i=0}^{\lfloor (n+1)/2 \rfloor} (2i)^{\oplus \binom{n+1}{2i}}, \qquad \mathbf{b} = \bigoplus_{i=1}^{\lfloor (n+2)/2 \rfloor} (2i-1)^{\oplus \binom{n+1}{2i-1}}, \tag{207}$$

where $\oplus$ denotes concatenation, so that e.g. $x^{\oplus k}$ is the length-k vector with all entries equal to x. For dipoles this gives the 2-body process $\mathbf{a} = (1, 3)$, $\mathbf{b} = (2, 2)$, for quadrupoles the 4-body process $\mathbf{a} = (1, 3, 3, 3)$, $\mathbf{b} = (2, 2, 2, 4)$, and so on.

scaling

Consider a value of n for which the minimal number of powers of ρ appearing in the expression for the current is the minimum value of $n + 1$ (as we saw above this will always be satisfied for all "reasonable" choices of n). Since the current will then contain $n + 1$ powers of ρ and $n + 1$ spatial derivatives, a single-variable scaling ansatz $\rho(x, t) = \rho(xt^{-1/z})$ yields

$$z = n(2 + d) + 2. \tag{208}$$

This is quite striking in that it explicitly depends on d, which is not something that happens for the regular (linear) diffusion equation ($n = 0$).

However, this single-variable scaling ansatz actually is only applicable in the cases of $n = 0, 1$. Indeed, suppose that $n > 1$. Then both $Q^{(0)}$ and $Q^{(2)}$ must be time-independent, which is impossible if $\rho(x, t) = \rho(xt^{-1/z})$, except in the trivial case when $Q^{(0)} = Q^{(2)} = 0$ or if we ignore (208) and take $z = \infty$. Physically, when $n > 1$ we always have a non-zero conserved quadrupole moment that defines a length scale in the problem.

For dipolar diffusion, a single-variable scaling ansatz works because we can always choose to define $Q^{(1)}$ with the origin located at x_{cm}, so that $Q^{(1)} = 0$. Thus when $Q^{(1)}$ is conserved but $Q^{(2)}$ is not, we expect that $Q^{(2)}$ evolves over time as

$$Q^{(2)}(t) \sim t^{\frac{1}{4+d}}. \tag{209}$$

Master equation and scaling limit

In this section we will derive the multipolar diffusion equations from lattice master equations. Doing so will require us to think about how to take a scaling limit where derivative expansions become valid, which conceptually works out in a way rather different as compared to conventional diffusion.

conventional diffusion

We begin by reviewing conventional diffusion. Let n_i be the number of particles on site i. If the probability for a single particle to hop within a time step dt is r, then

$$\partial_t n_i = \frac{r}{dt}(n_{i+1} + n_{i-1} - 2n_i). \tag{210}$$

Let a be the lattice spacing and $\mathcal{N} \in \mathbb{N}$ be the number of sites. Define the density $\rho_x \equiv n_i/a$, where the switch between i and x is merely suggestive notation. Consider the continuum limit, where $a \to 0$ with fixed $\mathcal{N}a$; here we usually say that we may take $x \in \mathbb{R}$ and that ρ_x is well-defined in this limit, meaning that ρ_x is some $O(1)$ number at any given $x \in \mathbb{R}$. In terms of the original lattice model, this means that the average occupancy of any lattice site is $n_i \sim a\rho_x \to 0$. This makes sense for thinking about the continuum — we hold fixed the total number of particles but increase the number of lattice spacings between particles, while at the same time making the lattice spacing smaller. In the continuum limit we would not usually take n_i to be $O(1)$, since then ρ_x does not have a well-defined limit. For the diffusion equation this is okay because it is non-interacting, and the way in which

a large number of particles diffuse is asymptotically equal to the average way that a single particle diffuses. Thus having the lattice limit be dilute is acceptable.

In the continuum limit we write the lattice diffusion equation as

$$\partial_t \rho_x = D \left(\partial_x^2 \rho_x + \frac{a^2}{12} \partial_x^4 \rho_x + \cdots \right), \qquad D \equiv \frac{ra^2}{dt}. \tag{211}$$

We then drop the higher order derivative terms on the grounds that $a \to 0$ and that all derivatives $\partial_x^n \rho$ are of the same size.

dipolar diffusion

Now we move on the to dipolar case. Consider a master equation generated by the processes $0110 \leftrightarrow 1001$. Then

$$\partial_t n_i = \frac{r}{dt} \left(n_{i-1} n_{i+2} + n_{i-2} n_{i+1} + n_{i+1} n_{i+2} + n_{i-1} n_{i-2} - n_i (n_{i+1} + n_{i-1} + n_{i+3} + n_{i-3}) \right). \tag{212}$$

Again define $\rho = n/a$. Then

$$\partial_t \rho_x = \frac{4ra^5}{dt} \partial_x^2 \left((\partial_x \rho)^2 - \rho \partial_x^2 \rho + a^2(\cdots) \right), \tag{213}$$

where the $\cdots$ have two ρs and six ∂s. Dropping the $(\cdots)$, the zero-current solutions are exponentials:

$$\rho^{\text{eq}}(x) = e^{\lambda x}. \tag{214}$$

It is illuminating to also consider the master equation generated by $020 \leftrightarrow 101$. Since the number of pairs to be chosen when two particles hop from the same site is $n_i(n_i - 1)$ — instead of n_i^2 — we get

$$\partial_t n_i = \frac{r}{dt} \left(2n_{i-1} n_{i+1} + n_{i+1}(n_{i+1} - 1) + n_{i-1}(n_{i-1} - 1) - n_i(2(n_i - 1) + n_{i+2} + n_{i-2}) \right). \tag{215}$$

This becomes

$$\partial_t \rho_x = \frac{ra^5}{dt} \partial^2 ([(\partial_x \rho)^2 - \rho \partial_x^2 \rho + a^2(\cdots)] - a^{-3} \rho). \tag{216}$$

Note in particular the appearance of the $-\frac{ra^2}{dt} \partial_x^2 \rho$ term on the RHS, which acts as a conventional diffusion term with *negative* diffusion constant, thereby favoring charge localization (as before the $\cdots$ represents terms with two ρs and six ∂_xs). Dropping the $(\cdots)$, the zero-current solutions are now of the form

$$\rho^{\text{eq}}(x) \propto \sinh^2(\alpha x + \beta) \tag{217}$$

for arbitrary α, β.

From (213) one might be tempted to take a continuum limit by letting $D = 4ra^5/dt$ be a constant (the power of a^5 is weird but we can scale dt with whatever z we wish) and taking $\rho, \partial\rho, \cdots \sim O(1)$. But in this limit the 3-site master equation is not well defined, possessing an infinitely negative diffusion term which completely localizes all of the particles. In fact this localization is very physical: in the continuum limit the particles in the lattice regularization are very dilute, and we know that in the dilute limit dipole-conserving particles are completely frozen, with trivial dynamics.

Thus interesting (non-frozen) dynamics does not occur in the continuum limit.

quadrupolar diffusion

A master equation containing only cubic terms in the n_i can be obtained by considering the process

$$1000110 \leftrightarrow 0110001. \tag{218}$$

A simpler (but still 3-body) process is $20010 \leftrightarrow 01002$. Becuase of the 2s, this process will contain a contribution to the current which is only quadratic in n_i. Indeed, the full master equation is

$$\frac{dt}{r}\partial_t n_i = 2n_{i-2}(n_{i-2} - 1)n_{i+1} + n_{i+1}(n_{i+1} - 1)n_{i+4} + 2n_{i-1}n_{i+2}(n_{i+2} - 1) + n_{i-4}n_{i-1}(n_{i-1} - 1)$$
$$- n_i \left(2(n_i - 1)n_{i+3} + n_{i-3}(n_{i-3} - 1) + n_{i+3}(n_{i+3} - 1) + 2(n_i - 1)n_{i-3}\right). \tag{219}$$

Expanding in derivatives,

$$\partial_t \rho_x = \frac{2ra^8}{dt}\partial_x^3 \left([\rho^3 \partial_x^3 \ln(\rho) + a^2(\cdots)] + a^{-3}\rho\partial_x\rho\right). \tag{220}$$

Examples

dipole

Consider first dipolar diffusion in 1d. We know the current will have $n + 1 = 2$ powers of ρ and also $n + 1 = 2$ derivatives. Thus

$$J = a(\partial_x\rho)^2 + b\rho\partial_x^2\rho \tag{221}$$

for some a, b, determined by requiring that $J = 0$ when evaluated on any entropy-maximizing function of the form $\rho(x) = e^{\lambda x}$. It is easy to check that $a = 1, b = -1$ is required, thus yielding the dipolar diffusion equation

$$\partial_t\rho = D\partial_x^2((\partial_x\rho)^2 - \rho\partial_x^2\rho). \tag{222}$$

An interesting fact is that this equation (along with the higher multipole version to follow) is not purely dissipative, meaning that the RHS cannot be written as $\delta H(\rho)/\delta\rho$ for any function $H(\rho)$. To see this, note that any such $H(\rho)$ must involve three powers of ρ and four derivatives. A rather simple-minded approach is thus to write H as

$$H = a\rho^2\partial^4\rho + b\rho\partial^3\rho\partial\rho + c\rho(\partial^2\rho)^2 + d\rho(\partial\rho)^2\partial^2\rho. \tag{223}$$

We then explicitly compute $\delta H/\delta\rho$ and attempt to match the resulting expression with the RHS of the above diffusion equation, which we can rewrite as $D[(\partial\rho)^2 - \rho\partial^4\rho]$. The variation of H gives (note that the d term is a total derivative and thus doesn't contribute)

$$\frac{\delta H}{\delta\rho} = (2a - b + c)(3(\partial^2\rho)^2 + 4\partial\rho\partial^3\rho + 2\rho\partial^4\rho), \tag{224}$$

which can never take on the desired form.

quadrupole

Consider now quadrupolar conservation, and remain in 1d. We know the current needs to have $n + 1 = 3$ powers of ρ, as well as 3 derivatives. Thus the minimal expression for the current reads

$$J = a\rho^2 \partial_x^3 \rho + b\rho \partial_x \rho \partial_x^2 \rho + c(\partial_x \rho)^3, \tag{225}$$

where a, b, c are to be determined by requiring that $J = 0$ when evaluated on any entropy-maximizing function of the form $\rho(x) \propto e^{-(x-x_0)^2/2\sigma^2}$. A bit of algebra shows that the correct choice is to let $a = -1, b = 3, c = -2$. Thus the minimal quadrupolar diffusion equation is

$$\partial_t \rho = D\partial_x^3 \left(-2(\partial_x \rho)^3 - \rho^2 \partial_x^3 \rho + 3\rho \partial_x \rho \partial_x^2 \rho\right). \tag{226}$$

A brute force approach like the one used for the dipole-conserving diffusion equation shows that this equation is also not purely dissipative, with the RHS not being able to be written as $\delta H(\rho)/\delta\rho$ for some H.

The above equation is indeed what is derived when one performs a graident expansion on the quadrupole-conserving 3-body process $(-1, 2, 0, -2, 1)$, viz. $\mathbf{a} = (1, 4, 4)$, $\mathbf{b} = (2, 2, 5)$. This can be easily verified by performing a gradient expansion on the microscopic current

$$J_i = \rho_{i-2}\rho_{i+1}^2 - \rho_{i-1}^2\rho_{i+2} \tag{227}$$

for which one obtains $D = 2$ in the present units.

When one employs the shorter-ranged 4-body term $\mathbf{a} = (1, 3, 3, 3), \mathbf{b} = (2, 2, 2, 4)$, one instead obtains

$$\partial_t \rho = D\partial_x^3 \left(\rho[2(\partial_x \rho)^3 + \rho^2 \partial_x^3 \rho - 3\rho \partial_x \rho \partial_x^2 \rho]\right), \tag{228}$$

now with $D = 1$, and with the extra power of ρ in the expression for the current. This is checked by performing a gradient expansion on the microscopic current, which for this hopping process reads

$$J_i = \rho_i^3 \rho_{i-2} - \rho_{i+1}\rho_{i-1}^3. \tag{229}$$

Thus the form of the derivatives in the constitutive relation is universal, but extra powers of ρ may always be tacked on by considering hopping processes with larger-than-necessary number of particles.

In infinite space, the asymptotic steady state is

$$\rho(x) = \frac{N}{\sqrt{2\pi Q^{(2)}}} e^{-(x-x_{\text{cm}})^2/2Q^{(2)}}. \tag{230}$$

Thus we have the rather remarkable result that the system spontaneously "congeals" itself into a Gaussian blob, which then simply sits motionless motionelss for eternity. In a finite box one still gets a Gaussian solution, but the peak is no longer generically centered on x_{cm}.

sextupole

The lowest-body sextupole-conserving process is a four-body process with $\mathbf{a} = (1, 4, 5, 8)$, $\mathbf{b} = (2, 2, 7, 7)$, while the shortest-range processes is an eight-body process obtained from Pascal's triangle as $\mathbf{a} = (1, 3, 3, 3, 3, 3, 3, 5)$ $\mathbf{b} = (2, 2, 2, 2, 4, 4, 4, 4)$.

Since the minimal expression for the current should contain 4 powers of ρ and 4 derivatives, we may write

$$J = a(\partial\rho)^4 + b\rho^2\partial\rho\partial^3\rho + c\rho^2\partial^2\rho\partial^2\rho + d\rho\partial^2\rho(\partial\rho)^2 + e\rho^3\partial^4\rho \tag{231}$$

for some constants a, b, c, d, e. Consider a solution of the form $\rho(x) = e^{f(x)}$. Then

$$J(x)e^{-f(x)} = f'^4(a+b+c+d+e) + f'^2 f''(3b+2c+d+6e) + f''^2(c+3e) + f'f'''(b+4e). \tag{232}$$

Requring that $f(x) = \alpha x^3/3 + \beta(x - x_0)^2$ give a zero-current steady state solution for all α, β, x_0 is easily seen to be equivalent to the vanishing of the coefficients in each of the various derivative terms above. Solving this system equations then gives the sextupolar constitutive relation

$$J = D\left(6(\partial\rho)^4 + 4\rho^2\partial\rho\partial^3\rho + 3\rho^2\partial^2\rho\partial^2\rho - 12\rho\partial^2\rho(\partial\rho)^2 - \rho^3\partial^4\rho\right). \tag{233}$$

The correctness of this bad boy can be verified in the usual way by taking a gradient expansion of the microscopic current operator, which for the four-body process written above is

$$J_i = \rho_{i-2}^2\rho_{i+3}^2 - \rho_{i-3}\rho_i\rho_{i+1}\rho_{i+4}, \tag{234}$$

which when expanded gives the above relation with $D = 6$.

n-pole

By looking at the previous examples, we notice that they all conform to the pattern of

$$J = D\rho^{n+1}\partial^{n+1}\ln(\rho), \tag{235}$$

which certainly makes sense on account of the fact that $\rho(x)$ being an exponential of a degree n polynomial always yields a steady state. Nevertheless, the fact that the lower bound of $n + 1$ on the number of particles that participate in an n-pole conserving hopping process is not tight means that the equation written above might not hold for very large values of n (e.g. $n > 12$).

subsystem symmetries

The situation in higher dimensions is similar if we restrict our attention to maximal multipole groups: in this case a J with $n+1$ derivatives in 1d is replaced by an $n+1$ component vector $J^{a_1...a_{n+1}}$, with each derivative getting its own index. While we will not investigate non-maximal multipole groups in much detail, one extreme example of interest is the subsystem symmetric case, where $\int_{\mathbf{r}} r_a^n \rho_{\mathbf{r}}$ is conserved for *all* n, but $\int_{\mathbf{r}} r_a^n r_b^m \rho_{\mathbf{r}}$ is *not* conserved as long as $n, m > 0$. As an example, in 2d the minimal hopping process consistent with this symmetry group (at least on the square lattice) is the ring exchange term; it is easy to check that this produces the subsystem-symmetric diffusion equation

$$\partial_t\rho = D\partial_x\partial_y(\partial_x\rho\partial_y\rho - \rho\partial_x\partial_y\rho), \tag{236}$$

for which $\rho(\mathbf{r}) = e^{f(x)+g(y)}$ is a solution for *any* functions f, g. In keeping with this, any density configuration independent of either x or y is a steady state of the dynamics.

Adding noise

We now discuss a general framework for properly incorporating noise into the multipolar diffusion equations derived above. We will do this by making use of the generating functional approach, which allows us to derive (more general versions of) FDTs that set the standard deviation of the noise fields in terms of the diffusion constants. In the following we will consider multipole diffusion within the framework of a discrete-time Markov process with hopping rate r. We will also define the "jump" field $\hat{\Delta}_i(t) \equiv \hat{\rho}_i(t+\varepsilon) - \hat{\rho}_i(t)$, where the hats denote fields appearing in a spacetime path integral — expectation values of such fields will be denoted simply by dropping the hats. We also define the generating functional

$$W[\hat{\Gamma}] \equiv \langle e^{\int \hat{\Gamma}\hat{\Delta}} \rangle, \tag{237}$$

where the expectation value is over all spacetime trajectories of $\hat{\rho}_i(t)$ (weighted by the probability for each configuration to occur), and $\int \hat{\Gamma}\hat{\Delta}$ is shorthand for $\sum_t \sum_i \hat{\Gamma}_i(t)\hat{\Delta}_i(t)$. Functional derivatives of $\log W$ wrt $\hat{\Gamma}_i(t)$ can be used to generate connected correlation functions of the spacetime field $\partial_t\hat{\rho}_i$.

0-*pole moment: standard diffusion*

Let us first review how regular diffusion works. At a given timestep, $\hat{\Delta}_i(t)$ has a probability $zr\rho_i(t)$ of being -1 (here z is the coordination number of the lattice) and a $r\sum_{j\in\partial i}\rho_j(t)$ probability of being $+1$ (recall $\rho_i(t) = \langle\hat{\rho}_i(t)\rangle$). Thus in the $r \to 0$ continuum time limit, we obtain

$$\begin{aligned}
W[\hat{\Gamma}] &\approx \prod_{i,t}\left(1 + \frac{1}{2}r\sum_{j\in\partial i}(\rho_j(t)[e^{\hat{\Gamma}_i(t)-\hat{\Gamma}_j(t)} - 1] + \rho_i(t)[e^{-\hat{\Gamma}_i(t)+\hat{\Gamma}_j(t)} - 1]\right) \\
&\to \exp\left(r\int_{i,t}\sum_{j\in\partial i}\rho_j(t)(e^{\hat{\Gamma}_i(t)-\hat{\Gamma}_j(t)} - 1)\right),
\end{aligned} \tag{238}$$

where the -1s come from the possibility of no hopping events involving site i occuring, and the $1/2$ on the first line comes from double-couting each hopping process. Differentiating with respect to $\hat{\Gamma}$, we get

$$\frac{\delta\ln W[\hat{\Gamma}]}{\delta\hat{\Gamma}_j(t)} = r\sum_{k\in\partial j}\left(\rho_k(t)e^{\hat{\Gamma}_j(t)-\hat{\Gamma}_k(t)} - \rho_j(t)e^{\Gamma_k(t)-\Gamma_j(t)}\right). \tag{239}$$

Sending $\hat{\Gamma}_i(t) \to 0$, we then see that

$$\partial_t\rho_i = r\sum_{j\in\partial i}(\rho_j(t) - \rho_i(t)) \to D\partial_i^2\rho_i(t), \tag{240}$$

correctly reproducing the diffusion equation (letting $D \equiv ra^2$ with a the lattice spacing).

    The power of the generating functional approach is that it lets us understand how to generalize the diffusion equation to a Langenvin equation in a way that properly accounts

for the effects of noise. To see this, consider the second moment obtained by taking a functional derivative of (239):

$$\langle \partial_t \hat{\rho}_i \partial_{t'} \hat{\rho}_j \rangle_c = r \delta_{t,t'} \sum_{k \in \partial i} (\rho_j(t) + \rho_k(t))(\delta_{ij} - \delta_{ik}). \tag{241}$$

Note that this expression passes the sanity checks of vanishing when we sum over either i or j, as it must due to $\partial_t Q^{(0)} = 0$:

$$\sum_i \langle \partial_t \hat{\rho}_i \partial_{t'} \hat{\rho}_j \rangle_c = \sum_j \langle \partial_t \hat{\rho}_i \partial_{t'} \hat{\rho}_j \rangle_c = 0. \tag{242}$$

Therefore we know that $\langle \partial_t \hat{\rho}_i \partial_{t'} \hat{\rho}_j \rangle_c = \delta_{t,t'} \partial_i \partial_j \mathcal{O}$ for some operator $\mathcal{O}$ (here $\partial_i = \frac{\partial}{\partial x_i}$ and we are using notation appropriate for 1d, *n.b* i is a lattice site and not the label of a spatial direction—sorry). Taking the continuum limit and expanding in derivatives gives[29]

$$\langle \partial_t \hat{\rho}_i \partial_{t'} \hat{\rho}_j \rangle_c = \delta_{t,t'} D \partial_i \partial_j ([\rho_i + \rho_j] \delta_{ij}). \tag{244}$$

Therefore we may write the Langevin equation as

$$\partial_t \hat{\rho}_i = D \partial_i^2 \rho_i(t) + \partial_i \eta(t), \tag{245}$$

where the noise field η_i has autocorrelators

$$\langle \eta_i(t) \eta_j(t') \rangle_c = 2D \delta_{t,t'} \delta_{ij} \rho_i(t). \tag{246}$$

Thus we have essentially derived a FDT, since the fluctuations of the noise are seen to be determined by the diffusion constant and the average density. The fact that it is the derivative of the noise field that appears on the RHS of the Langevin equation (rather than the noise field itself) is of course due to charge conservation.

It is rather unsavory that the standard deviation of the noise is explicitly dependent on the density, although physically this makes sense as absolute particle number fluctuations will be higher in regions with higher density. One might try to get around this by writing the noise term in the Langevin equation as $\partial_i(\sqrt{2D\rho_i}\widetilde{\eta}(t))$ where $\langle \widetilde{\eta}_i(t)\widetilde{\eta}_j(t') \rangle_c = \delta_{t,t'}\delta_{i,j}$, but this only works if one then writes $\partial_i \partial_j (\sqrt{\rho_i \rho_j} \delta_{ij}) \overset{?!}{=} \partial_i \partial_j (\rho_i \delta_{ij})$.

An application of this Langevin equation is the calculation of the structure factor that governs the spectrum of fluctuations about the equilibrium steady state. Write $\rho(x,t) = \rho^{\text{eq}}(x) + \gamma(x,t)$, where $\rho^{\text{eq}}(x)$ is a steady-state. Then in Fourier space, the Langevin equation is

$$\gamma = \frac{ik}{i\omega + Dk^2}\eta. \tag{247}$$

Now

$$\langle \eta_{k\omega} \eta_{q\nu} \rangle_c = 2D \delta_{\omega,-\nu} \rho^{\text{eq}}_{k+q}. \tag{248}$$

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[29]In higher dimensions, this equation is written in more canonical notation as

$$\langle \partial_t \hat{\rho}_{\mathbf{r}} \partial_{t'} \hat{\rho}_{\mathbf{r'}} \rangle_c = \delta_{t,t'} D \sum_{a=1}^d \frac{\partial}{\partial r^a} \frac{\partial}{\partial r'^a} ([\rho_i + \rho_j]\delta_{ij}). \tag{243}$$

We will assume that $\rho^{\text{eq}}(x)$ varies on scales much longer than the relevant fluctuations in η, so that ρ^{eq}_{k+q} can be approximated locally as $\rho^{\text{eq}}(x)\delta_{k,-q}$. Then the local correlation functions of γ read

$$\langle\gamma_{k\omega}\gamma^*_{k\omega}\rangle_c = 2D\rho^{\text{eq}}(x)\frac{k^2}{\omega^2 + D^2 k^4}. \tag{249}$$

In particular, the equal-time correlators yield the structure factor

$$S(k) \equiv \langle\gamma_k(t)\gamma^*_k(t)\rangle_c = \rho^{\text{eq}}(x), \tag{250}$$

which is independent of k.

dipolar diffusion

Based on the analysis for regular diffusion, it is tempting to guess that noise can be added to the dipolar diffusion equation simply by adding a term $\partial_i^2 \eta(t)$ where now $\eta_i(t)$ has auto-correlators equal to $2D\delta_{t,t'}\delta_{i,j}\rho_i^2(t)$. We will see that this is fact correct.

Specializing to 1d for simplicity, consider the $101 \leftrightarrow 020$ dipolar diffusion process generated by taking $\mathbf{a} = (1,3)$, $\mathbf{b} = (1,1)$. Following the same steps as in the analysis for regular diffusion (and being a bit more laconic now that we know how things work), we find

$$\ln W[\hat{\Gamma}] = r \int_{i,t} \left(\rho_{i-1}(t)\rho_{i+1}(t)(e^{-\partial_i^2 \Gamma_i(t)} - 1) + \rho_i(t)^2(e^{\partial_i^2 \Gamma_i(t)} - 1) \right). \tag{251}$$

Taking one functional derivative and sending $\hat{\Gamma} \to 0$ gives

$$\partial_t \rho_i = \partial_i^2 \frac{\delta \ln W[\hat{\Gamma}]}{\delta \partial_i^2 \Gamma_i(t)} = D\partial_i^2(\rho_i^2(t) - \rho_{i-1}(t)\rho_{i+1}(t)), \tag{252}$$

with the the expression in parenthesis correctly becoming $(\partial\rho)^2 - \rho\partial^2\rho$ in the continuum limit.

Taking two functional derivatives on the other hand gives

$$\langle\partial_t\rho_i \partial_{t'}\rho_j\rangle_c = 2D\delta_{t,t'}\partial_i^2\partial_j^2(\rho_i(t)^2\delta_{i,j}), \tag{253}$$

where we have dropped higher derivatives of the density. Note that we correctly have $\sum_i i^m \langle\partial_t\rho_i \partial_{t'}\rho_j\rangle_c = \sum_j j^m \langle\partial_t\rho_i \partial_{t'}\rho_j\rangle_c$ for $m = 0, 1, 2$. We also see that we may thus write the Langevin equation as

$$\partial_t\rho = D\partial^2((\partial\rho)^2 - \rho\partial^2\rho) + \partial^2\eta, \tag{254}$$

where now the noise field has autocorrelators

$$\langle\eta_i(t)\eta_j(t')\rangle_c = 2D\delta_{t,t'}\delta_{i,j}\rho_i^2(t). \tag{255}$$

As before, we can use the Langevin equation to derive the structure factor for the density fluctuations about local equilibirum. We again write $\rho(x,t) = \rho^{\text{eq}}(x) + \gamma(x,t)$, but the nonlinearity of the dipolar diffusion equation forces us to make an additional assumption, namely that gradients of ρ^{eq} are all much smaller than ρ^{eq} itself. Even though ρ^{eq} is an exponential function of position in the present case, the length scale of this exponential is

thermodynamically large as long as x_{cm} is. So as long as the center of mass $x_{\mathrm{cm}} = \omega(L^0)$, derivatives of ρ^{eq} can indeed be dropped. Then the linearized Langevin equation for γ reads

$$\gamma = -\frac{k^2}{i\omega + \widetilde{D}k^4}\eta, \tag{256}$$

where the effective subdiffusion constant $\widetilde{D} \equiv D\rho^{\mathrm{eq}}(x)$. Again assuming that ρ^{eq} is slowly varying to compute the η correators, we obtain

$$\langle \gamma_{k\omega}\gamma_{k\omega}^* \rangle_c = 2\widetilde{D}\rho^{\mathrm{eq}}(x)\frac{k^4}{\omega^2 + (\widetilde{D}k^4)^2}. \tag{257}$$

Thus the structure factor is in fact exactly the same as in the case of conventional diffusion, viz.

$$S(k) = \rho^{\mathrm{eq}}(x). \tag{258}$$

quantum multipolar diffusion

It is straightforward to understand the equilibirum states that occur for multipole-conserving quantum particles; all one has to do is replace classical distinguishable particles with bosons or fermions, as appropriate. For simplicity we will mostly consider dipole conserving particles in 1d box, $x \in [-L/2, L/2]$. As before we will let $N \equiv Q^{(0)}$, $x_{\mathrm{cm}} \equiv Q^{(1)}/N$.

fermions

Denote the Lagrange multiplier for dipole moment as β, and the multiplier for total charge as $-\beta\mu$. Then

$$N = \int_{-L/2}^{L/2} \frac{dx}{e^{\beta(x-\mu)} + 1} \implies \mu = \frac{1}{\beta}\ln\left(\frac{e^{\beta L/2} - e^{\beta N}}{e^{\beta N} - e^{\beta L}}\right). \tag{259}$$

The analagous equation for x_{cm} is rather complicated, and the explicit expression involves polylogarithms. Thus we specify to the simple case of half-filling, where $N = L/2$. This forces $\mu = 0$, with x_{cm} then determining the effective "temperature": high T corresponds to $x_{\mathrm{cm}} = 0$, while $T = 0^+$ corresponds to $x_{\mathrm{cm}} = -L/4$ and $T = 0^-$ has $x_{\mathrm{cm}} = +L/4$.

Various cute things are possible when we consider higher multipole moments. For example, consider an infinite system with quadrupole moment conservation. Then the equilibrium state is a "Fermi surface" in real space: taking $Q_a^{(2)}$ to be independent of a for simplicity (so that the FS is spherical), the FS "radius" is then roughly fixed by the total number of particles, while the temperature is determined by the size of $Q^{(2)}$.

bosons

Now we discuss the bosonic case. First consider a dipole conserving system in finite box of size $[0, L]^d$. The interesting question to ask is when a "real space BEC" occurs, with all of the bosons spontaneously condensing at a given spatial point.

A BEC will occur when $\mu \to 0$, which means (assuming equal dipole moments along all spatial directions for simplicity)

$$N = \int_{\mathbb{R}^d} \frac{d^d r}{e^{\beta_* \sum_a r_a} - 1} \implies T_* = \left(N^{-1} \int_0^{\beta_* L} \frac{d^d r}{e^{\sum_a r_a} - 1} \right)^{-1/d}. \tag{260}$$

The integral on the RHS has a UV divergence (in the conventional Bose gas context for BECs, the role of position is swapped with that of momentum, and it is instead an IR divergence) when $d = 1$, but is finite when $d > 1$. Assuming that $\beta_* L = \Omega(L^0)$, in $d > 1$ we then have

$$T_* \propto N^{1/d}, \tag{261}$$

so that our assumption $\beta_* L = \Omega(L^0)$ is satisfied if we are at fillings $N/L^d = O(L^0)$.

We now ask to what dipole moment this temperature corresponds to. This is determined by

$$Q^{(1)} = T_*^{d+1} \int_0^{\beta_* L} d^d r \frac{r}{e^{\sum_a r_a} - 1}, \tag{262}$$

with the integral UV-finite in all dimensions. Thus

$$T_* \propto (Q^{(1)})^{1/(1+d)}, \tag{263}$$

and so the transition occurs when the center of mass $x_{\text{cm}} = D/N$ satisfies

$$x_{\text{cm}} \leq C N^{1/d} \tag{264}$$

where here and below C will be used to denote unimportant numerical constants. Thus the transition occurs when x_{cm} is thermodynamically large

Consider now a quadrupole conserving system in infinite volume. The condition for a BEC to occur reads

$$N = \int \frac{d^d r}{e^{\beta_* r^2} - 1} \implies \beta_*^{d/2} N = S^{(d-1)} \int_0^\infty dr \frac{r^{d-1}}{e^{r^2} - 1}. \tag{265}$$

The integral on the RHS is finite if $d > 2$, for $d \leq 2$ it has a UV divergence. When $d > 2$ we thus get a critical temperature that goes as

$$T_* \propto N^{2/d}. \tag{266}$$

More meaningful is the quadrupole moment to which this temperature corresponds. Assuming rotational invariance for simplicity, this quadrupole moment is

$$Q_a^{(2)} = \frac{1}{d} \int dr \frac{r^{d+1}}{e^{\beta r^2} - 1} = C T_*^{1+d/2}. \tag{267}$$

Thus using the above scaling for T_*, we see that a BEC forms when the quadrupole moment

$$Q_a^{(2)} \leq C N^{1+2/d}, \tag{268}$$

which is parametrically much smaller than its maximum value $Q^{(2)}_{a,max} \propto N^{2+d}$. The standard deviation of the particles is $\sigma = \sqrt{N^{-1}Q^{(2)}}$, so that a BEC forms when the standard deviation satisfies

$$\sigma \leq CN^{1/d}, \tag{269}$$

which has the same scaling as the critical center of mass in the dipole conserving case. In fact this is not a conincidence, and it is easy to check that the condition for a BEC to form in general is that

$$l^{(n)}_* = O(N^{1/d}), \qquad d > n, \qquad N = O(L^d), \tag{270}$$

where

$$l^{(n)}_* \equiv (Q^{(n)}/N)^{1/n}. \tag{271}$$

Gibbs ensemble from KMS

Today's entry is very short: we will show that the Gibbs ensemble can be derived from the KMS condition (away from phase transition points, and assuming no SSB). This provides another way to motivate the Boltzmann weights, distinct from the maximization of S argument.

First let us discuss why we would like a way of singling out the Gibbs state from other possible thermal density matrices. What requirements should we have of a thermal density matrix ρ? First, it must have $\text{Tr}[\rho] = 1$. Second, it must correctly reproduce expectation values of all thermodynamic quantities, e.g. $\text{Tr}[\rho H] = \langle E \rangle$.[30] Furthermore if we to be in equilibrium, with thermal expectation values independent of time, we need $e^{-iHt}\rho e^{iHt} = \rho$ for all t, which tells us that $\rho = \rho(H)$. The Gibbs state certainly fits the bill so far. But in fact the actual functional form of $\rho(H)$ isn't uniquely singled out by thermodynamics: we really just need that $\text{Tr}[\rho(H)] = 1$ and $\text{Tr}[\rho(H)H] = \langle E \rangle$, but these conditions can be satisfied by multiple density matrices, corresponding to different possible thermodynamic ensembles. For example, we could also use $\rho(H) = \Pi_{\langle E \rangle}$, where $\Pi_{\langle E \rangle}$ has support only on a small energy window around $\langle E \rangle$ (or right at $\langle E \rangle$ in the TDL), on which it is constant. This choice is of course the microcanonical ensemble, and looks very different from $e^{-\beta H}/Z$

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[30]In what follows we will make the assumption that there are only a finite number of conserved quantities to keep track of, and that they are all "explicit" variables like E, N, V, etc. We are therefore assuming ETH holds, with the system being non-integrable.

as a matrix. The heuristic way of understanding why these ensembles are equivalent in the TDL is to recognize that fluctuations about the expectation value of quantities whose expectation values are imposed with Lagrange multipliers are vanishingly small in the TDL. For example, consider the canonical ensemble. We claim that $\sigma_E/\langle E\rangle \sim 1/\sqrt{N} \to 0$ in the TDL. Intuitively, this just comes from the CLT: we can break the system up into $\sim N$ chunks with constant energy density, which all more or less behave independently, and considering the probability distribution for the energy of the sum of these blocks gives us the result. Alternatively, we can argue that since the specific heat $C_V = \partial_T\langle E\rangle \propto \langle E^2\rangle - \langle E\rangle^2$ and $\langle E\rangle$ are both extensive, we have $C_V/\langle E\rangle^2 \propto \sigma_E^2/\langle E\rangle^2 \propto 1/N$.

Now for the KMS condition. While the KMS condition is often derived assuming a density matrix following the Gibbsian form, one could take the view that this reasoning is rather backwards from a formal point of view, and view the KMS condition as more fundamental. This perspective is nice because it singles out the Gibbs state over the states for other ensembles (e.g. the microcanonical ensemble), resolving the ambiguity mentioned above.

The KMS condition is that for any two operators A, B, we have

$$\mathrm{Tr}[\rho_\beta A\alpha_{t+i\beta}(B)] = \mathrm{Tr}[\rho_\beta\alpha_t(B)A], \tag{272}$$

where ρ_β is the density matrix and $\alpha_z(\mathcal{O}) = e^{izH}\mathcal{O}e^{-izH}$ is the time evolution operator extended to the domain $\mathbb{R} \times iS_\beta^1$. Note that if we take B to commute with H so that it is invariant under α_t (i.e. $B = B(H)$), then the KMS condition tells us that $[\rho_\beta, B(H)] = 0$, which re-derives the fact that $\rho_\beta = \rho_\beta(H)$.

We now choose A and B to be the projectors $A = |n\rangle\langle m|, B = A^T$, where $|n\rangle$ is the nth eigenstate of H. The KMS condition then reads

$$[\rho_\beta]_{nn}e^{it(E_m-E_n)}e^{\beta(E_n-E_m)} = [\rho_\beta]_{mm}e^{it(E_m-E_n)}, \tag{273}$$

which in order to hold must mean that $[\rho_\beta]_{nn} \propto e^{-\beta E_n}$. Since we know that ρ_β can only be a function of H, we know that ρ_β must be diagonal in the energy eigenbasis. Therefore the KMS condition (and $\mathrm{Tr}[\rho_\beta] = 1$) indeed imply that $\rho = e^{-\beta H}/Z$.

Note that in the presence of more conserved thermodynamic quantities besides just energy, the correct density matrix is obtained by adding the generators of these symmetries into the automorphism α_t. For example, in the case of $U(1)$ particle number conservation, α_t instead becomes (we would often just relabel $H - \mu N$ as H; this is the AQFT notation)

$$\alpha_z(\mathcal{O}) = e^{i(H-\mu N)z}\mathcal{O}e^{-i(H-\mu N)z} \tag{274}$$

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Gibbs trivialities

Today's entry is devoted to proofs of a few trivial facts about Gibbs distributions.

classical case

Consider a classical system with state space Ω and energy $E(x), x \in \Omega$. Define the Gibbs distribution

$$g_T(x) \equiv \frac{e^{-E(x)/T}}{\sum_{y \in \Omega} e^{-E(y)/T}}, \tag{275}$$

and for a probability distribution p, let the free energy be defined as

$$F(p) \equiv \mathbb{E}_{x \sim p}[E(x)] - TH(p). \tag{276}$$

We claim that $g_T(x)$ minimizes $F(p)$. To see this, we simply functionally differentiate $F(p) - \lambda p$, where λ is a Lagrange multipler ensuring $\sum_{x \in \Omega} p(x) = 1$ and allowing the variational derivative to be taken in an unconstrained way. Then

$$\frac{\delta F}{\delta p(x)} = E(x) + T \ln(p(x)) - T - \lambda. \tag{277}$$

Setting this to zero and solving for $p(x)$ indeed gives $g_T(x)$, after choosing λ to account for normalization.

quantum case

Define the Gibbs state

$$\gamma_T \equiv \frac{e^{-H/T}}{\text{Tr}[e^{-H/T}]} \tag{278}$$

and the free energy

$$F(\rho) \equiv \text{Tr}[H\rho] - TS(\rho). \tag{279}$$

We claim that γ_T minimizes $F(\rho)$. One way of doing this is as follows. Let $H = U_H^\dagger \Lambda_H U_H$, and $\rho = U_\rho^\dagger \Lambda_\rho U_\rho$, with U_α unitary and Λ_α diagonal. Then

$$F(\rho) = \text{Tr}[\Lambda_H V^\dagger \Lambda_\rho V] - TS(\Lambda_\rho), \tag{280}$$

where $V = U_\rho U_H^\dagger$. Letting $\boldsymbol{\lambda}_\alpha$ be the vector of diagonal entries of Λ_α, the first term is

$$\text{Tr}[\Lambda_H V^\dagger \Lambda_\rho V] = \boldsymbol{\lambda}_H^T M \boldsymbol{\lambda}_\rho, \tag{281}$$

where $M = \sum_{i,j} |V_{ij}|^2 |i\rangle\langle j|$. The unitarity of V implies the stochasticity of M. $F(\rho)$ will be minimized when M is an extremal point in the set of stochastic matrices, viz. when M

is a permutation (which basically means that H and ρ can be simultaneously diagonalized, generically implying that $\rho = \rho(H)$). But after doing so, we can replace λ_H^i with $E(i)$ and λ_ρ^i with $\rho(i)$, and the problem becomes equivalent to the classical case.

We can also just directly take the variational derivative. To linear order in the variation $\delta\rho$, this gives

$$\delta F = \text{Tr}[\delta\rho(H - \lambda\mathbf{1}) + T\delta\rho\ln(\rho) + T\rho\int_0^\infty dz \frac{1}{\rho + z\mathbf{1}}\delta\rho\frac{1}{\rho + z\mathbf{1}}], \tag{282}$$

where λ enforces $\text{Tr}[\rho] = 1$ and we have used

$$\ln(A + B) = \ln(A) + \int_0^\infty dz \frac{1}{A + z\mathbf{1}}B\frac{1}{A + B + z\mathbf{1}} \tag{283}$$

with $A = \rho, B = \delta\rho$, with going to linear order allowing us to drop the B in the denominator. By the cyclicity of the trace and the fact that ρ commutes with $(\rho + z\mathbf{1})^{-1}$, we can re-arrange the last term so that it becomes $\int_{\mathbb{R}^+}\rho\frac{dz}{(\rho + z\mathbf{1})^2}$. But this is actually just equal to $\mathbf{1}$, as one can see by evaluating the integral in ρ's eigenbasis. Thus we just get

$$\delta F = \text{Tr}[\delta\rho(H - \lambda\mathbf{1} + T\ln(\rho))]. \tag{284}$$

Since this must vanish for all $\delta\rho$ when F is extremized, ρ must be equal to γ_T.

convexity

Since $S(\rho)$ and $H(p)$ are convex and $\text{Tr}[H\rho], \mathbb{E}[E]$ are linear, both classical and quantum free energies are concave. Thus g_T and γ_T are in fact global (not just local) minima of F.

relative entropy

For any ρ, consider the difference $F(\rho) - F(\gamma_T)$. Using $H = -T(\ln(\gamma_T) + \ln Z)$, we have

$$\begin{aligned}
F(\rho) - F(\gamma_T) &= T\text{Tr}[-(\ln(\gamma_T) + \ln Z)(\rho - \gamma_T) - S(\rho) + S(\gamma_T)] \\
&= T\text{Tr}[-\rho\ln\gamma_T + \gamma_T\ln\gamma_T + \rho\ln\rho - \gamma_T\ln\gamma_T] \\
&= TD(\rho||\gamma_T),
\end{aligned} \tag{285}$$

with the fact that $D(\rho||\sigma) \geq 0$ with equality iff $\rho = \sigma$ thus explaining why $F(\rho)$ has a global minimum at $\rho = \gamma_T$. This means that even approximate minimizers of F are close to γ_T, which is formalized using the quantum Pinsker inequality $D(\rho||\sigma) \geq \frac{1}{2}||\rho - \sigma||_1^2$ (note that here we are defining $D(\rho||\sigma)$ in terms of natural logs, hence there is no $1/\ln 2$):

$$F(\rho) \geq \frac{T}{2}||\rho - \gamma_T||_1^2. \tag{286}$$

Random energy model

This diary is a concatenation and elaboration on a couple exercises in Mezard's book on computation and physics. The goal is to familiarize ourselves with a family of random energy models and their phase transitions.

edit: This problem has been removed to serve as a physics benchmark question for evaluating LLMs.

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