Diffusion Recap

\# Left mover = L

\# Right " = R

$n = R - L$ = total displacmt

$N = R + L$ = total # of steps

$$\text{Prob}(R) = {}^{N}C_{R}\, p^{R} q^{L} \qquad R = \frac{N+n}{2} \qquad L = \frac{N-n}{2}$$

Dist $x = na$ time $t = N\tau$

Apply Stirling to $\dfrac{N!}{\left(\frac{N+n}{2}\right)!\left(\frac{N-n}{2}\right)!} p^{\frac{N+n}{2}} q^{\frac{N-n}{2}}$ and get a gaussian distrn peaked around $n = (p-q)N$

Alternatively $n = \sum_{i=1}^{N} d_i$ $\quad d_i = \begin{matrix} +1 \leftarrow \text{prob } p \\ -1 \leftarrow \text{prob } q \end{matrix}$

Each d_i is indept. $\langle d_i \rangle = p - q$

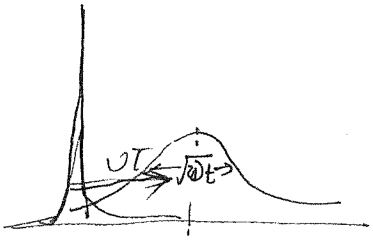
$$\text{Var}(d_i) = \langle d_i^2 \rangle - \langle d_i \rangle^2 = 1 - (p-q)^2 = 4pq$$

$x = na$ $\quad \langle x \rangle = (p-q)Na = \frac{(p-q)a}{\tau} t$

$$\text{Var}(x) = 4Npqa^2 = \frac{4pqa^2}{\tau} t$$

Call $\frac{(p-q)a}{\tau} = v \qquad \frac{2pqa^2}{\tau} = D$

$$P(x,t) \approx \frac{e^{-(x-vt)^2/4Dt}}{\sqrt{4\pi D t}}$$



Would like

A Continuum description of diffusion: $\nearrow$ Eqn for $x(t)$, $\searrow$ Eqn for $P(x,t)$

In practice, we are interested in situations where $\sqrt{2Dt} \sim vt$

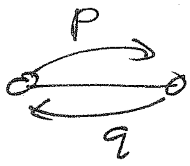
$\Rightarrow \sqrt{4pqn} \sim (p-q)n$. For large n, this means p-q is small.

Eqn for $P(x,t)$ [Fokker Planck Approach]

$$P(n,N+1) = p\,P(n-1,N) + q\,P(n+1,N)$$

Reorganize :

$$P(n,N+1) - P(n,N) = \left(p\,P(n-1,N) - q\,P(n,N)\right) - \left(p\,P(n,N) - q\,P(n+1,N)\right)$$

Note that 

$J_{n\,n+1}(N) = p\,P(n,N) - q\,P(n+1,N)$

is the current across the link $[n\ n+1]$

$$P(n,N+1) - P(n,N) = -\left[J_{n\,n+1}(N) - J_{n-1\,n}(N)\right]$$

Increase of prob = − div. of curret.

Def $p(x,t) = \frac{1}{a} P(x/a, t/\tau)$ $\quad j(x+\frac{a}{2},t) = \frac{1}{\tau} J_{\frac{x}{a}\,\frac{x}{a}+1}\left(\frac{t}{\tau}\right)$

$$a\left\{P(x,t+\tau) - P(x,t)\right\} = \tau\left\{j(x-\frac{a}{2}t) - j(x+\frac{a}{2},t)\right\}$$

Or $$\frac{\partial}{\partial t} p(x,t) = -\frac{\partial}{\partial x} j(x,t)$$

Conservation of probability!

However, to get the evolution of $p(x,t)$, we need $j(x,t)$ in terms of $p(x,t)$

$$J_{n\,n+1}(N) = p\,P(n,N) - q\,P(n+1,N) = \frac{p+q}{2}\left\{P(n,N) - P(n+1,N)\right\} + \frac{p-q}{2}\left\{P(n,N) + P(n+1,N)\right\}$$

$$= -\frac{1}{2}\left\{P(n+1,N) - P(n,N)\right\} + \frac{p-q}{2}\left\{P(n,N) + P(n+1,N)\right\}$$

$$j\left(x+\tfrac{a}{2},t\right) = \frac{1}{\tau} J_{\frac{x}{a}\,\frac{x}{a}+1}\left(\frac{t}{\tau}\right)$$

$$= -\frac{1}{2\tau}\, a\left(p(x+a,t) - p(x,t)\right) + \frac{(p-q)a}{\tau}\, \frac{p(x,t)+p(x+a,t)}{2}$$

$$= -\frac{a^2}{2\tau}\frac{\partial}{\partial x} P\left(x+\tfrac{a}{2},t\right) + \frac{(p-q)a}{\tau} P\left(x+\tfrac{a}{2},t\right) + o(a^4)$$

We will restrict ourselves to the situation when $p-q=\epsilon$ is small. $p=\frac{1+\epsilon}{2}$. $q=\frac{1-\epsilon}{2}$

$$D = \frac{2pq\,a^2}{\tau} = \frac{a^2}{2\tau}(1-\epsilon^2) \approx \frac{a^2}{2\tau}$$

$$\frac{\epsilon a}{\tau} = \frac{(p-q)a}{\tau} = v$$

$$j(x,t) = -D\frac{\partial}{\partial x}P(x,t) + v\,p(x,t)$$

$$\frac{\partial}{\partial t}p(x,t) = \underbrace{D\frac{\partial^2}{\partial x^2}P(x,t)}_{\text{Diffusion}} \underbrace{- v\frac{\partial}{\partial x}P(x,t)}_{\text{Drift.}}$$

Altenative description: Evolution of $x(t)$ [Langevin eqn]

$$x_{N+1} = x_N + d_{N+1}$$

$$\langle d_{N+1} \rangle = p - q = \epsilon$$

$$\frac{dx}{dt} = \frac{x(t+\tau) - x(t)}{\tau} = \frac{(n_{N+1} - n_N)a}{\tau} = \frac{a d_{N+1}}{\tau}$$

$$= \frac{a\epsilon}{\tau} + \underbrace{\frac{a}{\tau}\left[d_{N+1} - \langle d_{N+1} \rangle\right]}_{\eta(t)}$$

$$\frac{dx}{dt} = v + \eta(t)$$

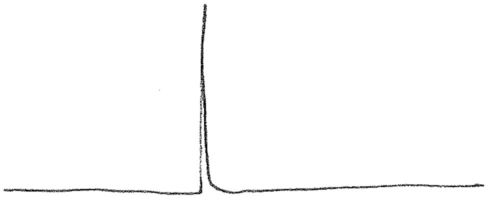
$\langle \eta(t)\ \eta(t') \rangle = 0$ when $t \neq t'$

$$\langle (\eta(t))^2 \rangle = \frac{a^2}{\tau^2} 4pq = \frac{2D}{\tau}$$

Note that $\left\langle \left(\int_{t_1}^{t_2} dt\, \eta(t) \right)^2 \right\rangle = \left\langle \left(\tau \sum_{N=t_1/a}^{t_2/a} \eta\left(\frac{N}{a}\right) \right)^2 \right\rangle$

$$= \tau^2 \sum_{t_1/a}^{t_2/a} \frac{2D}{\tau} = 2D\tau \left(\frac{t_2 - t_1}{\tau}\right)$$

Same if we assumed $\langle \eta(t)\, \eta(t') \rangle = 2D\,\delta(t-t')$



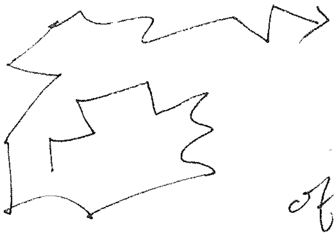
$$\int dx\, \delta(x) f(x) = f(0)$$

$$\frac{dx}{dt} = \vartheta + \eta(t)$$

Langevin Term

$$\langle \eta(t) \rangle = 0$$

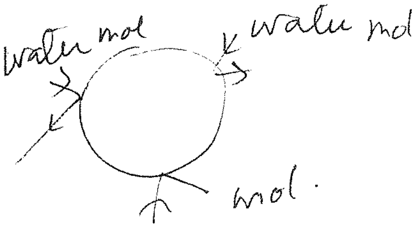
$$\langle \eta(t)\eta(t') \rangle = 2D\delta(t-t')$$

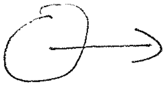


Brownian Motion motivated much of the research.

Brown 1827 (Pollen moving stochastically in water)

Physicist interested because this was an indirect verification of Atomicity. For example gas law $PV = Nk_BT$ gives us $R = Nk_B$ but not N or k_B separately





$$m\ddot{x} = \text{Force} = \text{External Force} + \overset{\text{Force}}{\text{moluculer collissons}}$$

$$m\ddot{x} = F_{ext} - \underset{\substack{\uparrow \\ \text{drag}}}{\gamma}\dot{x} + \underset{\substack{\uparrow \\ \text{random}}}{\xi}(t)$$

$m\ddot{x} + \gamma\dot{x} = F_{ext} + \xi(t)$. In the overdamped region, the inertial term could be thrown away

For example

$m\ddot{x} + \gamma\dot{x} = F$ Starting with $\dot{x} = 0$

Solves to give $\dot{x} = \frac{F}{\gamma}(1 - e^{-\frac{\gamma t}{m}})$

That means that within a time scale of $\frac{m}{\gamma}$, the $\dot{x}$ goes to $\frac{F}{\gamma}$. If that time is short compared to time scale of other changes we could ignore $m\ddot{x}$ term and have $\Gamma\dot{x} = F$

$$\gamma\dot{x} = F_{ext} + \xi(t)$$

viscosity, not noise

For a sphere in a fluid $F = 6\pi\eta a\dot{x}$

So $\gamma = 6\pi\eta a$

$\frac{1}{\gamma} = \mu$, mobility $\dot{x} = \mu F_{ext}$

Let $F_{ext}(x) = -\frac{\partial}{\partial x}V_{ext}(x)$

$$J(x) = -D\frac{\partial}{\partial x}p(x,t) + v(x)p(x,t)$$

$$= -D\frac{\partial}{\partial x}p(x,t) - \mu\frac{\partial V(x)}{\partial x}p(x,t)$$

Thermal Eqm $\Rightarrow$ $J(x) = 0$

$$\Rightarrow \frac{\partial}{\partial x}p(x,t) = -\frac{\mu}{D}\frac{\partial V_{ext}(x)}{\partial x}p(x,t)$$

But Stat. mech. says $P(x,t) = cst\ e^{-V_{ext}(x)/k_BT}$

$$\frac{1}{k_B T} = \frac{\mu}{D} \quad \text{or} \quad D = \mu k_B T$$

If we know μ & ~~B~~ measure D we could get k_B out.

Let us write Langevin eqn as

$$\dot{x} = \Gamma F + \Gamma \zeta = \Gamma F + \eta \,, \qquad \Gamma = \gamma^{-1} = \mu$$

where ~~[illegible]~~

$$\langle \eta(t) \rangle = 0$$

$$\langle \eta(t)\eta(t') \rangle = 2D\,\delta(t-t') \qquad = 2\Gamma k_B T\,\delta(t-t')$$

To gain some experience in how to use this think of a particle trapped in a harmonic potn.

$$V(x) = \frac{1}{2} K x^2 \qquad F = -Kx$$

$$\dot{x} = -\Gamma K x + \eta(t)$$

Let us call $\Gamma K = \frac{1}{\tau}$ $\quad \left[\Gamma = \frac{1}{\gamma},\ K = m\omega_0^2,\ \frac{1}{\tau} = \Gamma K = \frac{\omega_0^2 m}{\gamma} = \omega_0^2 \tau_{\text{Damping}}\right]$

$$\dot{x} + \frac{1}{\tau} x = \eta(t) \Rightarrow \frac{d}{dt}\left(e^{t/\tau} x(t)\right) = e^{t/\tau}\eta(t)$$

$$e^{t/\tau} x(t) = \int_{t_0}^{t} dt'\, e^{t'/\tau}\eta(t') + e^{t_0/\tau} x(t_0)$$

effect of initial condn

$$x(t) = e^{-(t-t_0)/\tau} x(T_0) + \int_{t_0}^{t} dt' \, e^{-(t-t')/\tau} \eta(t')$$

effect of thermal noise

Effect of initial condition dissappears as $t - t_0 \to \infty$

$$x(t) = \int_{-\infty}^{t} dt' \, e^{-(t-t')/\tau} \eta(t)$$

We can calculate correlators

$$\langle x(s)\, x(t+s) \rangle = \int_{-\infty}^{t+s} dt'' \int_{-\infty}^{s} dt' \, e^{-(t+s-t')/\tau - \frac{(s-t'')}{\tau}} \langle \eta(t')\eta(t'') \rangle \quad s > 0$$

$$= 2\Gamma k_B T \int_{-\infty}^{s} dt' \, e^{-(t+s-t')/\tau} e^{-(s-t')/\tau}$$

$$= e^{-t/\tau} \times 2\Gamma k_B T \int_{-\infty}^{s} dt' e^{-2(s-t')/\tau}$$

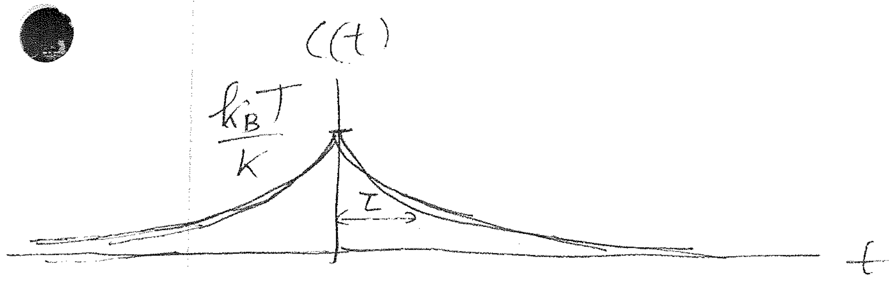
$$= \Gamma k_B T \tau \, e^{-t/\tau} = \Gamma k_B T \frac{1}{\Gamma K} e^{-t/\tau} = \frac{k_B T}{K} e^{-t/\tau}$$

Correlation function

$$C(t) = \langle x(s)\, x(t+s) \rangle = \frac{k_B T}{K} e^{-t/\tau}$$

Notethat when $t=0$ $\langle x(s)^2 \rangle = \frac{k_B T}{K} \Rightarrow \langle \frac{1}{2} K x^2 \rangle = \frac{1}{2} k_B T$

Equiparition.



Now let us figure out the response func.

$$\dot{x} = \Gamma\big(F(x) + \underset{\overset{\uparrow}{\text{perturbation}}}{f(t)}\big) + \eta(t)$$

$F(x) = -Kx$

$$x(t) = \int_{-\infty}^{t} e^{(t-t')/\tau}\big(\Gamma f(t') + \eta(t')\big)$$

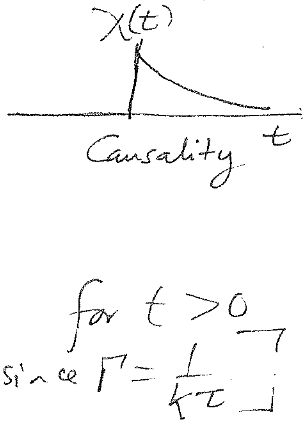
$$\langle x(t)\rangle = \Big\langle \Gamma\int_{-\infty}^{t} e^{-(t-t')/\tau} f(t')\Big\rangle + \Big\langle \underbrace{\int_{-\infty}^{t} dt' e^{-(t-t')/\tau}\eta(t')}_{\hookrightarrow\ 0}\Big\rangle$$

$$\langle x(t)\rangle = \Gamma\int_{-\infty}^{t} e^{-(t-t')/\tau} f(t')$$

Response function $\chi(t) = \Gamma e^{-t/\tau}$ [illegible] $t \geq 0$

$= 0$ $t \leq 0$

$$\langle x(t)\rangle = \int_{-\infty}^{\infty} \chi(t-t')\, f(t')\, dt'$$



Causality

Note that $C(t) = \frac{k_BT}{K} e^{-|t|/\tau}$

$\chi(t) = \frac{1}{K\tau} e^{-t/\tau}$ for $t > 0$

$\left[\text{since } \Gamma = \frac{1}{K\tau}\right]$

$\Rightarrow C'(t) = -k_BT\,\chi(t)$ for $t > 0$

This turns out to be general relationship
Called the fluctuation dissipation theorem
Define x st. $\langle x\rangle = 0$ at $f=0$

For small Uniform f. Eqm distrn is

$$P_f(x) = \frac{e^{-\beta(H_0(x) - f x)}}{Z(f)} = \frac{e^{-\beta H_0(x)}\left(1+\frac{fx}{k_BT}+\cdots\right)}{Z(0)\left(1+f\underset{=0}{\langle x\rangle}+\frac{1}{2}f^2\langle x^2\rangle\right)}$$

$$\approx P_0(x)\left(1+\frac{fx}{k_BT}+O(f^2)\right)$$

Lets ~~da~~ say f was on till time zero and then got turned off.

$$P(x,t) = \int dx' P(x, x'|t)\, P_f(x')$$

$$= \int dx' P(x, x'|t) \left\{ P_{0}(x') + \frac{fx'}{k_BT} P_0(x') + O(f^2) \right]$$

$$\langle x(t)\rangle = \int dx\, x\, P(x,t) = \int dx\, dx'\, P(x, x'|t)\, P_0(x')\, x\, x' \frac{f}{k_BT}$$

$$= \frac{1}{k_BT} f \langle x(t)\, x(0)\rangle_{f=0}$$

$$= \frac{f}{k_BT}\, C(t)$$

However $\langle x(t)\rangle = f\int_{-\infty}^{0} dt' \chi(t-t')$

$$\int_{-\infty}^{0} dt'\, \chi(t-t') = \frac{C(t)}{k_BT}$$

$$C'(t) = k_B T \int_{-\infty}^{0} \chi'(t-t')\,dt'$$

$$= -k_B T \left[\chi(t-t')\right]_{t=-\infty}^{t'=0}$$

$$= -k_B T \chi(t)$$

assuming $\chi(t) \to 0$ as $t \to \infty$

This just says response function and correlation fnc. are ~~as~~ related. for examp.

$$C(0) = -\int_0^\infty C'(t)\,dt \qquad (\text{assuming } C(\infty) = 0)$$

$$= k_B T \int_0^\infty \chi(t)\,dt = k_B T \chi$$

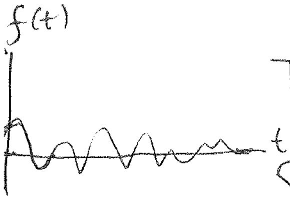
Where χ is the response to a constant perturbation f.

$$\langle x \rangle = \frac{\int_x e^{-\beta H_0(x) + \beta f x}\, x}{\int_x e^{-\beta H_0(x) + \beta f x}} = \frac{\int_x e^{-\beta H(x)}\, x + \beta f \int_x x^2 e^{-\beta H_0(x)}}{\int e^{-\beta H_0(x)} + O(f^2)}$$

$$= \frac{0 + \beta f \langle x^2 \rangle}{1 + O(f^2)}.$$

$$\langle x \rangle_f = \frac{\langle x^2 \rangle_{f=0}}{k_B T} \times f \qquad \chi = \frac{\langle x^2 \rangle_0}{k_B T}$$

$$\chi = \frac{C(0)}{k_B T}$$



What has it got to do with dissipation?
That is better seen in the frequency space

Suppose we drive the system with some transient force $f(t) = \frac{1}{2\pi} \int d\omega\, \hat{f}(\omega) e^{-i\omega t}$

Work done on the system is $\int dW = \int f dx$
$= \int_{-\infty}^{\infty} f \dot{x}\, dt = -\int dt\, \dot{f}(t)\, x(t)$

The average work done $\langle W \rangle = -\int dt\, \dot{f}(t) \langle x(t) \rangle$

$$= -\int dt dt' \dot{f}(t)\, \chi(t-t')\, f(t')$$

$$= \frac{i}{(2\pi)^2} \int d\omega\, \omega\, \hat{f}(\omega)\, \hat{f}(\omega') \int dt dt' e^{-i(\omega t + \omega' t')} \chi(t-t')$$

Call $t - t' = s$

$$\int dt dt' e^{-i(\omega t + \omega' t')} \chi(t-t') = \int ds\, \chi(s) e^{-i\omega s} \int dt' e^{-i(\omega+\omega')t}$$

$$= \int ds\, \chi(s) e^{-i\omega s}\, 2\pi\, \delta(\omega+\omega')$$

$$= 2\pi\, \delta(\omega+\omega')\, \hat{\chi}(-\omega)$$

$$\langle W \rangle = \frac{i}{(2\pi)} \int d\omega d\omega'\, \delta(\omega+\omega')\, \omega \hat{f}(\omega)\, \chi(-\omega)\, \hat{f}(\omega')$$

$$= \frac{i}{2\pi} \int d\omega\, \omega \hat{f}(\omega) \chi(-\omega) \hat{f}(-\omega) = -\frac{i}{2\pi} \int d\omega\, \omega\, \chi(\omega)\, |\hat{f}(\omega)|^2 \quad (\omega \to -\omega)$$

Since $f(t)$ is real
$\hat{f}(\omega) = \int dt f(t) e^{i\omega t}$ has the property $\hat{f}(-\omega) = \hat{f}(\omega)^*$

$|\hat{f}(\omega)|^2 = \hat{f}(\omega)\hat{f}(-\omega) = |\hat{f}(-\omega)|^2$ is an even function of ω

$$\hat{\chi}(\omega) = \int_{-\infty}^{\infty} dt\, \chi(t) e^{i\omega t} = \int_{-\infty}^{\infty} dt\, \chi(t)\cos\omega t + i\int_{-\infty}^{\infty} dt\, \chi(t)\sin\omega t$$

$$\underset{\substack{\uparrow \\ \text{even in } \omega}}{\chi'(\omega)} + i\, \underset{\substack{\uparrow \\ \text{odd in } \omega}}{\chi''(\omega)}$$

$$\langle W \rangle = -\frac{i}{2\pi}\int d\omega\, \omega\left(\chi'(\omega) + i\chi''(\omega)\right)|\hat{f}(\omega)|^2$$

$$= -\frac{i}{2\pi}\int d\omega\, \underbrace{\omega\,\chi'(\omega)\,|\hat{f}(\omega)|^2}_{\substack{\text{odd fnc} \\ \text{of } \omega \\ \text{integral vanishes}}} + \frac{1}{2\pi}\int d\omega\, \underbrace{\omega\,\chi''(\omega)\,|\hat{f}(\omega)|^2}_{\substack{\text{even fnc} \\ \text{of } \omega}}$$

$\langle W \rangle$ is work done on the system that gets dissipated by interaction with the bath, since the average energy before and long time after the application of force remains the same.

So dissipated energy $= \frac{1}{2\pi}\int d\omega\, \underbrace{\omega\,\chi''(\omega)}\,|\hat{f}(\omega)|^2$

decides how much dissipation happens in a particular freq.

Now let us write the eqn $C'(t) = -k_B T\,\chi(t)$ for $t > 0$

in Fourier space

Even in t   odd in t   one sided

$$C'(t) = -k_BT\left[\chi(t)-\chi(-t)\right] \quad \text{for all } t.$$

Fourier

$$-i\omega\hat{C}(\omega) = -k_BT\Big[\underbrace{\hat{\chi}(\omega)}_{\chi'(\omega)+i\chi''(\omega)} - \underbrace{\hat{\chi}(-\omega)}_{\chi'(\omega)-i\chi''(\omega)}\Big] = -2ik_BT\,\chi''(\omega)$$

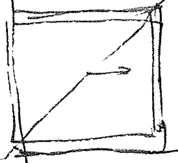
$$\hat{C}(\omega) = 2k_BT\,\frac{\chi''(\omega)}{\omega}$$

note that $\omega\chi''(\omega)$ is related to dissip.n

$\hat{C}(\omega)$ is related to the spectral density of fluctuations

$$\hat{x}(\omega) = \frac{1}{\sqrt{T}}\int_0^T d\omega\, e^{i\omega t}\, x(t)$$

$$\langle|\hat{x}(\omega)|^2\rangle = \frac{1}{T}\int_0^T dt\int_0^T dt' \quad \langle x(t)\,x(t')\rangle e^{i\omega(t-t')}$$



$$= \frac{1}{T}\int_0^T dt\int_0^T dt'\, C(t-t') \approx \frac{1}{T}\int_0^T dt' \int ds\, C(s)e^{i\omega s} = \hat{C}(\omega)$$

when $T\to\infty$

$$\underset{\text{fluctuation in the } \omega \text{ component}}{\hat{C}(\omega)} = \overbrace{2k_BT}^{\text{Thermal strength}} \frac{(\omega\, \overset{\text{dissipation}}{\chi''(\omega)})}{\omega^2}$$

In our simple model with a harmonic oscillator

$$\hat{\chi}(\omega) = \frac{1}{K\tau}\int_0^\infty dt\, e^{-t/\tau} e^{i\omega t} = \frac{1}{K\tau}\,\frac{1}{-i\omega + 1/\tau}$$

$$= \frac{1}{K\tau}\,\frac{\frac{1}{\tau} + i\omega}{\omega^2 + \frac{1}{\tau^2}}$$

$$\chi'(\omega) = \frac{1}{K\tau}\,\frac{1/\tau}{\omega^2 + 1/\tau}$$

$$\chi''(\omega) = \frac{1}{K\tau}\,\frac{\omega}{\omega^2 + \frac{1}{\tau^2}}$$

$$\hat{C}(\omega) = \frac{k_BT}{K}\int_{-\infty}^{\infty} e^{-|t|/\tau} e^{i\omega t} = \frac{k_BT}{K}\left[\int_0^\infty dt\, e^{-t/\tau} e^{i\omega t} + \int_{-\infty}^0 dt\, e^{t/\tau} e^{i\omega t}\right]$$

$$= \frac{k_BT}{K}\left[\frac{1}{\frac{1}{\tau} - i\omega} + \frac{1}{\frac{1}{\tau} + i\omega}\right]$$

$$= \frac{2k_BT/K\tau}{\frac{1}{\tau^2} + \omega^2}$$

$$\int_0^\infty e^{-zt}\,dt = \frac{1}{z}$$

If $\mathrm{Re}\, z > 0$

$$= \frac{2k_BT}{\omega}\,\chi''(\omega)$$

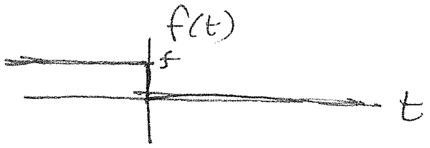
One way to think about it that fluctuation at a particular frequency is related to the response to thermal noise driving the system.

Retake on the derivn of fluctuation dissipation theorem with better notation

$\langle x(t) \rangle = ?$ for $t > 0$

when $f(t) = f$ for $t < 0$

$\qquad\quad = 0$ for $t > 0$



$$\langle x(t) \rangle = \int dx'\, x'\, P(x(t) = x')$$

$$= \int dx'\, x' \int P_{f=0}(x(t)=x' \,|\, x(0)=x)\, P_f(x(0)=x)\, dx$$

Note that $P_f(x(0)=x) = P_f^{eq}(x) = \dfrac{e^{-\beta(H(x)-fx)}}{\int dx'\, e^{-\beta[H(x')-fx']}}$

$$= \frac{e^{-\beta H(x)}\left(1+\frac{fx}{k_BT}+o(f^2)\right)}{\left(\int dx' e^{-\beta H(x')}\right)\left(1+\frac{f}{k_BT}\frac{\int dx' x' e^{-\beta H(x')}}{\int dx' e^{-\beta H(x')}}+o(f^2)\right)}$$

$$= \frac{e^{-\beta H(x)}}{\int dx' e^{-\beta H(x')}}\left(1+\frac{fx}{k_BT}+o(f^2)\right)$$

$$= P_{f=0}^{eq}(x) \text{ [redacted] } \left(1+\frac{fx}{k_BT}+o(f^2)\right)$$

$$\langle x(t) \rangle = \int dx'\, x'\, P_{f=0}(x(t)=x' \,|\, x(0)=x)\, P_{f=0}^{eq}(x)\left(1+\frac{fx}{k_BT}\right. \left. + o(f^2)\right)$$

$$= \int dx'\, x'\, P_{f=0}(x(t)=x' \,|\, x(0)=x)\, P_{f=0}^{eq}(x(0)=x) + \frac{f}{k_BT}\int dx'\, dx\, x'\, x\, P_{f=0}(x(t)=x' \,|\, x(0)=x)\, P_{f=0}^{eq}(x(0)=x)$$

$$+ o(f^2)$$

$= \int dx'\, x' \int dx\, P^{eq}_{f=0}(x(t)=x'$ [redacted] $\text{AND } x(0)=x)$

$+ \frac{f}{k_BT} \int dx' dx\ x'x\ P^{eq}_{f=0}(x(t)=x' \text{ AND } x(0)=x)$

$= \underbrace{\int dx'\, x'\ P^{eq}_{f=0}(x(t)=x')}_{\uparrow} + \frac{f}{k_BT} \langle x(t)\, x(0) \rangle_{f=0}$

[redacted] zero

$\langle x(t) \rangle = \frac{f}{k_BT} \left[C(t) \right]_{f=0}$

$\langle x(t) \rangle = \int_{-\infty}^{t} dt'\ \chi(t-t')$ [redacted] $f(t)$

$= f \int_{-\infty}^{0} dt'\ \chi(t-t')$

$C(t) =$ [redacted] $k_BT \int_{-\infty}^{0} dt'\ \chi(t-t')$

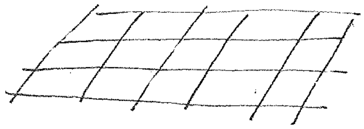
$C'(t) = k_BT \int_{-\infty}^{0} dt'\ \chi'(t-t')$

$= -k_BT \left[\chi(t-t') \right]_{t'=-\infty}^{t'=0}$

$= -k_BT\, \chi(t)$ $\blacksquare$ assuming $\chi(\infty)=0$

Dissipative dynamics for extended systems.

$$\dot{x} = -\Gamma \frac{\partial V}{\partial x} + \eta$$



$$\frac{d}{dt} m_i(t) = -\Gamma_{Lattice} \frac{\delta F[m]}{\delta m_i} + \eta_i$$

$$\langle \eta_i(t)\, \eta_j(t') \rangle = \overset{2k_BT}{\Gamma_{lattice}} \delta_{ij}\, \delta(t-t')$$

If we goto continuous limit with magnetization density $m(x,t) = \frac{m_i}{a^D}$ $\quad \Gamma = \frac{\Gamma_{Lattice}}{a^D}$ $\quad \eta(x,t) = \frac{\eta_i}{a^D}$

$$\frac{\partial}{\partial t} m(\vec{x},t) = -\Gamma \frac{\delta F[m]}{\delta m(\vec{x},t)} + \eta(\vec{x},t)$$

$$F[m] = \int d^Dx \left[\frac{1}{2}(\nabla m)^2 + \frac{r}{2} m^2 + \frac{u}{4} m^4 - hm\right]$$

$$\langle \eta(x,t)\, \eta(x',t') \rangle = 2\Gamma k_B T\, \delta(t-t')\, \delta^D(\vec{x}-\vec{x}')$$

$$\frac{\partial}{\partial t} m = -\Gamma\left(-\nabla^2 m + rm + um^3\right) + \eta$$

Ignoring the nonlinear term, as in Landau theory

$$\frac{\partial}{\partial t} m = \Gamma(\nabla^2 m - rm) + \eta$$

$M = \int d^Dx\, m$

If m is uniform and we ~~b~~ $\qquad \frac{\partial}{\partial t} M = -\Gamma r M + \int \eta\, d^Dx$

$\frac{\partial}{\partial t}\langle M \rangle = -\Gamma r \langle M \rangle$

$\langle M(t) \rangle = \langle M(0) \rangle e^{-\Gamma r t}$. We with call $\Gamma r = \frac{1}{\tau}$

Note that in Landau mean field theory, as we approach the critical point, r gets smaller and correlation length $\xi \sim \frac{1}{\sqrt{r_0}}$ diverges. The timescale τ diverges as well as $\frac{1}{\Gamma r_0}$.

$\tau \sim \xi^2$ in Mean field theory. More careful analysis shows $\tau \sim \xi^z$, z is the dynamic critical exponent $z = 2 + o(\epsilon^2)$ in ϵ expansion.

[Could go more explicit on $m_i \to m(x,t)$

$$F[\{m_i\}] = \sum_i \phi(m_i) + \sum_{\langle ij \rangle} K(m_i, m_j) + \cdots$$

$$= \sum_i a^D \frac{1}{a^D} \phi(m_i) + \cdots \simeq \int d^D x \, f(m)$$

$$f(m) = \frac{1}{a^D} \phi(m_i)$$

$$\dot{m}_i = -\Gamma_{Lattice} \phi'(m_i) + \cdots$$

e.g., $\phi(m_i) = \frac{1}{2} r_{lattice} m_i^2 + \cdots$

$$\dot{m}_i = -\Gamma_{Lattice} r_{lattice} m_i + \cdots$$

$\phi = a^D f$

$m_i = a^D m$

$$a^D \dot{m} = -\Gamma_{lattice} \frac{a^D}{a^D} \frac{\partial f}{\partial m}$$

$$\dot{m} = -\frac{\Gamma_{lattice}}{a^D} \frac{\partial f}{\partial m} = -\Gamma \frac{\partial f}{\partial m}$$

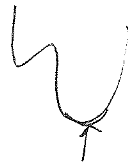
Hence $\Gamma = \frac{\Gamma_{lattice}}{a^D}$]

In fact, in Fourier space

$$\frac{\partial}{\partial t} \hat{m}(k) = -\Gamma(k^2+1)\hat{m}(k) + \eta(k) \Rightarrow \langle m_k(k) \rangle \sim e^{-\Gamma(k^2+1)t}$$

What we saw was that as we go closer and closer to the critical point, dynamics slows down. This is known a critical slowing down.

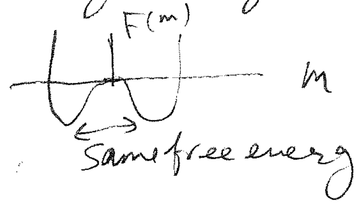
What about dynamics in the ordered phase: Small perturbations from genuine ordered state could be analyzed as in Landau Theory



Find the effective r around the nontrivial minimum. $\tau \sim \frac{1}{r_{eff}}$.

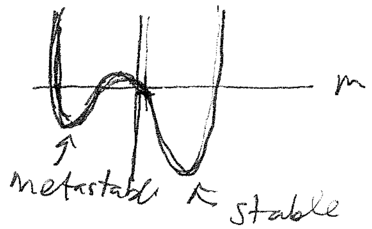
What if we need a large changes.

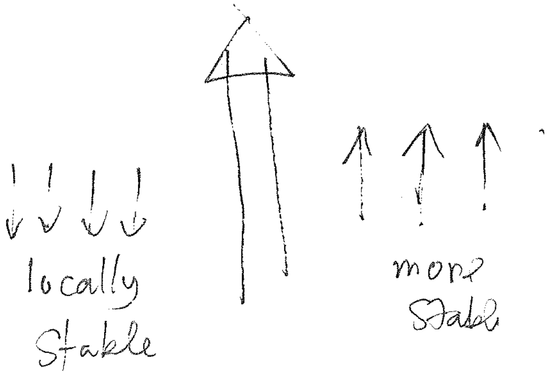
At $h = 0$

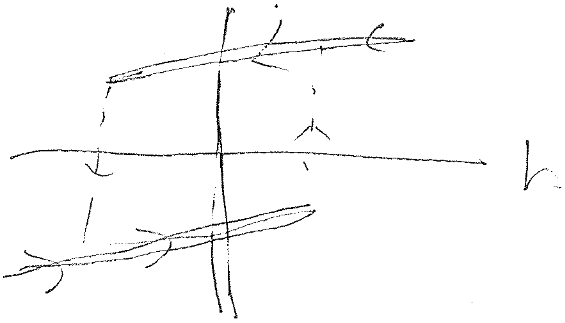


At $h \neq 0$

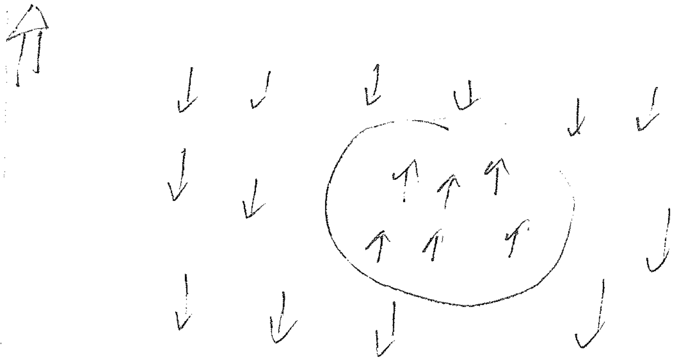
A





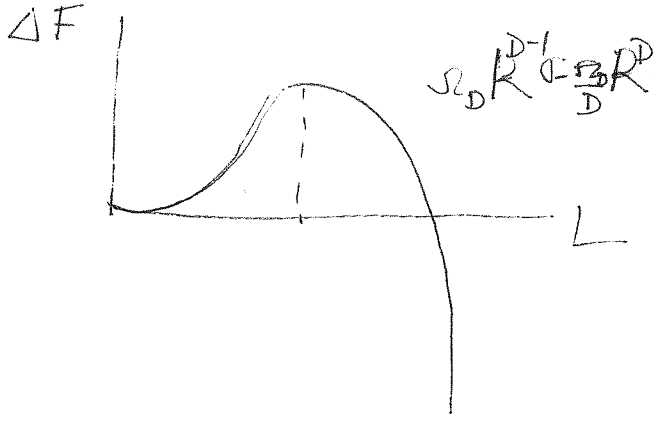


What if you are stuck to to the ~~wrong~~ metastable state



gain $\frac{1}{D}\Omega_D R^D \Delta f$

loss boundary $\Omega_D R^{D-1}\sigma$



$\Omega_D R^{D-1}\sigma - \frac{\Omega_D}{D} R^D \Delta f$

maxima at $\Omega_D (D-1) R_c^{D-1}\sigma = \cancel{D} R_c^D \frac{\Omega_D}{\cancel{D}}\Delta f$

at $R_c = \frac{(D-1)}{\cancel{D}}\frac{\sigma}{\Delta f}$

~~For~~ Barrier $\sim \Delta F_{\text{Droplet}} = \Omega_D\left[(D-1)\frac{\sigma}{\Delta f}\right]^{D-1}\sigma - \frac{1}{D}\Omega_D\left((D-1)\frac{\sigma}{\Delta f}\right)^{D}\Delta f$

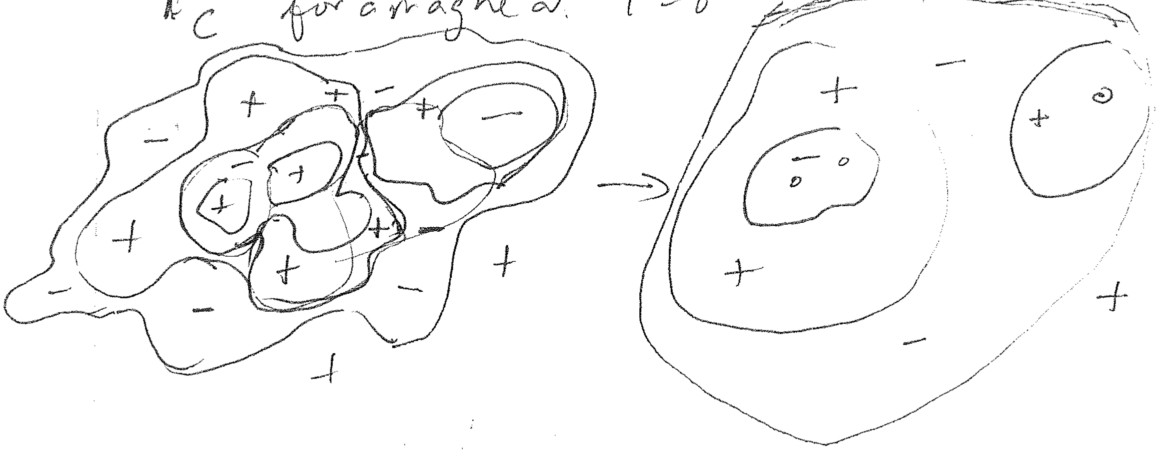
$= \Omega_D (D-1)^{D-1}\left[1-\frac{D-1}{D}\right]\frac{\sigma^D}{\Delta f^{D-1}} = \Omega_D\frac{(D-1)^{D-1}}{D}\frac{\sigma^D}{\Delta f^{D-1}}$

In 3D $\Delta F = 4\pi\frac{2^2}{3}\frac{\sigma^3}{\Delta f^2} = \frac{16\pi}{3}\frac{\sigma^3}{\Delta f^2}$

Rate $\sim e^{-\beta\Delta F}$

This would be slow
esply if Δf is small.

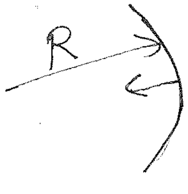
What if we start from a high temperature state and quench ~~it~~ into ~~To~~ temperature below T_c for a magnet at $T=0$



Coarsening

Size of correlated region $\sim L(t)$

$L(t) \sim t^{1/2}$



$$v = \frac{dR}{dt} \sim \frac{\Gamma\sigma}{R}$$

$$\frac{dR}{dt} \sim \frac{\Gamma\sigma}{R} \Rightarrow R \sim \sqrt{\Gamma\sigma t}$$

If $L \sim R$ we have $L \sim t^{1/2}$

Comments on dynamics beyond dissipative dynamics [Model A]

What if something is conserved? Total # of particles

$\Rightarrow$ Hydrodynamics

$$\frac{\partial\varphi}{\partial t} = -\nabla\cdot J_{\varphi} \qquad \int \varphi\, d^D x = \text{fixed}$$

$$J = \nabla\left[-\lambda\frac{\delta F}{\delta\varphi} + \eta\right] \Rightarrow \frac{\partial\varphi}{\partial t} = -\lambda\nabla^2 \frac{\delta F}{\delta\varphi} + \nabla\eta$$

When $\frac{\delta F}{\delta\varphi} = r\varphi + \cdots\cdots$

$$\langle \eta(x,t)\eta(x',t')\rangle = 2T\lambda\,\delta(x-x')\delta(t-t')$$

$$\frac{\partial\varphi}{\partial t} = \lambda\nabla^2\varphi + \lambda\nabla\eta$$

Note that τ is not finite.

Diffusive response: (Model B)

Other interesting cases: Goldstone modes, ...