Mathematical Statistical Physics II

Course given at LMU in the WS13/14

S. Bachmann.

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Part I: Classical results on phase transitions for quantum spin systems.

① Quantum spin systems & Phase transitions

a) Background & Setting

- Physical background: magnetic materials (Ferromagnetism)

Description: free energy $F(\beta, h)$ $\quad \beta = \frac{1}{kT}$: the inverse temp.

h: external magnetic field.

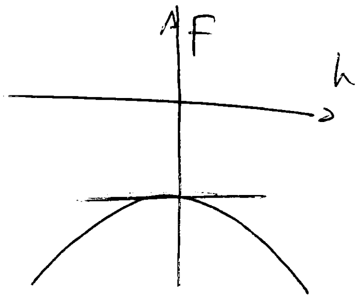
→ magnetization: $m(\beta, h) = -\frac{\partial F}{\partial h}$

magnetic susceptibility $\chi(\beta, h) = \frac{\partial m}{\partial h} = -\frac{\partial^2 F}{\partial h^2}$

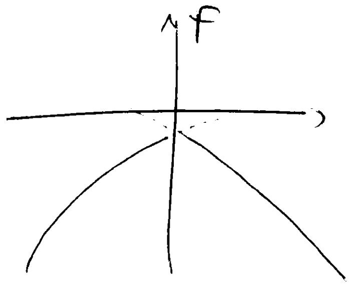
F is piecewise analytic, & phase transition is signalled by a non-analyticity of.

Observation:

$\beta < \beta_c$



$\beta > \beta_c$



T_c is the Curie temperature

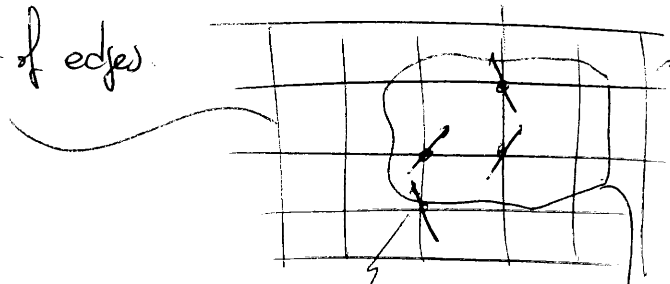
Low temperature: $-\left.\frac{\partial F}{\partial h}\right|_{0^+} \neq 0$: Spontaneous magnetization.

High temperature: $\left.\frac{\partial F}{\partial h}\right|_{0^+} = 0$: no magnetization.

Challenge: Understand the emergence of these phenomena from many-particle (quantum) mechanics

- A simple model (or a class of simple models) QSS.

$\mathcal{E}$: set of edges



lattice or graph Γ (countable set equipped with a ~~distance~~ metric $d(x,y)$, $x,y \in \Gamma$)

at each point (site) there is a spin (electron or nucleus, ...)

Λ: finite subset.

At each site: Hilbert space $\mathcal{H}_x$ of finite dimension.
Usually $\mathcal{H}_x = \mathcal{H}$ $\forall x \in \Gamma$ and carries ~~the~~ the $(2S+1)$-dimensional representation of $su(2)$, i.e. $\mathcal{H} = \mathbb{C}^{2S+1}$, the Hilbert space of a spin S, $S \in \mathbb{N}$ or $\frac{1}{2}\mathbb{N}$.

Λ finite: $\mathcal{H}_\Lambda = \bigotimes_{x\in\Lambda} \mathcal{H}_x$

Ex: Refresh representation theory of $su(2)$: $[S^i, S^j] = i\varepsilon^{ijk} S^k$

Recall: $S = \frac{1}{2}$: Pauli matrices

$$S^1 = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \quad S^2 = \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad S^3 = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$S = 1$:

$$S^1 = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}; \quad S^2 = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}; \quad S^3 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

Also: If $\vec{a} \in \mathbb{R}^3$, $S^{\vec{a}} = \vec{a}\cdot\vec{S}$ is the generator of rotations around the $\vec{a}$ axis

($SU(2)$: quantum mechanical rotation group)
universal cover of $SO(3)$

~~An interaction is a map $X \subset \Gamma$ (finite) $\mapsto$~~

Observables at x: $\mathcal{A}_x = \mathcal{B}(\mathcal{H}_x)$ (matrices!)

at Λ: $\mathcal{A}_\Lambda = \bigotimes_{x\in\Lambda} \mathcal{A}_x = \mathcal{B}(\mathcal{H}_\Lambda)$

Natural embedding: $\Lambda_1 \subset \Lambda_2$: $\mathcal{A}_{\Lambda_1} \hookrightarrow \mathcal{A}_{\Lambda_2}$:

$$A \in \mathcal{A}_{\Lambda_1} \Rightarrow A \otimes \mathbb{1}_{\Lambda_2\setminus\Lambda_1} \in \mathcal{A}_{\Lambda_2}.$$

Also: $\Lambda_1 \cap \Lambda_2 = \emptyset \Rightarrow \mathcal{A}_{\Lambda_1} \subset \mathcal{A}_{\Lambda_2}'$

$\mathcal{A}_{\Lambda_2} \subset \mathcal{A}_{\Lambda_1}'$

Algebra of quasi-local observables: it is a C^*-algebra $\|x\|^2 = \|x^* x\|$

$$\overline{\bigcup_{\substack{\Lambda\in\Gamma \\ \Lambda \text{ finite}}} \mathcal{A}_\Lambda}^{\|\cdot\|} =: \mathcal{A}$$

Def: Interaction: Map: $(X \subset \Gamma, \text{ finite}) \longmapsto \Phi_X \in \mathcal{A}_X$

with $\Phi_X^* = \Phi_X$ for all X.

Hamiltonian on Λ: $H_\Lambda = \sum_{X\subset\Lambda} \Phi_X$.

Note: There is (of course!) no limit $\nexists \lim_{\Lambda\nearrow\Gamma} H_\Lambda$ as an operator on some tensor product space. → real interacting system.

But the dynamics it generates may extend to Γ.

Typically: 1) $\|\Phi_X\|$ decays rapidly with the size of X

even: $\Phi_X = 0$ if $\operatorname{diam}(X) \geq R$: finite range interaction.

e.g. $\|\Phi\| = \sum_{X\ni 0} \frac{\|\Phi(X)\|}{N(X)} < \infty \Rightarrow \|H_\Lambda\| = N(\Lambda)\|\Phi\|$.

2) There is an action $\tau_{\vec a}$ of $\mathbb{Z}^d$ on the algebra $\mathcal{A}$ and

$$\tau_{\vec a}(\Phi_X) = \Phi_{(X+\vec a)}$$

translation-invariant interaction.

3) Rotations are represented by the action of $SU(2)$ on the algebra.

$A \in \mathcal{A}_x$: rotation around $\vec{a} \in \mathbb{R}^3$:

$$U_{\vec{a}}^* A U_{\vec{a}} =: \gamma_{\vec{a}}^{x}(A) \qquad \text{(unitary implementation)}$$

where $U_{\vec{a}} = e^{iS\vec{a}}$

— extends to any finite $\Lambda \subset \Gamma$:

Rotation-invariant interaction: $\gamma_{\vec{a}}^{X}(\Phi_X) = \Phi_X \quad \forall X, \vec{a}$

Examples:

Ising model: $S = \frac{1}{2}$

$$H_{\Lambda,h} = -\sum_{(x,y) \in \mathcal{E}_\Lambda} S_x^1 \cdot S_y^1 \mp h \sum_{x \in \Lambda} S_x^3 \quad , \quad h \in \mathbb{R}$$

Heisenberg model: any S

$$H_{\Lambda,h}^{F,AF} = \mp \sum_{(x,y) \in \mathcal{E}_\Lambda} \underbrace{\vec{S}_x \cdot \vec{S}_y}_{= S_x^1 S_y^1 + S_x^2 S_y^2 + S_x^3 S_y^3} - h \sum_{x \in \Lambda} S_x^3$$

and variants: * space-dependent coefficients J_{xy}

* "orientation-dependent" — " — $J_{xy}^{(1)}, J_{xy}^{(2)}, J_{xy}^{(3)}$

<u>EX</u>: Prove that $H_{\Lambda,0}^{F,AF}$ is rotation-invariant $\Leftarrow$ $J_{xy}^{(1)} = J_{xy}^{(2)} = J_{xy}^{(3)}$

translation-invariant $\Leftarrow$ $J_{xy}^{(i)} = J_{xy}^{(j)} \quad \forall i,j \in \Gamma$

- Thermodynamic description

$$f_\Lambda^{F,AF}(\beta,h) := -\frac{1}{\beta|\Lambda|} \log \operatorname{Tr}_{\mathcal{H}_\Lambda} e^{-\beta H_{\Lambda,h}^{F,AF}}$$

Phase transitions arise as non-analyticity of f_Λ in (β,h).

... can only arise in the limit $|\Lambda| \to \Gamma$

Theorem (existence of the thermodynamic limit): Let $\Lambda_L = \{1, \dots, L\}^d$ and $\mathcal{E}_L$ be the nearest-neighbours in Λ_L. Then there exists $f(\beta, h)$:

$$\lim_{L\to\infty} f_{\Lambda_L}(\beta,h) = f(\beta,h)$$

the convergence is uniform on compact sets.

Proof (for ferrom.): Choose $n \in \mathbb{N}$, fixed. $L = k\cdot n + r$, $0 \le r < n$.

Let

$$h_{xy} = 2(\vec{S}_x \cdot \vec{S}_y) + C$$

where C is chosen so that $h_{xy} > 0$.

$$\mathrm{Tr}\, e^{-\beta H^{F;AF}_{\Lambda_L,h}} = e^{-\beta C|\mathcal{E}_L|}\, \mathrm{Tr}\, e^{\beta\sum_{(x,y)\in\mathcal{E}_L} h_{xy} + \beta h \sum_{x\in\Lambda_L} S_x^3}$$

$$\geq e^{-\beta C|\mathcal{E}_L|}\left[\mathrm{Tr}_{\mathcal{H}_{\Lambda_n}}\, e^{\beta\sum_{(x,y)\in\mathcal{E}_n} h_{xy} + \beta h\sum_{x\in\Lambda_n} S_x^3}\right]^{k^d}$$

$$= \left(\mathrm{Tr}\, e^{-\beta H_{\Lambda_n,h}}\right)^{k^d} e^{-\beta C|\mathcal{E}_L|}\, e^{k^d\beta C|\mathcal{E}_n|}$$

where we used:

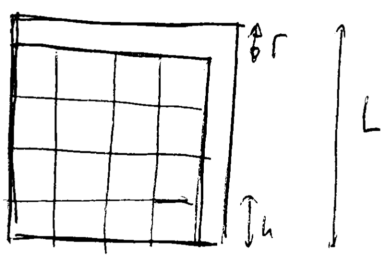
1) $\mathrm{Tr}\, e^{A+B} \geq \mathrm{Tr}\, e^{A}$ for A,B hermitian and $B \geq 0$. (h_{xy} terms connecting boxes and in the slab)

2) $\mathrm{Tr}\, e^{\beta h S_x^3} \geq 1$ for the sites in the slab of width r. (by explicit calculation in any rep: $1 + \sum \cosh(\dots)$)

Now:

$$|\mathcal{E}_L| \leq \underbrace{k^d|\mathcal{E}_n|}_{\text{bulk}} + \underbrace{k^d d\, n^{d-1}}_{\text{edges of small boxes}} + \underbrace{r d^2 L^{d-1}}_{\text{in the slab}}$$

$rdL^{d-1} \geq$ # of points in slab. each of them has $2d$ neighbours.



$$- f_{\Lambda_L}(\beta,h) \leq \frac{k^d n^d}{L^d} f_{\Lambda_n}(\beta,h) + \frac{k^d d n^{d-1}}{L^d} C + \frac{r d^2}{L} C$$

i) $\limsup_{L\to\infty} f_{\Lambda_L}(\beta,h) \leq f_{\Lambda_n}(\beta,h) + \frac{d}{n} C$

as $\frac{kn}{L} \to 1 \quad (L\to\infty)$

ii) Now $n \to \infty$:

$$\limsup_{L\to\infty} f_{\Lambda_L}(\beta,h) \leq \liminf_{n\to\infty} f_{\Lambda_n}(\beta,h)$$

$\Rightarrow$ The limit exists.

Uniform convergence follows from equicontinuity, see exercise. □

Notes. * Proof relies on subadditivity

Ex: Prove Fekete's lemma: (simple form)

Let $(a_n)_{n\geq 1}$ be a real sequence, $a_n > 0$ s.t.

$$a_{n+m} \leq a_n + a_m \quad \forall m,n \geq 1.$$

Then

$$\lim_{n\to\infty} \frac{a_n}{n} = \inf_{n\geq 1} \frac{a_n}{n}$$

* Prove equicontinuity and therefore uniform convergence (by Arzelà - Ascoli): If $\frac{|\mathcal{E}_\Lambda|}{|\Lambda|} \leq C$

$$|\beta f_\Lambda(\beta,h) - \beta' f_\Lambda(\beta',h')| \leq \underbrace{K(C,d,S)}_{\text{does not depend on } \Lambda}\left(|\beta-\beta'| + |h-h'|\right)$$

→ uniform boundedness.

* f exists for any interaction $\Phi \in \mathcal{B}$, and $|f(\Phi) - f(\Psi)| \leq \|\Phi - \Psi\|$

∘ Lemma 1.5: $\beta f_\Lambda(\beta,h)$ is concave in $(\beta, \beta h)$.

Proof: by explicit calculation of the Hessian.

- For any $\Lambda \subset \Gamma$, let $\Lambda^{(r)} := \{x \in \Gamma : d(x, \Lambda) \leq r\}$.
- Let $\{\Lambda_n\}_{n \in \mathbb{N}}$ be a sequence of volumes s.t.
  i) $\forall x \in \Gamma$, $\exists n_0 : \Lambda_{n_0} \ni x$ (absorbing)
  ii) $\Lambda_n \subset \Lambda_m$ if $n \leq m$ (increasing)
- Introduce a norm on interactions: (translation-invariant)

$$\|\Phi\| = \sum_{X \ni 0} \frac{\|\Phi(X)\|}{|X|} \to \text{Banach space } \mathcal{B}.$$

- Theorem: For $\{\Lambda_n\}$ as above and $\Phi \in \mathcal{B}$,
  $\exists\, f(\beta, \Phi) < \infty$:

$$\lim_{\Lambda \to \Gamma} f_\Lambda(\beta, \Phi) = f(\beta, \Phi)$$

see Ruelle.

• Now: We have a well-defined thermodynamics. Phase transitions?

Magnetization: $M_\Lambda := \frac{1}{|\Lambda|} \sum_{x\in\Lambda} S_x^3$

Order parameters: (note $\langle M_{\Lambda_L} \rangle_{\Lambda_L,\beta,0} = 0$ (at $h=0$) by symmetry)

(a) Thermodynamic magnetization: $m_{th}(\beta) := -\lim_{h\to 0^+} \frac{1}{h}\left(f(\beta,h) - f(\beta,0)\right)$

(b) Residual magnetization: $m_{res}(\beta) := \lim_{h\to 0^+} \liminf_{L\to\infty} \langle M_{\Lambda_L} \rangle_{\Lambda_L,\beta,h}$

(c) Spontaneous magnetization: $m_S(\beta) = \liminf_{L\to\infty} \langle |M_{\Lambda_L}| \rangle_{\Lambda_L,\beta,0}$.

<u>Proposition</u>: $m_{th}(\beta) \overset{(1)}{=} m_{res}(\beta) \overset{(2)}{\geq} m_S(\beta)$.

<u>Note</u>: One could also consider $\langle M_{\Lambda_L}^2 \rangle_{\Lambda_L,\beta,h}$. This is equivalent to m_S

<u>Lemma</u>: $\langle |M_\Lambda| \rangle^2 \leq \langle (M_\Lambda)^2 \rangle \leq S \langle |M_\Lambda| \rangle$ #

* Proof at the back:
(i.e. these are both zero or both non-zero).

It is useful as

$$\langle (M_\Lambda)^2 \rangle = \frac{1}{|\Lambda|^2} \sum_{x,y\in\Lambda} \langle S_x^3 S_y^3 \rangle$$

expressed in terms of spin-spin correlations.

$\Rightarrow$ Necessary condition for $m_S(\beta) \neq 0$: $\langle S_x^3 S_y^3 \rangle \not\to 0$ $(|x-y| \to \infty)$.

Proof of proposition left as an exercise. Uses properties of concave functions (1) and (a) $[H_\Lambda, M_\Lambda] = 0$, (b) eigenvalues of M_Λ are symmetric around 0 for (2).

~~Message: $\langle S_x^3 S_y^3 \rangle \not\to 0 \Rightarrow \langle M_\Lambda^2 \rangle$~~

Message: $\langle S_x^3 S_y^3 \rangle \to 0 \Rightarrow \langle (M_\Lambda)^2 \rangle \to 0 \Rightarrow m_S(\beta) = 0$

<u>But</u>: does not exclude phase transitions...

A remark on correlations. One expects correlations are increasing functions of both β & interaction strength.

* for β : ???
* but : correlations are stronger in directions where interactions are stronger. Let

$$H_\Lambda = -\sum_{x,y\in\Lambda} \left(J^1_{xy} S^1_x S^1_y + J^2_{xy} S^2_x S^2_y + J^3_{xy} S^3_x S^3_y \right)$$

If $|J^2_{xy}| \leq J^1_{xy}$ $\forall x,y$, then

$$|\langle S^2_x S^2_y \rangle| \leq \langle S^1_x S^1_y \rangle$$

Proof: Let $\{|\sigma\rangle, \sigma \in \{-S, \dots, S\}\}$ be an ON basis of eigenvectors of S^3 and s.t. matrix elements of S^1, $S^+ = S^1 + iS^2$ and $S^- = S^1 - iS^2$ are all non-negative. Also: matrix elements of S^2 are less or equal those of S^1 in absolute value.

Trotter:
$$\text{s-}\lim \left(e^{-\frac{A}{n}} e^{-\frac{B}{n}} \right)^n = e^{-(A+B)}$$

$$|\mathrm{Tr}_{\mathcal{H}_\Lambda} S^2_x S^2_y e^{-\beta H_\Lambda}| \leq \lim_{n\to\infty} \sum_{\substack{\sigma_0 \dots \sigma_n \\ \in\{-S,\dots,S\}^n}} |\langle \sigma_0, S^2_x S^2_y \sigma_1 \rangle \cdot$$

$$\cdot \prod_{i=1}^{n} \underbrace{\langle \sigma_i, e^{\frac{\beta}{n}\sum J^3_{ij} S^3_i S^3_j} \sigma_i \rangle}_{>0} \langle \sigma_i, e^{\frac{\beta}{n}(\sum J^1_{ij} S^1_i S^1_j + J^2_{ij} S^2_i S^2_j)} \sigma_{i+1} \rangle|$$

where $\sigma_{n+1} = \sigma_0$.

Note: 1) $J^1_{ij} S^1_i S^1_j + J^2_{ij} S^2_i S^2_j$
$$= \frac{1}{4}(J^1_{ij} - J^2_{ij})(S^+_i S^+_j + S^-_i S^-_j)$$
$$+ \frac{1}{4}(J^1_{ij} + J^2_{ij})(S^+_i S^-_j + S^-_i S^+_j)$$

$\Rightarrow$ all matrix elements are non-negative

$\Rightarrow$ all matrix elements of $e^{\cdot}$ are non-negative (take Taylor series of the exponential)

2) $|\langle \sigma_0, S^2_x S^2_y \sigma_1 \rangle| \leq \langle \sigma_0, S^1_x S^1_y \sigma_1 \rangle$

Done

$\square$

b) 2d spin systems: Absence of phase transitions

- We will prove:
  - Decay of correlations for the 2d-Heisenberg model (1)
    $\to$ absence of spontaneous magnetization.
  - Absence of symmetry breaking for general 2d models. (2)

Note: $(2) \not\Rightarrow (1)$: there exist examples in classical systems.

- (1) Consider:

$$H_\Lambda = \sum_{(x,y)\in\mathcal{E}_\Lambda} -2\left(S_x^1 S_y^1 + S_x^2 S_y^2 + u S_x^3 S_y^3\right) \quad , u \in [-1,1]$$

Theorem: for $i = 1,2,3$:

$$\left|\langle S_0^i S_x^i\rangle_{\Lambda,\beta,0}\right| \le 2 S^2 e^{-\xi_\beta(x)}$$

where $\xi_\beta(x) = \sup_{\phi_y \in \mathbb{R}^\Lambda}\left[(\phi_x - \phi_0) - 4\beta S^2 \sum_{(y,z)\in\mathcal{E}_\Lambda}\left(\cosh(\phi_y - \phi_z) - 1\right)\right]$

Note: If $(\Lambda, \mathcal{E}_\Lambda)$ is 2d-like: $\exists K$ s.t. $\forall \ell \ge 1$

$$\left|\{x \in \Lambda : d(0,x) = \ell\}\right| \le K\ell$$

Then: $\exists\, C = C(\beta, S, K) > 0$, independent of x, s.t.

$$\xi_\beta(x) \ge \frac{1}{16\beta S^2 K^2}\log\left(d(0,x)+1\right) - C$$

Which implies:

$$e^{-\xi_\beta(x)} \le C_1\left(1 + d(0,x)\right)^{-C_2/\beta}$$

algebraic decay of correlations for $\beta < \infty$.

- Note: It is expected that some of these systems undergo a "Kosterlitz-Thouless" phase transition: correlation functions go from exponential decay at low β to algebraic decay at high β.
  Expected to happen for abelian symmetry groups, [Fröhlich-Spencer]
- Proof: (essentially Fröhlich)

We introduce complex rotations: $e^{\theta S^3} S^{\pm} e^{-\theta S^3} = e^{\pm\theta} S^{\pm}$, $\theta \in \mathbb{C}$.
note: this is not unitary unless $\theta \in i\mathbb{R}$.
We consider

$$H_\Lambda = - \sum_{(y,z)\in\mathcal{E}_\Lambda} \left(S_y^+ S_{\cancel{z}}^- + S_z^+ S_y^- + 2u\, S_y^3 S_z^3 \right)$$

For any function $\{\phi_y\}_{y\in\Lambda}$, let $A_\phi := \prod_{y\in\Lambda} e^{\phi_y S_y^3}$.
Then:

$$\mathrm{Tr}\left(S_0^+ S_x^- e^{-\beta H_\Lambda}\right) = \mathrm{Tr}\left(A_\phi S_0^+ S_x^- A_\phi^{-1} e^{-\beta A_\phi H_\Lambda A_\phi^{-1}}\right)$$

where

$$A_\phi H_\Lambda A_\phi^{-1} = - \sum_{(y,z)\in\mathcal{E}_\Lambda} \left(e^{(\phi_y-\phi_z)} S_y^+ S_z^- + e^{(-\phi_y+\phi_z)} S_y^- S_z^+ + 2u\, S_y^3 S_z^3 \right)$$

$$= H_\Lambda - \sum_{(y,z)\in\mathcal{E}_\Lambda} \Big[\left(\cosh(\phi_y-\phi_z)-1\right)\left(S_y^+ S_z^- + S_z^+ S_y^-\right) + \sinh(\phi_y-\phi_z)\left(S_y^+ S_z^- - S_z^+ S_y^-\right) \Big]$$

$$=: H_\Lambda + B + C$$

with $B^* = B$ and $C^* = -C$ as $(S^{\pm})^* = S^{\mp}$

Hence: $\mathrm{Tr}\left(S_0^+ S_x^- e^{-\beta H_\Lambda}\right) = e^{\phi_0-\phi_x}\,\mathrm{Tr}\left(S_0^+ S_x^- e^{-\beta H_\Lambda - \beta B - \beta C}\right)$

Use: (a) Trotter

(b) Hölder: $\|AB\|_1 \le \|A\|_p \|B\|_q$, $\frac{1}{p}+\frac{1}{q}=1$

and $|\mathrm{Tr}(B^* A)| \le \|B^* A\|_1 \le \|B\|_p \|A\|_q$

$$|\mathrm{Tr}(\dots)| \le \lim_{N\to\infty} \|S_0^+ S_x^-\|_\infty \left\| \left(e^{-\frac{\beta}{N}H_\Lambda} e^{-\frac{\beta}{N}B} e^{-\frac{\beta}{N}C}\right)^N \right\|_1$$

$$\le \lim_{N\to\infty} \|S_0^+ S_x^-\|_\infty \left\| \left(\text{———} \,\text{"}\, \text{———} \right) \right\|_N^N$$

$$\le \lim_{N\to\infty} \|S_0^+ S_x^-\|_\infty \left\|e^{-\frac{\beta}{N}H_\Lambda}\right\|_N^N \left\|e^{-\frac{\beta}{N}B} e^{-\frac{\beta}{N}C}\right\|_\infty^N$$

$$\le \lim_{N\to\infty} \underbrace{\|S_0^+ S_x^-\|_\infty}_{\le 4S^2} \underbrace{\left\|e^{-\frac{\beta}{N}H_\Lambda}\right\|_N^N}_{= Z(\beta)} \underbrace{\left\|e^{-\frac{\beta}{N}B}\right\|_\infty^N}_{\le e^{\beta\|B\|}} \underbrace{\left\|e^{-\frac{\beta}{N}C}\right\|_\infty^N}_{=1}$$

as $|e^{-\frac{\beta}{N}H_\Lambda}| = e^{-\frac{\beta}{N}H_\Lambda}$, $H_\Lambda^* = H_\Lambda$; as $C^* = -C$

and $\|B\| \le 4S^2 \sum_{(y,z)\in\mathcal{E}_\Lambda} \left(\cosh(\phi_y - \phi_z) - 1\right)$

All in all: $\langle S_0^+ S_x^- \rangle_\beta \le 4S^2 e^{\phi_0 - \phi_x} e^{4\beta S^2 \sum_{(y,z)\in\mathcal{E}_\Lambda} \left(\cosh(\phi_y-\phi_z)-1\right)}$

gives $\xi_\beta(x) = (\phi_x - \phi_0) - 4\beta S^2 \sum_{(y,z)\in\mathcal{E}_\Lambda} \left(\cosh(\phi_y - \phi_z) - 1\right)$

To conclude: $\langle S_0^1 S_x^2 \rangle = -\langle S_0^2 S_x^1 \rangle$ by rotation invariance of H_Λ around 3-axis.

$= -\langle S_x^1 S_0^2 \rangle = -\langle S_0^1 S_{-x}^2 \rangle$ by translation inv.

$= -\langle S_0^1 S_x^2 \rangle$ by inv. under $x \to -x$.

$\Rightarrow \langle S_0^1 S_x^2 \rangle = 0$

$\Rightarrow \langle S_0^+ S_x^- \rangle = \langle (S_0^1 + i S_0^2)(S_x^1 - i S_x^2) \rangle$

$= \big(\underbrace{\langle S_0^1 S_x^1 \rangle + \langle S_0^2 S_x^2 \rangle}_{\text{equal by rot. inv.}} \big)$

$\Rightarrow \langle S_0^1 S_x^1 \rangle = 2^{-1} \langle S_0^+ S_x^- \rangle \le \frac{1}{2} S^2 e^{-\xi_\beta(x)}$

□

- Look for a bound for $\xi_\beta(x)$.

for any $x \in \Gamma$, $\quad \phi_y^{(x)} := \begin{cases} c \log \frac{d(0,x)+1}{d(0,y)+1} & d(0,y) \le d(0,x) \\ 0 & \text{otherwise} \end{cases}$

$$\Rightarrow \quad \phi_y - \phi_z = \begin{cases} c \log \frac{d(0,z)+1}{d(0,y)+1} & \text{if } d(0,y) = d(0,z) \pm 1 \text{ and both } \le d(0,x) \\ 0 & \text{otherwise} \end{cases}$$

$$\Rightarrow \sum_{(y,z)\in \mathcal{E}_\Lambda} \left(\cosh\left(\phi_y - \phi_z\right) - 1\right) = \sum_{d=0}^{d(0,x)-1} \sum_{y: d(0,y)=d} \sum_{\substack{z: \\ d(0,z)=d(0,y)+1 \\ (y,z)\in\mathcal{E}_\Lambda}} \left(\cosh\left(c \log \frac{d+2}{d+1}\right) - 1\right)$$

$$\le K^2 \sum_{d=0}^{d(0,x)-1} d\left(\cosh\left(c \log\left(1 + \frac{1}{1+d}\right)\right) - 1\right) \quad \text{(2D-like graphs)}$$

$$\le K^2 \sum_{d=0}^{d(0,x)-1} c^2 \frac{d}{(1+d)^2} \le K^2 c^2 \sum_{d=1}^{d(0,x)} \left(\frac{1}{d} - \frac{1}{d^2}\right)$$

$$\le K^2 c^2 \left[\left(1 + \log(d(0,x))\right) - 0\right] \le K^2 c^2 \log\left(d(0,x)+1\right) + K^2 c^2$$

$$\Rightarrow \xi_\beta(x) \ge \underbrace{-c \log\left(d(0,x)+1\right) - 4\beta K^2 S^2 c^2 \log\left(d(0,x)+1\right)}_{(*)} - 4\beta (SKc)^2$$

Choose c so that $(*)$ is maximal: $c = -\frac{1}{8\beta K^2 S^2}$, i.e.

$$\xi_\beta(x) \ge \frac{1}{16\beta K^2 S^2} \log\left(d(0,x)+1\right) - C$$

$\square$

- Conclusion: Decay of correlations $\Rightarrow m_{sp.}(\beta) = 0$, in (one-) and (two-)d-like models.
- That is for the Heisenberg model. What can we say in general?

↳ Absence of symmetry breaking for 2D-models, classical and quantum.

(original version of Mermin-Wagner).

- The original statement of Mermin & Wagner:

$$H_\Lambda = - \sum_{x,y\in\Lambda} J(x-y)\, S_x \cdot S_y - h \sum_{x\in\Lambda} S_x^3$$

for $\Lambda \subset \mathbb{Z}^\nu$.

If $\nu \leq 2$, then $m_{th}(\beta) = 0$

- The proof relies on Bogoliubov's inequality:

<u>Lemma</u>: Let $\mathcal{H}$ s.t. $\dim \mathcal{H} < \infty$, $H = H^* \in \mathcal{B}(\mathcal{H})$, $\beta > 0$.

$$\tfrac{1}{2}\beta\, \omega_\beta\left(\{A, A^*\}\right) \cdot \omega_\beta\left(\left[[C,H], C^*\right]\right) \geq \left|\omega_\beta\left([C,A]\right)\right|^2$$

for any operators $A, C \in \mathcal{B}(\mathcal{H})$.

<u>Proof</u>: Exercise. Relies on the introduction of a good scalar product, the inequality is just Schwarz's.

- Another, modern, version of M-W: more general, but weaker.

<u>Theorem</u> [Fröhlich-Pfister] Let G be a compact, connected Lie group, $g \mapsto U(g)$ a unitary representation of G on $\mathcal{H}_x$ and γ_g the action of G on $\mathcal{A}_{\mathbb{Z}^2}$. Let Φ be s.t.

i) $\Phi_X = 0$ if $|X| \neq 2$ (2-body interaction)

ii) $\gamma_g(\Phi_X) = \Phi_X \quad \forall g \in G$ (symmetry)

iii) $\|\Phi_{\{x,y\}}\| \leq C \cdot (1 + d(x,y))^{-4}$ (decay)

Then, for any thermal state at inverse temp. β:

$$\omega_\beta \circ \gamma_g = \omega_\beta$$

i.e. Any thermal state is invariant under the action of G
"absence of (symmetry / continuous) breaking".

- <u>Note</u>: A thermal state here: A state satisfying the <u>KMS condition</u>:

$$\omega\left(A\,\tau^{\Gamma}_{i\beta}(B)\right) = \omega(BA)$$

where τ^{Γ}_t is the automorphism of $\mathcal{A}$:

$$\tau^{\Gamma}_t(A) = \lim_{\Lambda \nearrow \Gamma} e^{itH_\Lambda} A\, e^{-itH_\Lambda}.$$

In finite volume and for a Gibbs state:

$$\omega_{\beta,\Lambda}\left(A\tau^{\Lambda}_{i\beta}(B)\right) = Z_\Lambda(\beta)^{-1}\,\mathrm{Tr}\left(e^{-\beta H_\Lambda} A\, e^{-\beta H_\Lambda} B\, e^{\beta H_\Lambda}\right)$$

$$= Z_\Lambda(\beta)^{-1}\,\mathrm{Tr}\left(e^{-\beta H} BA\right) = \omega_{\beta,\Lambda}(BA).$$

by cyclicity.

c) 3d Heisenberg model : Long-range order

1) Learn methods on the classical system.
2) Extend to the quantum case.

Key element : reflection positivity.

1) Classical Heisenberg : periodic boundary conditions.

$\Lambda_L = \{-\frac{L}{2}+1, \dots, \frac{L}{2}\}^d$, $L \in 2\mathbb{N}$, $\mathcal{E}_\Lambda$: nearest-neighbours.

Configuration space : $\Omega_\Lambda = \times_{x\in\Lambda} S^2$ ← sphere in $\mathbb{R}^3$

"classical spins"

Energy : $H_\Lambda : \Omega_\Lambda \to \mathbb{R}$:

$$H_\Lambda(\sigma) = -2\sum_{(x,y)\in\mathcal{E}_\Lambda} \sigma_x \cdot \sigma_y - h\sum_{x\in\Lambda} \sigma_x^3$$

Partition function:

$$Z_\Lambda(\beta,h) := \int_{\Omega_\Lambda} d\sigma\, e^{-\beta H(\sigma)} \quad ; \quad d\sigma : \text{Lebesgue measure on } \Omega_\Lambda .$$

Gibbs state : $\mu_{\Lambda,\beta,h} : C^0(\Omega_\Lambda) \to \mathbb{R}$

$$\mu_{\Lambda,\beta,h}(f) = Z_\Lambda(\beta,h)^{-1} \int_{\Omega_\Lambda} d\sigma\, f(\sigma)\, e^{-\beta H_\Lambda(\sigma)}$$

Let Λ^* be the dual lattice: $\Lambda^* = \frac{2\pi}{L}\{-\frac{L}{2}+1, \dots, \frac{L}{2}\}^d$

Theorem [Fröhlich-Simon-Spencer].

Let $h=0$ and let $E(k) := 2\sum_{i=1}^d (1-\cos(k_i))$.

$$\frac{1}{|\Lambda|}\sum_{x\in\Lambda} \mu_{\Lambda,\beta,0}(\sigma_0^3\sigma_x^3) \geq \frac{1}{3} - \frac{1}{\beta|\Lambda|}\sum_{k\in\Lambda^*\setminus\{0\}} \frac{1}{E(k)}$$

- Consequence:

$$\liminf_{L\to\infty} \mu_{\Lambda_L,\beta,0}\left(\left(\frac{1}{|\Lambda|}\sum_{x\in\Lambda}\sigma_x\right)^2\right) = \liminf_{L\to\infty} \mu_{\Lambda_L,\beta,0}\left(\frac{1}{|\Lambda|}\sum_x \sigma_0\sigma_x\right)$$

$$\geq \liminf_{L\to\infty}\left(\frac{1}{3} - \frac{1}{\beta|\Lambda_L|}\sum_k \frac{1}{E(k)}\right)$$

$$= \frac{1}{3} - \frac{1}{(2\pi)^d\beta}\int_{[-\pi,\pi]^d}\frac{dk}{E(k)}.$$

To conclude: $(1-\cos(k_i)) \leq \frac{1}{2}k_i^2 \Rightarrow E(k) \leq |k|^2$

$$\Rightarrow \liminf_{L\to\infty}\mu_{\Lambda_L,\beta,0}\left(\left(\frac{1}{|\Lambda_L|}\sum_{x\in\Lambda}\sigma_x\right)^2\right) \geq 1 - \frac{1}{(2\pi)^d\beta}\int_{[-\pi,\pi]^d}\frac{dk}{|k|^2}$$

The integral is convergent for $d\geq 3$

$\Rightarrow$ $\liminf(\dots) > 0$ for β large enough, $d\geq 3$.

$\Rightarrow$ The classical Heisenberg model exhibits spontaneous magnetization at $T < T_c$.

- Notation: $C_L(x) := \mu_{\Lambda_L,\beta,0}\left(\sigma_0^3\sigma_x^3\right)$
- Proof: Reflection positivity $\underset{\text{Lemma}(3)}{\Rightarrow}$ Gaussian domination $\underset{\text{Lemma}(2)}{\Rightarrow}$ <u>infrared bounds</u> $\underset{\text{Lemma}(1)}{\Rightarrow}$ Theorem.

  We'll go backwards, and Reflection positivity is lemma 4.

FT: $\hat{f}(k) = \sum_{x\in\Lambda} e^{-ikx} f(x)$; $f(x) = \frac{1}{|\Lambda|}\sum_{k\in\Lambda^*} e^{ikx}\hat{f}(k)$.

<u>Lemma 1</u>: $\left(\hat{C}_L(k) \leq \frac{1}{\beta E(k)}\right) \Rightarrow$ Theorem.

Proof of L.1: First note: $\frac{1}{|\Lambda_L|}\sum_{x\in\Lambda_L} C_L(x) = \frac{1}{|\Lambda_L|}\hat{C}_L(0)$

But $\frac{1}{|\Lambda_L|}\hat{G}_L(0) = G_L(0) - \frac{1}{|\Lambda_L|}\sum_{k\in\Lambda^*\setminus\{0\}} \hat{G}_L(k)$

conclusion follows from

$$C_L(0) = Z(\beta)^{-1}\int_{\Omega_L} d\sigma\, (\sigma_0^3)^2 e^{-\beta H_\Lambda} \underset{\uparrow}{=} Z(\beta)^{-1}\int_{(S^2)^\Lambda} d\sigma\, \frac{1}{2}\|\sigma_0\|^2 e^{-\beta H_\Lambda} = \frac{1}{3}$$

$SO(3)$-invariance of $H_\Lambda(h=0)$ $\square$

and the assumption.

- Now: introduce a scalar <u>product</u> on $\ell^2(\Lambda)$:

$$\langle f|g\rangle_\Lambda := \sum_{(x,y)\in\mathcal{E}_\Lambda} (f_x - f_y)(g_x - g_y) \quad \left(\|f\|_\Lambda^2 := \langle f|f\rangle_\Lambda \right)$$

(symmetric quadratic form of the discrete Laplacian).

With it: $-2\sum_{(x,y)\in\mathcal{E}_\Lambda} \sigma_x\cdot\sigma_y = \langle\sigma|\sigma\rangle_f - \underset{\sim}{2d}|\Lambda|$

↖ # of neighbours at any point.

and define $\tilde{Z}_\Lambda(\beta, g) := \int_{\Omega_\Lambda} d\sigma\, \exp\left(-\beta\langle\sigma - g|\sigma - g\rangle\right)$

with $g_x = g_x \cdot e_3$ ("external field in the 3rd direction")

<u>Lemma 2</u>: $\left(\tilde{Z}_\Lambda(\beta, g) \le \tilde{Z}_\Lambda(\beta, 0)\right) \Rightarrow \left(\hat{C}_L(k) \le \frac{1}{\beta E(k)}\right)$

<u>Proof of L2</u>: Observe:

$$\tilde{Z}_\Lambda(\beta, g) = e^{2\beta d|\Lambda|}\mu_{\Lambda,\beta,h=0}\left(e^{2\beta \mathrm{Re}\langle\sigma|g\rangle_\Lambda}\right)\underbrace{e^{-\beta\langle g|g\rangle_\Lambda}\cdot Z_\Lambda(\beta, h=0)}_{\text{indep of }\sigma.}$$

i.e. $\tilde{Z}_\Lambda(\beta, g) \le \tilde{Z}_\Lambda(\beta, 0) \Leftrightarrow \mu\left(e^{2\beta \mathrm{Re}\langle\sigma|g\rangle_\Lambda}\right) \le e^{\beta\langle g|g\rangle_\Lambda}$

We take a small field g: $g \mapsto \varepsilon g$, $\varepsilon > 0$ and expand to second order to obtain:

$$\beta\varepsilon\Big[\underbrace{\mu(\langle\sigma|\rho\rangle_\Lambda)}_{=0 \text{ by symmetry } \sigma\leftrightarrow-\sigma}+\underbrace{\mu(\langle\rho|\sigma\rangle_\Lambda)}_{=0}\Big] + 2\beta^2\varepsilon^2\mu\big((\mathrm{Re}\langle\sigma|\rho\rangle_\Lambda)^2\big) + O(\varepsilon^3)$$

$$\le \beta\varepsilon^2\langle\rho|\rho\rangle_\Lambda + O(\varepsilon^4)$$

$$\rightarrow \quad 2\beta\mu\big[(\mathrm{Re}\langle\sigma|\rho\rangle_\Lambda)^2\big] \le \langle\rho|\rho\rangle_\Lambda \qquad (\star)$$

Now note that $\langle f|g\rangle_\Lambda = \sum_x f_x(-\Delta g)_x = (f,-\Delta g)$

where $(-\Delta g)_x = \sum_{(y,x)\in\mathcal{E}_\Lambda}(g_x - g_y)$

Choose ρ to be an eigenvector of $-\Delta$ for the eigenvalue $\lambda(k)$.

$-\Delta\psi_k = \lambda_k\psi_k \quad : \quad (\psi_k,\psi_k) = |\Lambda|$

easy: $\psi_k = e^{ikx}$, $\lambda_k = E(k) = 2\sum_{j=1}^{d}(1-\cos k_j) \in \mathbb{R}$

so that $\langle\sigma|\rho\rangle = E(k)\sum_x \sigma_x e^{-ikx}$ and

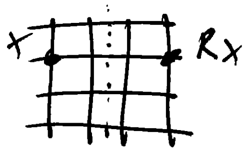
$$2\beta\mu\big[(\mathrm{Re}\langle\sigma|\rho\rangle_\Lambda)^2\big] = \beta E(k)^2 \big(C_L(t)\big)\sum_t e^{-ikt}\cdot|\Lambda|$$

and $\langle\rho|\rho\rangle = E(k)\,|\Lambda|$

$(\star) \Rightarrow \hat{C}_L(k) \le \frac{1}{\beta E(k)}$

□

• Reflection map : $R:\Lambda\to\Lambda$:



i.e. $\Lambda = \Lambda_1\cup\Lambda_2$; $\Lambda_1\cap\Lambda_2 = \emptyset$

and $\Lambda_2 = R\Lambda_1$ take $\Lambda = \mathbb{Z}^2$!

for any field ρ : $\rho = (\rho_1,\rho_2)$, $\rho_i = \rho|_{\Lambda_i}$.

• Lemma 3 If

$$\tilde{Z}_{\mathbb{Z}^2}(\beta,\rho)^2 \le \tilde{Z}_{\mathbb{Z}^2}(\beta,(\rho_1,R\rho_1))\,\tilde{Z}_{\mathbb{Z}^2}(\beta,(R\rho_2,\rho_2))$$

for any reflection R, then

$$\tilde{Z}_\Lambda(\beta,\rho) \le \tilde{Z}_\Lambda(\beta,0) \qquad \forall \text{ fields } \rho.$$

$$\beta\varepsilon\Big[\underbrace{\mu(\langle\sigma|\rho\rangle_\Lambda)}_{=0 \text{ by symmetry } \sigma\leftrightarrow-\sigma} + \underbrace{\mu(\langle\rho|\sigma\rangle_\Lambda)}_{=0}\Big] + 2\beta^2\varepsilon^2\mu\big((\mathrm{Re}\langle\sigma|\rho\rangle_\Lambda)^2\big) + O(\varepsilon^3)$$
$$\le \beta\varepsilon^2\langle\rho|\rho\rangle_\Lambda + O(\varepsilon^4)$$

$$\to \quad 2\beta\mu\left[(\mathrm{Re}\langle\sigma|\rho\rangle_\Lambda)^2\right] \le \langle\rho|\rho\rangle_\Lambda \qquad (*)$$

Now note that $\langle f|g\rangle_\Lambda = \sum_x \bar f_x(-\Delta g)_x = (f,-\Delta g)$

where $(-\Delta g)_x = \sum_{(y,x)\in\mathcal{E}_\Lambda}(g_x-g_y)$

Choose ρ to be a eigenvector of $-\Delta$ for the eigenvalue $\lambda(k)$

$-\Delta\psi_k = \lambda_k\psi_k \quad : \quad (\psi_k,\psi_k) = |\Lambda|$

easy: $\psi_k = e^{ikx}$, $\lambda_k = E(k) = 2\sum_{j=1}^{d}(1-\cos k_j)\in\mathbb{R}$

so that $\langle\sigma|\rho\rangle = E(k)\sum_x\sigma_x e^{-ikx}$ and

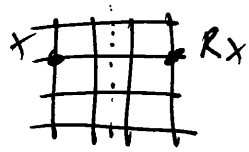
$$2\beta\mu\left[(\mathrm{Re}\langle\sigma|\rho\rangle_\Lambda)^2\right] = \beta E(k)^2 \sum_t C_L(t) e^{-ikt}\cdot|\Lambda|$$

and $\langle\rho|\rho\rangle = E(k)|\Lambda|$

$(*) \Rightarrow \hat C_L(k) \le \frac{1}{\beta E(k)}$

$\square$

- Reflection map : $R:\Lambda\to\Lambda$:



i.e. $\Lambda = \Lambda_1\cup\Lambda_2$; $\Lambda_1\cap\Lambda_2=\emptyset$
and $\Lambda_2 = R\Lambda_1$ take $\Lambda = \mathbb{Z}^2$!

for any field ρ : $\rho=(\rho_1,\rho_2)$, $\rho_i = \rho|_{\Lambda_i}$.

- Lemma 3 If

$$\tilde Z_{\mathbb{Z}^2}(\beta,\rho)^2 \le \tilde Z_{\mathbb{Z}^2}(\beta,(\rho_1,R\rho_1))\,\tilde Z_{\mathbb{Z}^2}(\beta,(R\rho_2,\rho_2))$$

for any reflection R, then

$$\tilde Z_\Lambda(\beta,\rho) \le \tilde Z_\Lambda(\beta,0) \qquad \forall \text{ fields } \rho .$$

<u>Proof of L3</u> Let ρ^* be a maximizer of the functional $\rho \mapsto \tilde{Z}(\beta,\rho)$, and let $\Pi := \tilde{Z}(\beta,\rho^*)$ (exists: $\tilde{Z}$ is continuous in ρ, $\tilde{Z} \geq 0$, and $\tilde{Z} \to 0$ as $\sup_{x\in\Lambda}|\rho_x| \to \infty$.)

If $\tilde{Z}_\Lambda(\beta,(\rho_1^*, R\rho_1^*)) < \Pi$ then,

$$\Pi^2 \underset{\text{Hyp.}}{\leq} \hat{Z}(\beta,(\rho_1^*, R\rho_1^*))\,\tilde{Z}(\beta,(R\rho_2^*,\rho_2^*))$$

$$< \Pi\,\tilde{Z}(\beta,(R\rho_2^*,\rho_2^*)) \quad \text{is a contradiction.}$$

Hence $(\rho_1^*, R\rho_1^*)$ is also a maximizer.

Now fix $x_0 \in \Lambda$ and let $\{R_n\}_{n\in\mathbb{N}}$ be a sequence of reflections s.t. $R_n \neq R_m$ if $n \neq m$ and $\exists\, n_0 \in \mathbb{N}$

$$\bigcup_{n \leq n_0} \{R_n \cdots R_1 x_0\} \supset \Lambda .$$

~~Then $x \in \Lambda$~~ Let $\rho^*_{n_0}$ be the associated fields.

Then $x \in \Lambda \Rightarrow \rho^*_{n_0}(x) = \rho^*_{n_0}(x_0)$

Hence constant fields are maximizers. But since

$$\tilde{Z}(\beta,\rho + \text{const.}) = \tilde{Z}(\beta,\rho)$$

Then, ~~constant~~ $\rho^* \equiv 0$ is a maximizer $\square$

- It remains to prove reflection positivity. (property of the Gibbs measure)

<u>Lemma 4</u>. For the classical ferromagnetic Heisenberg model

$$\tilde{Z}_\Lambda(\beta,\rho)^2 \leq \tilde{Z}_\Lambda(\beta,(\rho_1, R\rho_1))\,\tilde{Z}_\Lambda(\beta,(R\rho_2,\rho_2)).$$

Technical key step:

$$e^{-\frac{1}{2}(a+b)^2} = \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}} dx\, e^{-\frac{1}{2}x^2} e^{ix(a+b)} \qquad (*)$$

Proof. Write $\tilde{Z}_\Lambda(\beta, g) = \int_{\Omega_1} d\sigma_1 \int_{\Omega_2} d\sigma_2\, e^{-S_1(\sigma_1, g_1)} e^{-S_2(\sigma_2, g_2)} \times e^{-\beta \sum \left((\sigma_1 - g_1) - (\sigma_2 - g_2) \right)^2}$

where the sum is over all $x \in \Lambda_1$, $y \in \Lambda_2$: $(x,y) \in \mathcal{E}_\Lambda$.
(i.e. neighbours across the reflection axis).
Now, use $(*)$

$$e^{-\beta \sum (\ )^2} = \prod_{\substack{x\in\Lambda_1 \\ y \in \Lambda_2 \\ (x,y)\in\mathcal{E}_\Lambda}} \prod_{i=1}^{3} \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} d\xi^i_{xy}\, e^{-\frac{1}{2}\xi^{i\,2}_{xy}} \underbrace{e^{i\sqrt{2\beta}\left((\sigma_1 - g_1)^i - (\sigma_2 - g_2)^i\right)}}_{= e^{i\sqrt{2\beta}(\sigma_1 - g_1)^i} e^{-i\sqrt{2\beta}(\sigma_2 - g_2)^i}}$$

→ Back into the integral, take the square, regroup integrals over Ω_1, resp. Ω_2, and use Cauchy-Schwarz

$$\int d\xi\, d\chi\, f_1(\xi) f_1(\chi) f_2(\xi) f_2(\chi)$$

$$= \langle f_1, f_2 \rangle^2 \le \|f_1\|^2 \|f_2\|^2 = \int d\xi\, f_1(\xi) f_1(\xi) \int d\chi\, f_2(\chi) f_2(\chi)$$

use $(*)$ backwards to conclude □

2) The quantum case. [Dyson-Lieb-Simon 78]

- This is restricted to the antiferromagnet. No proof to this day of spontaneous magnetization for the ferromagnet!
- Same strategy as in the classical case.
  But: IRB holds easily for the so-called Duhamel's two-point function. Work is needed to obtain IRB for the thermal two-point function.
- We consider

$$H^{(u)}_\Lambda = -2 \sum_{(x,y)\in\mathcal{E}_\Lambda} \left(S^1_x S^1_y + S^2_x S^2_y + u S^3_x S^3_y \right) \quad \text{on } \Lambda = \left\{-\tfrac{L}{2}+1, \dots, \tfrac{L}{2}\right\}^d$$
periodic, $L \in 2\mathbb{N}$

$u = +1$: usual isotropic ferromagnet
$u = 0$: XY model

$u=-1$: unitarily equivalent to the isotropic antiferromagnet.
Let $U_\Lambda := \prod_{x\in\Lambda_A} e^{i\pi S_x^3}$ on a bipartite lattice.

where $\Lambda = \Lambda_A \cup \Lambda_B$ and $(x,y)\in\mathcal{E}_\Lambda \Rightarrow \begin{pmatrix} x\in\Lambda_A \\ y\in\Lambda_B\end{pmatrix}$ or $\begin{pmatrix} x\in\Lambda_B \\ y\in\Lambda_A\end{pmatrix}$

(bipartite lattice)

$\rightarrow$ $e^{i\pi S_x^3}$ rotated S_x^1 & S_x^2 by π i.e.
$S_x^{1,2} \rightarrow -S_x^{1,2}$

$$\Rightarrow U_\Lambda^{-1} H_\Lambda^{u} U_\Lambda = 2\sum_{(x,y)\in\mathcal{E}_\Lambda}\left(S_x^1S_y^1 + S_x^2S_y^2 - uS_x^3S_y^3\right).$$

<u>Theorem</u>. Consider $H_\Lambda^{(u)}$ for $u\in[-1,0]$. Then

$$\frac{1}{|\Lambda|}\sum_{x\in\Lambda}\omega_\beta(S_0^3S_x^3) \geq \frac{1}{3}S(S+1) - \frac{1}{\sqrt{2}|\Lambda|}\sum_{k\in\Lambda^*\setminus\{0\}}\left(\frac{E_u(k)}{E(k)}\right)^{1/2}$$

$$- \frac{1}{2\beta|\Lambda|}\sum_{k\in\Lambda^*\setminus\{0\}}\frac{1}{E(k)}$$

where
$$E_u(k) = \sum_{\alpha=1}^{d}\Big[(1-u\cos k_\alpha)\omega_\beta(S_0^1S_{e_\alpha}^1) + (u-\cos k_\alpha)\,\omega_\beta(S_0^2S_{e_\alpha}^2)\Big]$$

• Note: * Again, the last term is summable for $d\geq 3$, and arb. small for β large
* Since $\sum_{i=1}^{3}(S_x^i)^2 = (S_x)^2 = S(S+1)$, then
* $|\omega_\beta(S_0^1S_{e_\alpha}^1)|^2 \leq \omega_\beta((S_0^1)^2)\,\omega_\beta((S_{e_\alpha}^1)^2) \leq (\omega_\beta((S)^2))^2 = (S(S+1))^2$

so that $E_u(k) \leq S(S+1)\sum_\alpha(1+u)(1-\cos k_\alpha)$ ~~$\leq dS(S+1)$~~

i.e. $\frac{E_u(k)}{E(k)} \leq S(S+1)$

and $-\frac{1}{\sqrt{2}}\frac{1}{|\Lambda|}\sum(\dots) \geq \frac{1}{\sqrt{2}}\sqrt{S(S+1)}$ in $\liminf_{L\to\infty}$

All in all

$$\liminf_{L\to\infty} \frac{1}{|\Lambda_L|} \sum_{x\in\Lambda_L} \omega_\beta(S_0^3 S_x^3) > 0$$

for $S \geq 2$, $d \geq 3$ and β large enough.

the estimates can be improved to obtain the result for $(d \geq 3, S \geq 1)$ or $(S \geq \frac{1}{2}, d$ large$)$

Later improved to cover $d \geq 3$, $S \geq \frac{1}{2}$.

* Case $\nu = -1$: Implement U_Λ to get

$$\liminf_{L\to\infty} \frac{1}{|\Lambda_L|} \sum_{x\in\Lambda_L} (-1)^{d(0,x)} \omega_{\beta,\text{Heis.antif.}}(S_0^3 S_x^3) > 0.$$

"Néel ordering":

$$\begin{array}{c} \vdots \\ \cdots \uparrow \downarrow \uparrow \downarrow \uparrow \downarrow \cdots \\ \cdots \downarrow \uparrow \downarrow \uparrow \downarrow \uparrow \cdots \\ \vdots \end{array}$$

* The usual IRB cannot hold as such. $(S = \frac{1}{2})$

i) $\underbrace{\omega_\beta(\vec{S}_0\cdot\vec{S}_0)}_{=3/4} - \underbrace{\omega_\beta(\vec{S}_0\cdot\vec{S}_x)}_{\leq 1/4} \geq \frac{1}{2} \quad \forall \beta.$ (eigenvalues of $\vec{S}_0\cdot\vec{S}_x$ are $-\frac{3}{4}; \frac{1}{4}$) + positivity of $\omega_\beta(\cdot)$.

ii) if IRB were to hold:

$$\left|\omega_\beta(\vec{S}_0\cdot\vec{S}_0) - \omega_\beta(\vec{S}_0\cdot\vec{S}_x)\right| = \frac{1}{|\Lambda|}\left|\sum_{k\in\Lambda^*} (1 - e^{ikx})\,\widehat{\omega_\beta(\vec{S}_0\cdot\vec{S}_\bullet)}(k)\right|$$

$$\leq \frac{C}{\beta|\Lambda|} \sum_{k\in\Lambda^*} \frac{|1-e^{ikx}|}{E(k)} \longrightarrow 0 \quad (\beta\to\infty)$$

(i) and (ii) are a contradiction

$\to$ the quantum case is truly harder; what holds is weaker:

$$\widehat{\omega_\beta(S_0^3 S_x^3)}(k) \leq \frac{1}{\sqrt{2}}\sqrt{\frac{E_k(k)}{E(k)}} + \frac{1}{2\beta E(k)}.$$

- Reflection positivity & Gaussian domination

The quantum separation lemma (i.e. RP!):

<u>Lemma 1</u>: $\mathcal{H} = \mathcal{K} \otimes \mathcal{K}$, $\dim \mathcal{K} < \infty$, $A, B, C_1, \dots, C_\ell \in \mathcal{B}(\mathcal{K})$, are <u>real</u> matrices, $h_1, \dots, h_\ell \in \mathbb{R}$. Then

$$\mathrm{Tr}\left(e^{A\otimes 1 + 1\otimes B - \sum_k (C_k \otimes 1 - 1 \otimes C_k - h_k)^2}\right)^2$$

$$\leq \mathrm{Tr}\left(e^{A\otimes 1 + 1\otimes A - \sum_k (C_k\otimes 1 - 1\otimes C_k)^2}\right) \mathrm{Tr}(A \leftrightarrow B)$$

The proof relies on the operator identity

$$e^{-D^2} = \frac{1}{\sqrt{4\pi}} \int e^{ihD} e^{-\frac{1}{4}h^2} dh,$$

again Trotter's product formula and Cauchy-Schwarz – exercise.

We consider the partition function:

$$\tilde{Z}_\Lambda(\beta, v) := \mathrm{Tr}\, e^{-\beta \tilde{H}_\Lambda(v)}$$

where $\tilde{H}_\Lambda(v) = \sum_{x\in\Lambda} ((S_x^1)^2 + u(S_x^2)^2 + (S_x^3)^2)(-2d)$

$$+ \sum_{(x,y)\in\mathcal{E}_\Lambda} \left[(S_x^1 - S_y^1)^2 + (\sqrt{u} S_x^2 - \sqrt{u} S_y^2)^2 + \left(S_x^3 + v_x - S_y^3 - v_y\right)^2 \right]$$

<u>Lemma 2</u>: $\tilde{Z}_\Lambda(\beta, v) \leq \tilde{Z}_\Lambda(\beta, 0)$. (G.D.).

By the same argument as in the classical case, this follows from RP:

<u>Lemma 3</u>: If $u \leq 0$, then for any reflection R:

$$\tilde{Z}_\Lambda(\beta, (v_1, v_2))^2 \leq \tilde{Z}_\Lambda(\beta, (v_1, Rv_1)) \tilde{Z}_\Lambda(\beta, (Rv_2, v_2))$$

Proof: Follows from Lemma 1 with the following identification: directly.

$A\otimes 1 = -\beta \tilde{H}_{\Lambda_1}(v)$; $1 \otimes B = -\beta \tilde{H}_{\Lambda_2}(v)$

$C_{h,1} = -\sqrt{\beta}\, S^1_{z_h}$; $C_{h,2} = \sqrt{\beta u}\, S^2_{z_h}$; $C_{h,3} = \sqrt{\beta}\, S^3_{z_h}$; $h_{h,i} = v_{z_h} \delta_{i,3}$.

and z_h is either x_h or y_h for each pair $(x,y) \in \mathcal{E}_\Lambda$: $x \in \Lambda_1, y \in \Lambda_2$.

Note: in the standard basis: S^1, S^3 are real, S^2 is purely imaginary; in order to apply Lemma 1, the condition $\boxed{u \leq 0}$ is therefore necessary. $\square$

Gaussian domination rewritten: let $(\partial_i v)_x = v_x - v_{x+e_i}$:

$$\tilde{Z}_\Lambda(\beta, v) \leq \tilde{Z}_\Lambda(\beta, 0) \iff \frac{\mathrm{Tr}\left(e^{-\beta H_\Lambda + 2S(\sum_i \partial_i v)}\right)}{\mathrm{Tr}\left(e^{-\beta H_\Lambda}\right)} \leq e^{\frac{\|\partial v\|^2}{\beta}}$$

where $S(h) = \sum_{x\in\Lambda} S_x \cdot h_x$ and $h_x = v_x e_3$,

and $\|\partial v\|^2 = \sum_{(x,y)\in\mathcal{E}_\Lambda} (v_x - v_y)^2$

- It remains to prove that GD $\Rightarrow$ the good IRB.

The main tool is Duhamel's two-point function:

$$(A,B)_\beta := Z_\Lambda(\beta)^{-1} \int_0^1 \mathrm{Tr}\left(e^{-s\beta H} A e^{-(1-s)\beta H} B\right) ds$$

with its relation to the thermal expectation value: (here at $\beta = 1$)

$$(\heartsuit) \quad \frac{1}{2}\omega(\{A^+, A\})\, \phi\left(\frac{\omega([A^+,[H,A]])}{2\omega(\{A^+,A\})}\right) \leq (A^+, A) \leq \frac{1}{2}\omega(\{A^+,A\})$$

non-trivial: Falk-Bruch inequality

simple

$\phi(x \tanh(x)) = x^{-1}\tanh(x)$

with $(\heartsuit)$, morally: controlling $(\cdot,\cdot)_\beta$ suffices to control $\omega_\beta(\cdot,\cdot)$

Lemma 4: If $\tilde{Z}(\beta,v) \leq \tilde{Z}(\beta,0)$, then

$$\widehat{(S_0^3, S_x^3)_\beta}(h) \leq \frac{1}{2\beta E(h)} \qquad h \in \Lambda^* \setminus \{0\}$$

Morally, the proof is simply to check that the Hessian of $\tilde{Z}$ is non-positive at $v=0$. In order to compute derivative of $\tilde{Z}$ w.r.t. v, we use Duhamel's formula:

$$e^{A+B} = e^{A} + \int_0^1 e^{sA} B e^{(1-s)(A+B)} dt$$

$$\left(= \sum_{k=0}^{\infty} \int_{0 \leq t_1 \leq \dots \leq t_k \leq 1} dt_1 \dots dt_k \, e^{t_1 A} B e^{(t_2 - t_1)A} B \dots B e^{(1-t_k)A} \right).$$

It follows from: $f(s) := e^{sA} + \int_0^s e^{tA} B e^{(s-t)(A+B)} dt$

satisfies $f'(s) = e^{sA} A + e^{sA} B + \int_0^s e^{tA} B e^{(s-t)}(A+B) dt$

$$= f(s)(A+B),$$

with $f(0) = \mathbb{1}$, hence

$$f(s) = e^{s(A+B)}$$

Proof: $\tilde{Z}(\beta,v) \leq \tilde{Z}(\beta,0)$ and $v \mapsto \tilde{Z}(\beta,v)$ continuously differentiable implies that $\left.\frac{\partial^2 \tilde{Z}}{\partial v_x \partial v_y}\right|_{v=0} \leq 0$. (concavity)

We write $\tilde{H}(v) = \underbrace{\tilde{H}(0)}_{=H} + 2\sum_{(x,y)\in \mathcal{E}_\Lambda} (S_x^3 - S_y^3)(v_x - v_y) + \sum_{(x,y)\in\mathcal{E}_\Lambda} (v_x - v_y)^2$

and $\tilde{Z}(\beta,v) = \mathrm{Tr}\left[\exp\left(-\beta H - 2\beta \sum (S_x^3 - S_y^3)(v_x - v_y)\right)\right] \exp\left(-\beta \sum (v_x - v_y)^2\right)$

$$=: \mathrm{Tr}\left(e^{A+B(v)}\right) f(v)$$

note: $-B(v) = 2\beta \sum_x S_x h_x$ where $h_x = \sum_y (v_x - v_y)$

$f(v) = \exp\left(-\beta \sum_x v_x h_x\right)$; $f(0) = 1$

and $\left.\frac{\partial}{\partial v_i} f\right|_{v=0} = -\beta \left[h_i + \sum_x v_x \frac{\partial}{\partial v_i} h_x\right] f(v)\Big|_{v=0} = 0$

Now: we choose $v_x^{(h)} = \varepsilon \cos hx$, $h \neq 0$ ($h=0$ is the maximizer.)
and recall $\sum_{xy} v_x^{(h)} - v_y^{(h)} = h_x^{(h)} = E(h)\, v_x^{(h)}$

$$\frac{d^2 \tilde{Z}}{d\varepsilon^2}\Big|_{\varepsilon=0} \le 0 \Rightarrow \frac{d^2}{d\varepsilon^2} \mathrm{Tr}\left(e^{A+B(\varepsilon)}\right)_{\varepsilon=0} + \mathrm{Tr}(e^A)\, f''(0) \le 0$$

Duhamel: $$e^{A+B(\varepsilon)} = e^A + \int_0^1 dt\, e^{tA} B(\varepsilon) e^{(1-t)A} + \int_0^1 dt \int_0^{1-t} ds\, e^{tA} B(\varepsilon) e^{sA} B(\varepsilon) e^{(1-t-s)(A+B(\varepsilon))}$$

Since $B(\varepsilon)$ is linear in ε:

$$\frac{d^2}{d\varepsilon^2} \mathrm{Tr}\left(e^{A+B(\varepsilon)}\right)\Big|_{\varepsilon=0} = 2 \int_0^1 dt \int_0^{1-t} \mathrm{Tr}\left(e^{tA} B'(0) e^{sA} B'(0) e^{(1-t-s)A}\right)$$

$$= 4\beta^2 Z(\beta) \sum_{x,y} E(h)^2 \cos hx \cos hy\, (S_x, S_y)_\beta$$

$$= 4\beta^2 Z(\beta) \sum_{x,z} E(h)^2 \cos hx \cos h(z+x)\, (S_0, S_z)_\beta$$

using $\sum_z \mathrm{Re}\, e^{ihx} e^{ihz} (S_0, S_z)_\beta = \cos hx\, \widehat{(S_0, S_z)_\beta}(h)$

F.T is real as $(S_0, S_z) = (S_0, S_{-z})$

$$= 4\beta^2 Z(\beta) \Big(\sum_x \cos^2 hx\Big) \widehat{(S_0, S_0)}(h)$$

on the other hand: $f''(0) = -2\beta E(h) \sum_x (\cos^2 hx)$

$$\Rightarrow \widehat{(S_0, S_0)}(h) \le \frac{1}{2\beta E(h)} \qquad h \in \Lambda^* \setminus \{0\}$$

$\square$

It remains to obtain the bound on the thermal correlation function.
We use Falk-Bruch's inequality:

$$\frac{1}{2} \omega_\beta(\{A^*, A\}) \le \frac{1}{2} \sqrt{(A^*, A)_\beta\, \omega_\beta([A^*, [H, A]])} + (A^*, A)_\beta$$

A explicit calculation gives, for $A = \widehat{S^3}(h) = \sum_x e^{-ihx} S_x^3$

$$\omega_\beta([A^*, [H, A]]) = 4\beta |\Lambda|\, \mathcal{E}_u(h)$$

$$(A^+, A) = \sum_{x,y} \int \mathrm{Tr}\left(e^{sH} S_x^3 e^{(1-s)H} S_y^3\right) e^{ik(x-y)}$$
$$= |\Lambda| \, \widehat{(S_0^3, S_\bullet^3)}(k)$$

$$\omega_\beta(\{A^+, A\}) = 2|\Lambda| \, \widehat{\omega_\beta(S_0^3, S_\bullet^3)}(k) \quad ,$$

All in all, this proves

<u>Lemma 5</u> : If $\widehat{(S_0^3, S_\bullet^3)_\beta}(k) \leq \frac{1}{2\beta E(k)}$, then

$$\widehat{\omega_\beta(S_0^3 S_\bullet^3)}(k) \leq \sqrt{\frac{E_u(k)}{E(k)}} + \frac{1}{2\beta E(k)} \qquad (IRB).$$

<u>Proof of DLS-Theorem:</u>

$$\frac{1}{|\Lambda|}\sum_x \omega_\beta(S_0^3 S_x^3) = \frac{1}{|\Lambda|}\widehat{\omega_\beta(S_0^3 S_\bullet^3)}(0)$$
$$= \underbrace{\omega_\beta(S_0^3 S_0^3)}_{=1/3} - \underbrace{\frac{1}{|\Lambda|}\sum_{k\in\Lambda^*\setminus\{0\}} \widehat{\omega_\beta(S_0^3 S_\bullet^3)}(k)}_{\text{conclude by lemma 5}}$$

$\square$

:-)

d) The $\beta=\infty$ case: ground states

- Understanding ground states (G.S.) and their properties can sometimes be achieved by taking the limit $\beta\to\infty$. But as we have seen, not always (LRO in 2d was restricted to $\beta<\infty$). The methods to understand G.S. can be quite different.
- We consider the Heisenberg models on graphs Λ that are connected, and for this chapter, restrict attention to $|\Lambda|<\infty$.

$$H_\Lambda^{F/AF} = -J\sum_{(x,y)\in\mathcal{E}_\Lambda} S_x\cdot S_y \qquad \begin{cases} J>0 : \text{Ferromagnet} \\ J<0 : \text{Antiferromagnet}\end{cases}$$

We'll prove:

Theorem 1 [Ferromagnet] $S=\frac{1}{2}$. Let $J>0$, Λ connected. Let E_Λ^F be the smallest eigenvalue of H_Λ^F.

Then, the eigenspace corresponding to E_Λ^F has dimension $|\Lambda|+1$ and consists of all vectors invariant under permutations of the vertices.

Theorem 2 [Antiferromagnet] any S. ~~Periodic chain~~ Let $J<0$, Λ connected. Let E_Λ^{AF} be the smallest eigenvalue of H_Λ^{AF}.

Then, there is a unique vector Ω_Λ^{AF} corresponding to E_Λ^{AF}, and it is totally antisymmetric under permutation of the vertices.

- In terms of representation of $SU(2)$:

Ferromagnet: Ground states ~~form~~ span the maximum spin irreducible representation of $\bigotimes_{x\in\Lambda} D_{1/2}$

Antiferromagnet: The unique ground state is the unique vector of the minimal spin representation of $\bigotimes_{x\in\Lambda} D_{1/2}$

• Proof of Thm 1 : * Denote by $\lambda_0(A)$ the smallest eigenvalue of the operator A.

* Note that

$$S_x \cdot S_y = \frac{1}{2} T_{xy} - \frac{1}{4}$$

where $T_{xy}(u \otimes v) = v \otimes u$ (transposition)

This is checked easily on the eigenbasis of $S_x \cdot S_y$:

$$\psi_a = \frac{1}{\sqrt{2}}\big(|+-\rangle - |-+\rangle\big) \qquad \text{eigenvalue } -\frac{3}{4}$$

$$\left.\begin{aligned} \psi_s^{(1)} &= \frac{1}{\sqrt{2}}\big(|+-\rangle + |-+\rangle\big) \\ \psi_s^{(2)} &= |++\rangle \\ \psi_s^{(3)} &= |--\rangle \end{aligned}\right\} \text{eigenvalue } \frac{1}{4}$$

$$\Rightarrow \quad H_\Lambda^F = -\frac{J}{2} \sum_{(x,y)\in \mathcal{E}_\Lambda} \Big(T_{xy} - \frac{1}{2}\Big) \quad ; \quad \mathrm{Spec}(T_{xy}) = \{-1 ; +1\}.$$

and it suffices to look at the eigenvectors of

$$\tilde{H}_\Lambda^F = - \sum_{(x,y)\in \mathcal{E}_\Lambda} T_{xy}$$

* Define ~~$|\Lambda|$~~ $|\Lambda| =: N$; $|\mathcal{E}_\Lambda| =: E$

* Now : $\lambda_0(\tilde{H}) \geq -E$

Indeed: for any $A = A^*$, $B = B^*$: $\lambda_0(A+B) \geq \lambda_0(A) + \lambda_0(B)$

$$\lambda_0(A+B) = \inf_{\|\psi\|=1} \langle \psi, (A+B)\psi \rangle = \inf \Big(\underbrace{\langle \psi, A\psi\rangle}_{\geq \lambda_0(A)} + \underbrace{\langle \psi, B\psi \rangle}_{\geq \lambda_0(B)} \Big).$$

and $\lambda_0(-T_{xy}) = -1$.

* for any ~~basis~~ ~~vec~~ vector $v \in \mathbb{C}^2$:

$$\tilde{H}_\Lambda^F\Big(\bigotimes_{x\in\Lambda} v\Big) = -E\Big(\bigotimes_{x\in\Lambda} v\Big)$$

$$\Rightarrow \quad \lambda_0(\tilde{H}_\Lambda^F) = -E \; .$$

Further claim: $\tilde{H}^F_\Lambda \Omega_\Lambda = -E\Omega_\Lambda$ only if

$$T_{xy}\Omega_\Lambda = \Omega_\Lambda \quad \forall (x,y)\in \mathcal{E}_\Lambda .$$

Indeed. Let ψ_0 be s.t. $(A+B)\psi_0 = \lambda_0(A+B)$. Then

$$\langle \psi_0, (A+B)\psi_0\rangle = \lambda_0(A+B) \underset{\uparrow \text{assumption}}{=} \lambda_0(A)+\lambda_0(B)$$

$$\overset{\shortparallel}{\underbrace{\langle\psi_0, A\psi_0\rangle}_{\geq \lambda_0(A)} + \underbrace{\langle\psi_0, B\psi_0\rangle}_{\geq \lambda_0(B)}}$$

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Since any permutation π of the set Λ can be written as a product of transpositions τ_{xy}, $(x,y)\in\mathcal{E}_\Lambda$; for any Ω_Λ, we have that

$$U_\pi \Omega_\Lambda \overset{!}{=} \Omega_\Lambda$$

where $U_\pi(v_1\otimes\cdots\otimes v_N) = v_{\pi_1}\otimes\cdots\otimes v_{\pi_N}$

Conclude: If Ω_Λ is a G.S., then $U_\pi\Omega_\Lambda = \Omega_\Lambda \;\forall\pi$.
Vice versa, if $U_\pi\Omega_\Lambda = \Omega_\Lambda\;\forall\pi$, then
$T_{xy}\Omega_\Lambda = \Omega_\Lambda \;\forall (x,y)\in\mathcal{E}_\Lambda$ $\quad (T_{xy} = U_{\tau_{xy}})$.

It remains to compute the dimension of the ground state space.
If $\{e_1, e_2\}$ is a basis of $\mathbb{C}^2$, the vectors

$$\psi_h := \frac{1}{N!}\sum_{\pi\in S(\Lambda)} U_\pi\Big(\underbrace{(e_1\otimes\cdots\otimes e_1)}_{h}\otimes\underbrace{(e_2\otimes\cdots\otimes e_2)}_{N-h}\Big)$$

form an ON-basis of permutation-invariant vectors $\square$

in particular that $\langle\psi_h, S^3_0 S^3_x\psi_h\rangle = C_h$, where
is independent of x.

• Proof of Thm 2 : Recall, $S_x^1 S_y^1 + S_x^2 S_y^2 = \frac{1}{2}(S_x^+ S_y^- + S_x^- S_y^+)$

Define $S_{tot} = \sum_{x\in\Lambda} S_x$, $S_{A,B} = \sum_{x\in\Lambda_{A,B}} S_x$

$S_{tot}^3 = \sum_{x\in\Lambda} S_x^3$, $S^2 := (S_{tot})^2$

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$$\Psi_\alpha := \prod_{x\in\Lambda_A} \exp(i\pi S_x^3) e_\alpha = \exp(i\pi S_A^3) e_\alpha$$

Symmetries : ~~$[H_\Lambda^{AF}, (S_{tot}^2)] = [H_\Lambda^{AF}, (S_{tot}^3)] = [(S_{tot}^2), S_{tot}^3] = 0$~~

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→ We search for joint eigenvectors of all three operators

Eigenvalues of S^2: $S(S+1)$

↳ $(2S+1)$-fold degenerate, one level for each M, with $-S \le M \le S$ and S_{tot}^3 has eigenvalue M.

Hence: (i) $H_\Lambda^{AF} = J\sum_{(x,y)\in\mathcal{E}_\Lambda} S_x^3 S_y^3 + \frac{J}{2}\sum_{(x,y)\in\mathcal{E}_\Lambda}(S_x^+ S_y^- + S_y^+ S_x^-)$

$=: H_\Lambda^d + H_\Lambda^{off}$

$H_\Lambda^d \Psi_\alpha = \varepsilon_\alpha \Psi_\alpha$ (H_Λ^d is diagonal)

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(ii) H_Λ^{AF} is block diagonal, with blocks indexed by M.

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Then, the eigenspace corresponding to E_Λ^F has dimension $|\Lambda|+1$ and consists of all vectors invariant under permutations of the vertices

<u>Theorem 2</u> [Antiferromagnet, any S, ~~periodic chain~~]. Let $J<0$, Λ connected. Let E_Λ^{AF} be the smallest eigenvalue of H_Λ^{AF}.

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⇒ any two vectors Ψ_α, Ψ_β, $\langle \Psi_\alpha, (H_\Lambda^{AF})^\ell \Psi_\beta \rangle \neq 0$ for ℓ sufficiently large.

→ By Perron-Frobenius, $\left(-H_\Lambda^{AF}\restriction_{\mathcal{H}^{(M)}}\right)$ has a unique eigenvector $\Omega_\Lambda^{(M)}$ for the largest eigenvalue, and it is strictly positive :

$$\Omega_\Lambda^{(M)} = \sum_\alpha c_\alpha \psi_\alpha^{(M)} \Rightarrow c_\alpha > 0 \quad \forall \alpha .$$

Define $\quad H_\Lambda^{AF} \Omega_\Lambda^{(M)} = E_\Lambda^{(M)} \Omega_\Lambda^{(M)}$

Finally, we look for ground states that are also eigenvectors for S^2, and by rotation invariance, $S^2\psi^{(S)} = S(S+1)\psi^{(S)}$ must be of the form $\psi^{(S)} = \sum_{-S\le M\le S} d_M^{(S)} \psi^{(S,M)}$, $\psi^{(S,M)} \in \mathcal{H}^{(M)}$

We observe : the G.S. of $\tilde{H}_\Lambda = S_A \cdot S_B$, $\tilde{\Omega}$, has $S_{tot}^2 \tilde{\Omega} = 0$, and as above $\tilde{\Omega}$ is positive.

Hence, $\langle \Omega_\Lambda^{(0)}, \tilde{\Omega} \rangle > 0$,

but $\langle \Omega_\Lambda^{(0)}, \tilde{\Omega} \rangle = \frac{1}{S(S+1)} \langle \Omega_\Lambda^{(0)}, \underbrace{S_{tot}^2 \tilde{\Omega}}_{=0} \rangle$

$$\Rightarrow \quad S_{tot}^2 \Omega_\Lambda^{(0)} = 0 .$$

By rotation invariance, $d_M^{(S)} \neq 0 \ \forall M$; i.e. any eigenvector of S^2 must have a component in $\mathcal{H}^{(0)}$. But the G.S of $H_\Lambda^{AF}\restriction_{\mathcal{H}^{(0)}}$ is an eigenvector for $S=0$. Hence, all others must have a higher energy and the G.S. Ω_Λ of H_Λ^{AF} is $\Omega_\Lambda = \Omega_\Lambda^{(0)}$ $\square$

- An interesting further spectral property: if the spin is <u>half-integer</u>, then the spectral gap above the ground state energy of a chain of length L is $O(\frac{1}{L})$ → gapless system in the thermodynamic limit. → see exercises.

Conjecture (Haldane) : for <u>integer</u> spins, $\liminf_{L\to\infty}$ (spectral gap) $= \gamma > 0$.

Poisson processes (Homogeneous)

- $\lambda > 0$. X_t is a Poisson process with rate λ if

  i) $X_0 = 0$ almost surely

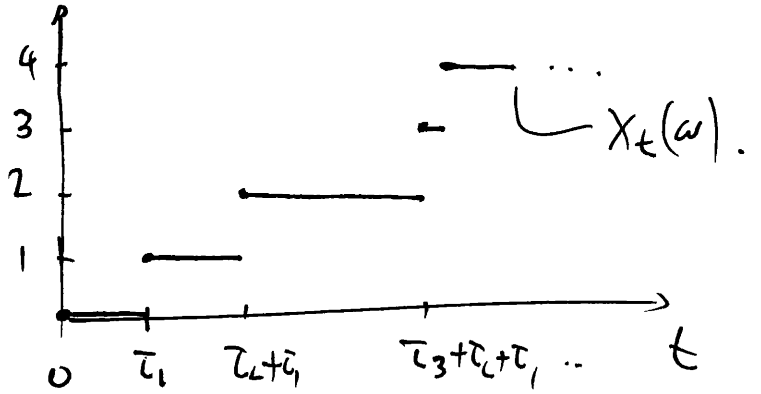
  ii) independent increments: $0 \le t_1 \le \dots \le t_n$:
  $X_{t_1}, X_{t_2} - X_{t_1}, \dots, X_{t_n} - X_{t_{n-1}}$ are independent random variables. (R.V.)

  iii) $0 \le s < t < \infty$: $X_t - X_s$ has Poisson distribution with parameter $\lambda(t-s) = \mu$:
  $$\mathbb{P}(X_t - X_s = k) = \frac{\mu^k}{k!} e^{-\mu} .$$

- Explicit construction: $\tau_1, \tau_2, \dots$: a sequence of i.i.d. R.V. with exponential distribution with parameter λ: density
$$~~p(\tau_i~~ \quad f(t) = \begin{cases} \lambda e^{-\lambda t} & t \ge 0 \\ 0 & t < 0 \end{cases}$$

Then define: $X_t : t \ge 0$:
$$X_t(\omega) = \sup \{ n : \sum_{i \le n} \tau_i(\omega) \le t \}$$

- Note: the t_i's are the "time between jumps", X_t the number of jumps, up to time t.



- Useful property: $\sigma_i := \sum_{j \le i} \tau_j$ "jump times".

then: given $\{X_t = k\}$, we have that

$$(\sigma_1, \dots, \sigma_k) \overset{d}{\sim} (U_{(1)}, \dots, U_{(k)})$$

where $U_1, \dots, U_k$ are i.i.d. uniform in $[0,t]$

and $U_{(1)} < U_{(2)} < \dots < U_{(k)}$ are the ordered values.

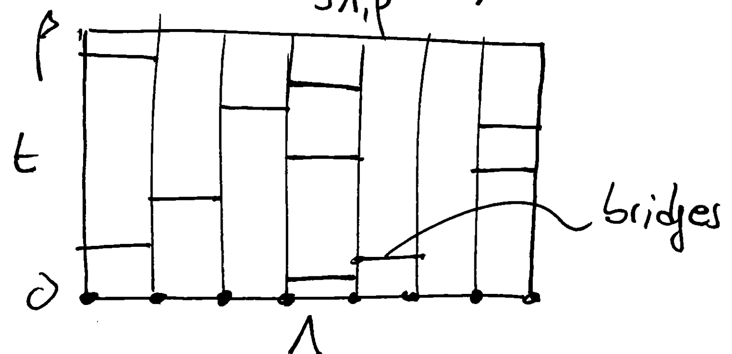
In other words: the jump times $\sigma_1, \dots, \sigma_k$ are uniformly distributed in the simplex $0 \le t_1 \le t_2 \le \dots \le t_k \le t \subset [0,t]^k$.

e) Stochastic representations of quantum spin chains

- It is useful to develop a different — though of course equivalent — point of view of physical models, or mathematical problems. e.g. harmonic analysis $\leftrightarrow$ Brownian motion.
- In classical lattice systems, a useful connection is with random walks: recurrence/transience $\leftrightarrow$ breaking/not of symmetry.
- These give mathematical insight and tools.
- Now: Some quantum spin chains can be related to classical probabilistic models of random loops/cycles.
- Define a Poisson edge process:
  $(\Lambda, \mathcal{E}_\Lambda)$ a finite graph.
  For each $e \in \mathcal{E}_\Lambda$, we attach a Poisson process on $[0,\beta]$ with intensity 1; processes for different edges are independent.
  A realization of that process is a finite sequence of pairs:

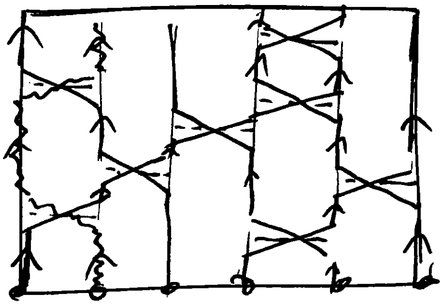
$$\omega = \big((e_1,t_1), \underbrace{(e_2,t_2)}_{\text{"bridge"}} \dots, (e_k,t_k) \big) \quad ; \quad t_i \in [0,\beta], \; e_i \in \mathcal{E}_\Lambda$$

  - \# of bridges per edge : Poisson r.v. with mean β
  - \# of bridges in total : —— " —— $\beta|\mathcal{E}_\Lambda|$
  - Conditional on there being k bridges, the times of arrival are uniformly distributed, and the edges are chosen uniformly in $\mathcal{E}_\Lambda$.
  - Denote the measure $d\rho_{\Lambda,\beta}(\omega)$.

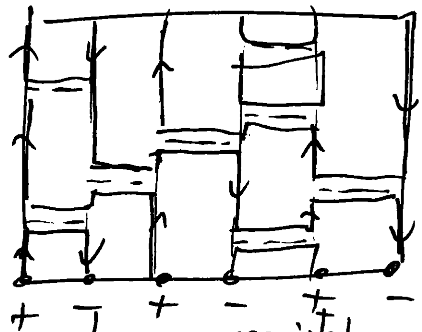


- To $\rho_{\Lambda,\beta}$, we associate cycles or loops.

Consider the cylinder $\Lambda \times [0,\beta]_{\text{periodic}}$



cycles associated to ω



loops associated with ω, on a bipartite lattice.

$C(\omega)$: config. of cycles
$|C(\omega)|$: # of cycles

length of a cycle: $\min\{L : \gamma(L) = \gamma(0)\}$ and $L = k \cdot \beta$, $k \in \mathbb{N}$

$\mathcal{L}(\omega)$: config. of loops.
$|\mathcal{L}(\omega)|$: # of loops.

length of a loop: $\min\{L : \gamma(L) = \gamma(0)\}$. here L can be anything.

Now: The Heisenberg models at $h=0$ are associated with the measures

$2^{|C(\omega)|} d\rho_{\Lambda,\beta}(\omega)$ for the ferromagnet

$2^{|\mathcal{L}(\omega)|} d\rho_{\Lambda,\beta}(\omega)$ for the antiferromagnet.

Precisely:

- <u>Theorem</u>: Let $\omega^F_{\beta,\Lambda,h}$ denote the Gibbs state at inverse temp. β for the Heisenberg ferromagnet, and $Z^F_\Lambda(\beta,h)$ its partition function.

$$Z^F_\Lambda(\beta,h) = e^{-\frac{\beta}{2}|\mathcal{E}_\Lambda|} \int d\rho_{\Lambda,\beta}(\omega) \prod_{\gamma \in C(\omega)} \left(2\cosh(hL(\gamma))\right).$$

$$\omega^F_{\beta,\Lambda,h}(S^3_x) = \frac{1}{2} e^{-\frac{\beta}{2}|\mathcal{E}_\Lambda|} \int d\rho_{\Lambda,\beta}(\omega) \prod_{\gamma \in C(\omega)} \left(2\cosh(hL(\gamma))\right) \cdot \tanh(hL(\gamma_x)).$$

and

$$\omega^{F}_{2\beta,\Lambda,h}\left(S^3_x S^3_y\right) = \frac{1}{4} e^{-\frac{\beta}{2}|\mathcal{E}_\Lambda|} \int d\rho_{\Lambda,\beta}(\omega) \prod_{\gamma\in C(\omega)} \left(2\cosh(hL(\gamma))\right) \cdot$$

$$\begin{cases} 1 & \text{if } \gamma_x = \gamma_y \\ \tanh(hL(\gamma_x))\tanh(hL(\gamma_y)) & \text{if } \gamma_x \neq \gamma_y \end{cases}$$

Before we prove this, let us rewrite it:

$$2\cosh(hL(\gamma)) = e^{hL(\gamma)}\left(1+e^{-2hL(\gamma)}\right)$$

$$\sum_{\gamma\in C(\omega)} L(\gamma) = \beta|\Lambda|$$

Define

$$\mathbb{P}_{\Lambda,\beta,h}(d\omega) := Z^F_\Lambda(2\beta,h)^{-1} e^{-\frac{\beta}{2}|\mathcal{E}_\Lambda| + \beta h|\Lambda|} \cdot \rho_{\Lambda,\beta}(d\omega) \prod_{\gamma\in C(\omega)} \left(1+e^{-2hL(\gamma)}\right)$$

Then:

$$\omega^F_{\Lambda,2\beta,h}(S^3_x) = \frac{1}{2}\mathbb{E}_{\Lambda,\beta,h}\left(\tanh(hL(\gamma_x))\right)$$

$$\omega^F_{\Lambda,2\beta,h}(S^3_x S^3_y) = \frac{1}{4}\mathbb{P}_{\Lambda,\beta,h}(\gamma_x=\gamma_y) + \frac{1}{4}\mathbb{E}_{\Lambda,\beta,h}\left(1_{\gamma_x\neq\gamma_y}\tanh\cdot\tanh\cdot\right).$$

and if $h=0$:

$$\omega^F_{\Lambda,2\beta,0}(S^3_x) = 0$$

$$\omega^F_{\Lambda,2\beta,0}(S^3_x S^3_y) = \frac{1}{4}\mathbb{P}_{\Lambda,\beta,h}(x \text{ and } y \text{ belong to the same cycle}).$$

:)

- Proof: Relies again on Duhamel's formula:

$$e^{A+B} = \sum_{n\geq 0}\int_{0\leq t_1\leq\dots\leq t_n\leq 1} dt_1\dots dt_n\, e^{t_1 A} B e^{(t_2-t_1)A} B \dots B e^{(1-t_n)A}$$

(exercise: prove that the series converges)

Apply this to $e^{-\beta H^F_{\Lambda,h}}$, where we write:

$$H^F_{\Lambda,h} = -\frac{1}{2}\sum_{e\in\mathcal{E}_\Lambda} T_e - h\sum_{x\in\Lambda} S_x^3 = -\sum_e \frac{1}{2}T_e - h\Pi_\Lambda$$

and dropped the constant $\frac{1}{4}\sum_{e\in\mathcal{E}_\Lambda} = \frac{|\mathcal{E}_\Lambda|}{4}$ that would cancel out in expectation values.

Taking $A = 2\beta h\Pi_\Lambda$, $B = \beta\sum_{e\in\mathcal{E}_\Lambda} T_e$, and rescaling all times $t_i \to \beta t_i$, we obtain

$$e^{-2\beta H^F_{\Lambda,h}} = \sum_{k\geq 0}\int_{0\leq t_1\leq\cdots\leq t_k\leq 1} dt_1\cdots dt_k\, e^{2\beta t_1 h\Pi_\Lambda} B \cdots B e^{2\beta(1-t_k)h\Pi_\Lambda}$$

$$= \sum_{k\geq 0}\int_{0\leq t_1\leq\cdots\leq t_k\leq\beta} dt_1\cdots dt_k \sum_{e_1,\dots,e_k\in\mathcal{E}_\Lambda} e^{2t_1 h\Pi_\Lambda} T_{e_1}\cdots T_{e_k} e^{2(\beta-t_k)h\Pi_\Lambda}$$

$$= \int d\rho_{\Lambda,\beta}(\omega)\, e^{2t_1 h\Pi_\Lambda} T_{e_1}\cdots T_{e_k} e^{2(\beta-t_k)h\Pi_\Lambda}$$

where $\omega = \big((t_1,e_1),\dots,(t_k,e_k)\big)$

To evaluate the trace of this, we use the product basis corresponding to S^3, which is an eigenbasis of Π_Λ so that

$$\langle \sigma_\Lambda, e^{2t_1 h\Pi_\Lambda} T_{e_1}\cdots T_{e_k} e^{2(\beta-t_k)h\Pi_\Lambda}\sigma_\Lambda\rangle$$

$$= \sum_{j=1}^{k-1} e^{2t_1 h\Pi_\Lambda(\sigma)} e^{2(t_2-t_1)h\Pi_\Lambda(\sigma^{(1)})}\cdots e^{2(\beta-t_k)h\Pi_\Lambda(\sigma)}$$

$$\langle\sigma_\Lambda, T_{e_1}\sigma_\Lambda^{(1)}\rangle \underbrace{\langle\sigma_\Lambda^{(1)}, T_{e_2}\sigma_\Lambda^{(2)}\rangle}\cdots\langle\sigma_\Lambda^{(k-1)}, T_{e_k}\sigma_\Lambda\rangle$$

non-zero iff, across e_2, $\sigma_\Lambda^{(1)}$ and $\sigma_\Lambda^{(2)}$ are $|a,b\rangle$ and $|b,a\rangle$, $a,b = \pm\frac{1}{2}$.

so that

$$\sum_{\substack{a,b\\c,d}}\langle a,b|T_{e_2}\,c,d\rangle = \sum_{\substack{a,b\\c,d}}\langle a,b|d,c\rangle$$

⇝ following the cylinder from 0 to β, the configuration $\sigma(t)$ is constant until t_1, where the spins across e_1 are exchanged, and so on until $t=\beta$ where one must recover $\sigma_\Lambda(0)$.

⇝ the non-vanishing spin configurations are characterized by a constant spin along each cycle!

all T_e's contribute 1.

so if the matrix element is non-zero, then it contributes

$$\langle \sigma_\Lambda, e^{2t_1 h \Pi_\Lambda} T_{e_1} \cdots T_{e_n} e^{2(\beta - t_n) h \Pi_\Lambda} \sigma_\Lambda \rangle = \prod_{\gamma \in C(\omega)} e^{2h L(\gamma) s(\gamma)}$$

where $s(\gamma)$ is the spin $(\pm \frac{1}{2})$ of the loop γ in configuration $C(\omega)$.
This follows from the fact that the sum

$$t_1 \Pi_\Lambda(\sigma) + (t_2 - t_1) \Pi_\Lambda(\sigma^{(1)}) + \dots + (\beta - t_n) \Pi_\Lambda(\sigma)$$

can immediately be reorganized according to the loop configuration.
Since $s(\gamma) \in \{\pm \frac{1}{2}\}$ for any admissible $C(\omega)$, we obtain

$$\tilde{Z}^f_\Lambda(2\beta, h) = \int d\rho_{\Lambda,\beta}(\omega) \prod_{\gamma \in C(\omega)} 2\cosh(hL(\gamma))$$

and $Z^f_\Lambda(2\beta, h) = e^{-2\beta \frac{|E_\Lambda|}{4}} \tilde{Z}^f_\Lambda(2\beta, h)$.

Furthermore : $\omega^f_{2\beta,\Lambda,h}(S^3_x) = \mathrm{Tr}\,(S^3_x e^{-2\beta H^f_{\Lambda,h}})$

gives rise to exactly the same picture, but the ~~loop~~ cycle containing $(x, t=0)$ picks up an additional weight $s(\gamma_x)$ so that it contributes $\sinh(hL(\gamma))$ instead of $2\cosh(hL(\gamma))$

$$\Rightarrow \omega^f_{2\beta,\Lambda,h}(S^3_x) = \frac{1}{2} e^{-\frac{\beta}{2}|E_\Lambda|} \int d\rho_{\Lambda,\beta}(\omega) \prod_{\gamma \in C(\omega)} (2\cosh(hL(\gamma))) \cdot \tanh(hL(\gamma_x)) .$$

Finally, we consider $\omega^f_{2\beta,\Lambda,h}(S^3_x S^3_y)$:

if x, y belong to the same loop, their signs cancel out otherwise, we get the above for the two loops γ_x and γ_y

$\square$

- Now, let us use this representation.

• <u>Proposition</u>: $\mathbb{E}_{\Lambda,\beta,0}\left(\sum_{x\in\Lambda} L(\gamma_x)\right) = \frac{4}{\beta}\frac{\partial^2}{\partial h^2}\log Z^F_{\Lambda}(\beta,h)\Big|_{h=0}$

In other words: the distribution of the length of the loops corresponds to magnetic susceptibility. If the length of loops is not summable (in expectation), then magnetic susceptibility is infinite and there is a phase transition, as $|\Lambda|\to\infty$.

<u>Proof</u>: Again using Duhamel's formula:

$$\mathrm{Tr}\, e^{-\beta H^F_{\Lambda,h}} = Z^F_\Lambda(\beta,0)\left(1+\frac{\beta}{2}h^2\sum_{x,y\in\Lambda}\underbrace{(S^3_x,S^3_y)_\beta}_{\text{Duhamel's two-point function}} + O(h^4)\right)$$

The proposition follows from:

$$\mathbb{E}_{\Lambda,\beta,0}\left(\sum_x L(\gamma_x)\right) = \sum_{x,y\in\Lambda}\int_0^\beta \mathbb{P}_{\Lambda,\beta,0}((x,0)\sim(y,t))\,dt$$
$$= 4\sum_{x,y\in\Lambda}\int_0^\beta \omega^F_{\Lambda,\beta,0}(S^3_x,S^3_y)(t)\,dt$$
$$\overset{\text{def}}{=} 4\sum_{x,y\in\Lambda}(S^3_x,S^3_y)_\beta$$
$$= \frac{4}{\beta}\frac{\partial^2}{\partial h^2}\log \mathrm{Tr}\, e^{-\beta H^F_{\Lambda,h}}\Big|_{h=0}$$

where $\underset{\omega(A,B_t)}{\underset{\shortparallel}{\omega^F_{\Lambda,\beta,h}(A,B)(t)}} = Z^F_\Lambda(\beta,h)\,\mathrm{Tr}\left(A e^{-(\beta-t)H^F_{\Lambda,h}}Be^{-tH^F_{\Lambda,h}}\right)$ $\square$

• It is thought that the Heisenberg ferromagnet at $h=0$ exhibits elementary excitations that behave like free bosons (spin waves, "magnons") in $\mathbb{Z}^d$. This is widely used but <u>not</u> proved. If this were true, then the free energy (or the pressure) would satisfy

$$\lim_{\beta\to\infty} \beta^{(d+2)/2} P(\beta, \overset{h=0}{0}) = -\frac{1}{(2\pi)^d}\int_{\mathbb{R}^d} \log\left(1-e^{-k^2}\right) dk$$

"free bose gas" comes in here through k^2 in the exponent, and the $-$ sign in $(1 - e^{-k^2})$.

see exercises.

Here is what can be proved:

- <u>Theorem</u> [Tóth, 93] if $d \geq 3$

$$\liminf_{\beta\to\infty} \beta^{\frac{d+2}{2}} P(\beta, 0) \geq (\log 2)\left(-\frac{1}{(2\pi)^d}\int \log(1-e^{-k^2})\,dk\right)$$

We will not prove this, but it uses the stochastic representation (similar works by Colon-Solovej)

- We conclude this chapter by stating the equivalent representation for the antiferromagnet. Here,

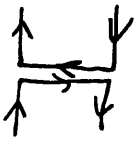
$$S_x \cdot S_y = \frac{1}{4} - P^{(0)}_{xy}$$

where $P^{(0)}_{xy}$ is the projection onto D_0 in $D_{1/2} \otimes D_{1/2}$:

$$P^{(0)}_{xy}|a, a\rangle = 0 \quad ; \quad P^{(0)}_{xy}|a,-a\rangle = \frac{1}{2}\left[|a,-a\rangle - |-a,a\rangle\right].$$

It turns out that the key notion here is not the length of the loops, but their winding number $w(\gamma)$: the number of times it goes around the cylinder before closing onto itself.

Note: $P^{(0)}_{xy}$ imposes antisymmetry, i.e.



All in all:

- **Theorem** [Aizenman-Nachtergaele 94]

$$Z_\Lambda^{AF}(2\beta,h) = e^{-\frac{\beta}{2}|\mathcal{E}_\Lambda|}\int d\rho_{\Lambda,\beta}(\omega)\prod_{\gamma\in\mathcal{L}(\omega)}\left(2\cosh(\beta h w(\gamma))\right)$$

$$\omega_{\Lambda,2\beta,h}^{AF}(S_x^3) = \frac{1}{2}(-1)^x e^{-\frac{\beta}{2}|\mathcal{E}_\Lambda|}\int d\rho_{\Lambda,\beta}(\omega)\prod_{\gamma\in\mathcal{L}(\omega)}\left(2\cosh(\beta h w(\gamma))\right)\cdot \tanh(\beta h w(\gamma_x)).$$

$$\omega_{\Lambda,2\beta,h}^{AF}(S_x^3 S_y^3) = \frac{1}{4}(-1)^x(-1)^y e^{-\frac{\beta}{2}|\mathcal{E}_\Lambda|}\int d\rho_{\Lambda,\beta}(\omega)\prod_{\gamma\in\mathcal{L}(\omega)}\left(2\cosh(\beta h w(\gamma))\right)\begin{cases}1 & \gamma_x=\gamma_y\\ \tanh(\beta h w(\gamma_x))\tanh(\beta h w(\gamma_y)) & \gamma_x\neq\gamma_y\end{cases}.$$

The proof follows similar lines.

Part II : Linear response theory for mechanical forces

2. Statistical mechanics of linear response

- **Setup**: System described by a Hamiltonian $H_X(t)$, time dependent and depending on parameters $X_1, \dots, X_n$, $X_i \in \mathbb{R}$.
Most often $X_i = X_i(t)$ is the only time-dependence.
$X_i(t)$: external "forces" s.t. $X(t) \to 0$ $(t \to -\infty)$.
can be mechanical or thermodynamical forces.

Goal: Understand the response of the system to the force $X(t)$

Typically: $B = B^*$: an observable
$$\Delta B(t) = \omega_t(B) - \omega_0(B)$$
where ω_0 is an equilibrium state ($X_i = 0 \ \forall i$):
$$[H_0, \rho_0] = 0 \qquad (\rho_0 \text{ is the density matrix of } \omega_0).$$
and ω_t is given by ρ_t solving
$$i\dot{\rho}_t = [H_X(t), \rho_t]$$

Question:
$$\Delta B(t) = \Delta B(t, X(\cdot)) \ ? \ = I_{B,t}[X]$$

Linear response: What is $\Delta B(t)$ "to first order in $X(\cdot)$" ?

Precisely: $H(t) = H_0 + H_I(t)$ with $H_I(t) = -X(t)A$.

We call $A = A^*$ a displacement.

Examples:
- Particles perturbed by a force $H_I(t) = \sum_{i=1}^{N} -\vec{F}_i(t) \cdot \vec{x}_i$.
- Atom in magnetic field: $H_I(t) = -\vec{B}(t) \cdot (\vec{L} + 2\vec{S})$
(A is the angular momentum operator)
- Open system with particle reservoir at chemical potential $\mu(t)$.
$H_I(t) = -\mu(t) \cdot N$.

<u>Assumption</u>: Linear response: There exists $\chi(t)$ s.t.

$$\Delta B(t) := \omega_t(B) - \omega_0(B) = \int_{-\infty}^{t} \chi(t-s)\, X(s)\, ds \qquad (*)$$

$\chi(t)$: (isolated) susceptibility.

We will drop $\omega_0(B)$. This is equivalent to considering $\tilde{B} := B - \omega_0(B)$ instead of B.

- <u>Note</u>: All the above allows for the discussion of mechanical forces, thermal perturbations are not included: reservoirs at different β's, temperature gradients, ...
- Causality: From $(*)$, the response depends on the past and the present, not the future. We extend $\chi(t)$ by 0:

$$\chi(t) = 0 \quad \text{for } t < 0,$$

so that

$$\Delta B(t) = \int_{-\infty}^{+\infty} \chi(t-s)\, X(s)\, ds.$$

(!!)

- Proposition: Assume $\chi \in \mathcal{L}^1(\mathbb{R})$. Then: $\hat{\chi}(\omega) = \int \chi(t) e^{i\omega t} dt$

i) $\operatorname{Re} \hat{\chi}(\omega) = \operatorname{Re} \hat{\chi}(-\omega)$ (even)

$\quad\operatorname{Im} \hat{\chi}(\omega) = -\operatorname{Im} \hat{\chi}(-\omega)$ (odd)

ii) $\hat{\chi}$ has an analytic extension in $\operatorname{Im} \omega > 0$, which is continuous up to $\operatorname{Im} \omega = 0$

iii) $\lim_{|\omega| \to \infty} \hat{\chi}(\omega) = 0$ ~~whenever~~

Proof: i) $B = B^* \Rightarrow \chi(t) \in \mathbb{R} \Rightarrow \overline{\hat{\chi}(\omega)} = \hat{\chi}(-\omega)$

ii) For $t \geq 0$, $|\exp(i\omega t)| = |\exp(i \operatorname{Re}\omega t) \exp(-\operatorname{Im}\omega t)|$

$$= \exp(-(\operatorname{Im}\omega) t).$$

Hence $\chi \in \mathcal{L}^1(\mathbb{R}) \Rightarrow \int |\chi(t) e^{i\omega t}| \leq \int |\chi(t)| e^{-(\operatorname{Im}\omega) t} dt < \infty.$

iii) This is Riemann-Lebesgue's lemma, which is simple:

$\mathcal{F}: \mathcal{S} \to \mathcal{S}$ and

$$\|\hat{f}\|_\infty \leq \frac{1}{(2\pi)^{1/2}} \|f\|_1$$

and the density of Schwartz space in L^1. $\square$

- Note: $\hat{\chi}(\omega)$ can be understood as the response to a harmonic driving: ~~instantaneous~~.

$$X(t) = e^{-i\omega t} \Rightarrow \Delta B(t) = \int_{-\infty}^{t} \cancel{e^{i\omega(t-s)}} \chi(t-s) e^{-i\omega s}\, ds$$

$$= \int_0^\infty \chi(r) e^{i\omega r}\, dr\; e^{-i\omega t} = \hat{\chi}(\omega) e^{-i\omega t}$$

on the other hand: for a pulse $X(t) = \delta(t)$: $\Delta B(t) = \chi(t)$

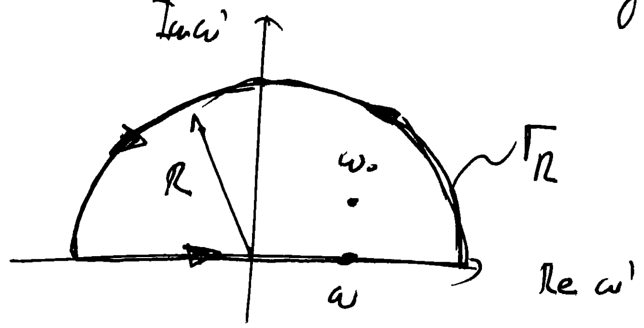
Define: $\hat{\chi}(0)$: "static susceptibility" (constant driving).

- Proposition (Kramers-Kronig dispersion relation)

For $\omega > 0$:

$$\begin{cases} \operatorname{Im} \hat{\chi}(\omega) = -\dfrac{2\omega}{\pi} \mathcal{P} \displaystyle\int_0^\infty \frac{\operatorname{Re} \hat{\chi}(\omega')}{\omega'^2 - \omega^2} d\omega' \\ \operatorname{Re} \hat{\chi}(\omega) = \dfrac{2}{\pi} \mathcal{P} \displaystyle\int_0^\infty \frac{\omega' \operatorname{Im} \hat{\chi}(\omega')}{\omega'^2 - \omega^2} d\omega' \end{cases}$$

Proof: Let $\omega_0 = \omega + i\varepsilon$ and use Cauchy's formula.



$$\hat{\chi}(\omega) = \lim_{\varepsilon \downarrow 0} \frac{1}{2\pi i} \lim_{R \to \infty} \int_{\Gamma_R} \frac{\hat{\chi}(\omega')}{\omega' - \omega - i\varepsilon} d\omega'$$

The semi-circle does not contribute by iii) above.

In the sense of distributions:

$$\lim_{\varepsilon\downarrow 0} \frac{1}{x-i\varepsilon} = \mathcal{P}\frac{1}{x} + i\pi\delta(x) \qquad \text{(Exercise)}$$

Hence:

$$\hat{\chi}(\omega) = \frac{1}{2\pi i}\left(\mathcal{P}\int_{-\infty}^{+\infty}\frac{\hat{\chi}(\omega')}{\omega'-\omega}d\omega' + i\pi\hat{\chi}(\omega)\right)$$

$$\Rightarrow \hat{\chi}(\omega) = \frac{1}{i\pi}\mathcal{P}\int_{-\infty}^{+\infty}\frac{\hat{\chi}(\omega')}{\omega'-\omega}d\omega'$$

Therefore:

$$\operatorname{Im}\hat{\chi}(\omega) = -\frac{1}{\pi}\mathcal{P}\int_{-\infty}^{+\infty}\frac{\operatorname{Re}\hat{\chi}(\omega')}{\omega'-\omega}d\omega' \underset{\operatorname{Re}\hat{\chi}\text{ is even.}}{=} -\frac{1}{\pi}\left[\mathcal{P}\int_0^\infty \frac{\operatorname{Re}\hat{\chi}(\omega')}{-\omega'-\omega} + \frac{\operatorname{Re}\hat{\chi}(\omega')}{\omega'-\omega}\right]$$

$$= -\frac{2}{\pi}\mathcal{P}\int_0^\infty\frac{\omega\operatorname{Re}\hat{\chi}(\omega')}{\omega'^2-\omega^2}d\omega'.$$

and similarly for $\operatorname{Re}\hat{\chi}$ using $\operatorname{Im}\hat{\chi}$ is odd $\square$

In other words: real and imaginary parts of $\hat{\chi}(\omega)$ are not independent functions.

It turns out that $\operatorname{Im}\hat{\chi}$ is related to <u>dissipation</u> (loss of energy).

- Define: Work done <u>on</u> the system (instantaneous)

$$W(t) = \omega_t(\dot{H}(t)).$$

$$\left(\text{see case } H_t = -\bar{F}(t)x\ ,\ \dot{H}_t = \dot{H} = \dot{\bar{F}}\cdot\tilde{x}\right)$$

indeed:

$$\frac{d}{dt}\omega_t(H(t)) = \frac{d}{dt}\operatorname{Tr}(\rho(t)H(t)) = \operatorname{Tr}\left(\dot{\rho}(t)H(t)\right) + \omega_t(\dot{H}(t))$$

compare with 1st law: $dU = Q + W$.

Here, the system is thermally isolated and

$$\operatorname{Tr}(\dot{\rho}(t)H(t)) = i\operatorname{Tr}([H,\rho]H) = 0 \quad \Big\}\ \text{no heat flux. indeed.}$$

• Recall: $\omega_t(B) - \omega_0(B) = \int_{-\infty}^{+\infty} \chi_B(t-s) X(s)\, ds$ (linear response)

where $H(t) = H_0 - X(t) A$

Causality: $\chi(t) = 0$ for $t < 0$.

$\Rightarrow$ $\hat{\chi}(\omega)$ has an analytic extension to $\mathrm{Im}\,\omega > 0$

$\Rightarrow$ Kramers-Kronig relation

• Now: $\mathrm{Im}\,\hat{\chi}(\omega)$ is related to dissipation (change of energy of the system)

Work observable: $W(t) = \dot{H}(t) = -\dot{X}(t) A$; $\quad W := \int_{\mathbb{R}} \omega_t(\dot{H}(t))\, dt$

Proposition: If $W \geq 0$, then

i) $\hat{\chi}_A(0) \geq 0$

ii) $\mathrm{Im}\,\hat{\chi}_A(\omega) \geq 0 \quad \forall \omega > 0$

(and $\mathrm{Im}\,\hat{\chi}_A(\omega) = 0 \quad \forall \omega > 0 \to W = 0$.)

Proof starts with $\int_{\mathbb{R}} -\dot{X}(t)\, \omega_t(A)\, dt = \int_{\mathbb{R}} X(t) \frac{d}{dt} \omega_t(A)\, dt$

Note: $\int$ "force · velocity"

Total work done:

$$W = \int_{-\infty}^{+\infty} \omega_t(\dot{H}(t))\,dt = -\int_{-\infty}^{+\infty} \dot{X}(t)\big(\omega_t(A) - \omega_0(A)\big)\,dt$$

$$\lim_{t \to \mp\infty} X(t) = 0$$

$$= -\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} \dot{X}(t)\,\chi_A(t-s)\,X(s)\,dt\,ds.$$

- Proposition If $W \geq 0$, then
  i) Static susceptibility: $\hat{\chi}_A(0) \geq 0$
  ii) $\operatorname{Im} \hat{\chi}_A(\omega) \geq 0 \quad \forall \omega > 0.$

  Moreover, $\operatorname{Im} \hat{\chi}_A(\omega) = 0 \quad \forall \omega > 0 \Rightarrow W = 0.$

Proof: Integrate by parts to get the more familiar form

$$W = \int_{-\infty}^{+\infty} X(t)\,\frac{d}{dt}\omega_t(A)\,dt$$

i) $\hat{\chi}_A(0)$ is obtained from a constant driving:

$X(t) = \theta(t)$ (strictly $\cdot e^{-\mu t}$, $\mu \downarrow 0$)

$$\omega_t(A) = \int_{-\infty}^{+\infty} \chi_A(t-s)\,\theta(s)\,ds = \int_{-\infty}^{t} \chi_A(r)\,dr$$

$$\Rightarrow \frac{d}{dt}\omega_t(A) = \chi_A(t)$$

so that $\quad 0 \leq W = \int_0^{\infty} \chi_A(t)\,dt = \int_{-\infty}^{+\infty} \chi_A(t)\,dt = \hat{\chi}_A(0)$

ii) Note: $\omega_t(A) = (\chi_A * X)(t)$

so that $\widehat{\omega_\cdot(A)}(\omega) = \hat{\chi}_A(\omega) \cdot \hat{X}(\omega).$

Moreover,

$$W = \langle X, \dot{\omega}_t(A) \rangle_{L^2(\mathbb{R}_t)}$$

By Parseval:

$$W = \langle \hat{X}, \widehat{\dot{\omega}_\cdot(A)} \rangle_{L^2(\mathbb{R}_\omega)} = \int_{\mathbb{R}} d\omega \, \overline{\hat{X}(\omega)} (-i\omega) \hat{\chi}_A(\omega) \hat{X}(\omega)$$

$$= \int_{\mathbb{R}} d\omega \, |\hat{X}(\omega)|^2 (-i\omega) \hat{\chi}_A(\omega).$$

Again: $X(t) \in \mathbb{R} \Rightarrow \overline{\hat{X}(\omega)} = \hat{X}(-\omega) \Rightarrow |\hat{X}(\omega)|^2 = |\hat{X}(-\omega)|^2$

$$0 \le W = \int d\omega \, |\hat{X}(\omega)|^2 \omega \, \mathrm{Im}\, \hat{\chi}_A(\omega)$$

$\square$

- Note: the imaginary part of $\hat{\chi}$ accounts for the change in energy due to mechanical forces: <u>dissipation</u>.
- <u>Proposition</u> (Kubo's formula)

Let $\rho(t)$ be the solution of $\quad i\dot{\rho} = [H(t), \rho]$
with $\rho(t) \to \rho_0$ as $t \to -\infty$.
Let

$$I_{B,t}[X] := \omega_t(B) - \omega_0(B)$$

and define

$$\chi_{BA}(t) := \frac{\delta I}{\delta X}\Big|_{X=0} \qquad B(t) = e^{itH_0} B e^{-itH_0}$$

Then

$$\chi_{BA}(t) = i\omega_0\big([B(t), A]\big)\Theta(t) \; ;$$

- <u>Remarks</u>: i) This is exactly a statement about linear response, as

$$\omega_t(B) = \omega_0(B) + \int_{-\infty}^{+\infty} \chi_{BA}(t-s) X(s) ds + O(X^2)$$

where $O(X^2)$ means $O(\varepsilon^2)$ for any variation $X(t) = \underbrace{0}_{\text{equilibrium}} + \varepsilon X(t)$.

ii) Crucial point: Linear response function χ_{BA} is expressed in terms of the equilibrium state and the isolated dynamics only!

Proof: "Interaction picture",
(Sketch) $\tilde{\rho}(t) := \exp(iH_0 t)\,\rho(t)\,\exp(-iH_0 t)$
$\tilde{H}_I(t) := \exp(iH_0 t)\,H_I(t)\,\exp(-iH_0 t)$.

$\tilde{\rho}$ satisfies the DE:

$$i\dot{\tilde{\rho}} = i e^{iH_0 t}\left(i[H_0, \rho(t)] - i[H(t), \rho(t)]\right)e^{-iH_0 t}$$
$$= \cancel{e^{iH_0 t}}\;[\tilde{H}_I(t), \tilde{\rho}(t)]$$

with $\tilde{\rho}(t) \to \rho_0$ as $t \to -\infty$. (ρ_0 is an eq. state).

Now:

$$\tilde{\rho}(t) = \tilde{\rho}(-\infty) - i\int_{-\infty}^{t} [\tilde{H}_I(s), \tilde{\rho}(s)]\,ds$$
$$= \rho_0 - i\int_{-\infty}^{t} \underbrace{[\tilde{H}_I(s), \rho_0]}_{= e^{+iH_0 s}[H_I(s),\, \rho_0]e^{-iH_0 s}}\,ds - \int_{-\infty}^{t}\int_{-\infty}^{s} [\tilde{H}_I(s), [\tilde{H}_I(r), \tilde{\rho}(r)]]\,dr\,ds.$$

and
$$I_{B,t}[X] = -i\int_{-\infty}^{t} \mathrm{Tr}\left(e^{-iH_0 t}\left(e^{iH_0 s}[H_I(s), \rho_0]e^{-iH_0 s}\right)e^{iH_0 t} B\right)ds$$
$$+ R_{B,t}[X].$$

the first term is
$$-i\int_{-\infty}^{t} \mathrm{Tr}\left(B(t-s)[A, \rho_0]\right)X(s)\,ds$$
$$= -i\int_{-\infty}^{t} \mathrm{Tr}\left(\rho_0\,[B(t-s), A]\right)X(s)\,ds$$

where we used $\cancel{[A,\rho B]} = [A, B\rho] = B[A,\rho] + [A,B]\rho$
and the trace of $[\cdot,\cdot]$ vanishes.

The rest is given by

$$R_{B,t}[X] = -\int_{-\infty}^{t}\int_{-\infty}^{s} \mathrm{Tr}\left(B(t)[A(s), [A(r), \tilde{\rho}(r)]]\right)X(r)X(s)\,dr\,ds.$$

Hence,

$$\frac{d}{d\varepsilon} I_{B,t}[\varepsilon X]\Big|_{\varepsilon=0} = -i\int_{-\infty}^{+\infty} ds\, \mathrm{Tr}\Big(\rho_0 [B(t-s), A]\Big)\Theta(t-s)X(s)\,ds \qquad \square$$

- Note: $\chi_{BA}(t)$ is real as

$$\overline{\mathrm{Tr}\big(\rho_0[B,A]\big)} = \mathrm{Tr}\big([A,B]\rho_0\big) = -\mathrm{Tr}\big(\rho_0[B,A]\big)$$

- Def: The observable B is called a flux if $\exists\, Q$:

$$B = i[H_0, Q]$$

Example: Q: charge operator, B is the current

In this case, we denote

$$L_{QA}(t) := \chi_{BA}(t).$$

- Corollary: [Onsager's reciprocal relations]:

$$L_{QA}(t) = L_{AQ}(-t)$$

Proof.

$$L_{QA}(t) = \mathrm{Tr}\Big(\big[[C(t), H_0], A\big]\rho_0\Big)$$
$$= -\mathrm{Tr}\Big(\big[[A, C(t)], H_0\big]\rho_0\Big) - \mathrm{Tr}\Big(\big[[H_0, A], C(t)\big], \rho_0\Big)$$

the first term is zero as it is equal to $\mathrm{Tr}\Big(\big[[A, C(t)]\rho_0, H_0\big]\Big)$, and the second one is

$$-\mathrm{Tr}\Big(\big[[H_0, A], C(t)\big]\rho_0\Big) = \mathrm{Tr}\Big(\big[[A(-t), H_0], C\big]\rho_0\Big) = L_{AQ}(-t) \qquad \square$$

- In a standard form:

Note: $-i[A,\rho_0] = i[\rho_0, A] \overset{i e^{-\beta H_0}(A - e^{\beta H_0} A e^{-\beta H_0}) Z(\beta)^{-1}}{=} -i e^{-\beta H_0}\int_0^\beta ds\, e^{sH_0}[H_0, A]e^{-sH_0} Z(\beta)^{-1}$

Hence:

$$\chi_{BA} = -i\,\mathrm{Tr}\Big(B(t)\int_0^\beta e^{-(\beta-s)H_0}[H_0, A]e^{-sH_0}\Big)Z(\beta)^{-1}$$

$$= \beta \Big(B(t),\, i[H_0, A]\Big)_\beta$$

Duhamel's two-point function!

We have proved the following:

- <u>Corollary</u>: If $B = i[H_0, Q]$, then

$$L_{QA}(t) = \beta \left(\dot{Q}(t), \dot{A}\right)_\beta \theta(t)$$

<u>Notes</u>: * The symmetry is now obvious from that of Duhamel's.
* "Response" = Current-current correlation function in the equilibrium state.

- Prove dissipativity?

<u>Proposition</u>: Let $H(t) = H(X(t))$ with $X(0) = X(T)$ and define $H = H(0) = H(T)$; U: evolution on $[0,T]$. Let

$$W := Tr(HU\rho U^*) - Tr(H\rho)$$

where the initial state $\rho = Z^{-1} e^{-\beta H}$. Then

$$W \geq 0.$$

<u>Proof</u>: Since $-\beta H = \log \rho + \log Z$, we have:

$$\beta \Delta E \underset{\substack{\uparrow \\ Tr\rho = 1.}}{=} Tr(\rho \log \rho) - \underbrace{Tr\left(U\rho U^* \log \rho\right)}_{Tr(\rho \log(U^*\rho U))}$$

$$= Tr(\rho \log \rho) - Tr(\rho \log(U^* \rho U))$$

$$\geq Tr\left(\rho - U^*\rho U\right) = 0$$

↑ relative entropy inequality (Klein's lemma) $\square$

<u>Note</u>: This assumes that all these manipulations with traces are legitimate, which not necessarily true in concrete (in particular thermodynamic!) systems.

- Time reversal: We start with an abstract definition:

Def: * Let τ^t be the time evolution on the algebra of observables $\mathcal{A}$ (τ^t is a strongly continuous group of *-automorphisms of $\mathcal{A}$). An *-automorphism Θ is time-reversal of $(\mathcal{A}, \tau^t)$ if
(anti-linear)

$$\Theta \circ \Theta = 1 \quad \text{and} \quad \tau^t \circ \Theta = \Theta \circ \tau^{-t}$$

* A state ω is time-reversal invariant if
$$\omega(\Theta(A)) = \omega(A^*) \quad \text{for all } A \in \mathcal{A}.$$

Consequences: Suppose $\exists\, U_\Theta$ on $\mathcal{H}$ that implements Θ:
$$\Theta(A) = U_\Theta A U_\Theta^{-1}.$$
Then:

i) U_Θ is anti-unitary

ii) $\mathrm{Tr}(\Theta(A)) = \mathrm{Tr}(A^*) = \overline{\mathrm{Tr}(A)}$

iii) If τ^t is generated by $H = H^*$: $\Theta(H) = H$

iv) If ω is given by a density matrix ρ as,
$$\omega = \omega \circ \Theta \iff U_\Theta^{-1} \rho\, U_\Theta = \rho$$

v) If $U_\Theta A U_\Theta^{-1} = A$, then $U_\Theta \tau^t(A) U_\Theta^{-1} = \tau^{-t}(A)$.

Note: * U is anti-unitary if it is an antilinear map s.t.
$$\langle U\psi, U\phi\rangle = \langle \phi, \psi\rangle$$

* In the Schrödinger representation, $(U_\Theta \psi)(x) = \overline{\psi(x)}$, i.e. U_Θ is just complex conjugation.

* Onsager's relations: Assume:
  a) Invariance of dynamics H_0
  b) Invariance of state (follows from a) for thermal states)
  c) Invariance of A, Q.

Then: $L_{QA}(t) = L_{AQ}(t)$.

This follows from $L_{QA}(t) = L_{AQ}(-t)$ and

$$L_{AQ}(-t) = \mathrm{Tr}\left([[A(-t), H_0], Q]\rho_0\right)$$
$$\overset{(i)}{=} \overline{\mathrm{Tr}\left([[U_\theta A(t) U_\theta^{-1}, H_0], Q]\rho_0\right)}$$
$$\overset{(ii)}{=} \overline{\mathrm{Tr}\left([[A(t), H_0], Q]\rho_0\right)} = \overline{L_{AQ}(t)} = L_{AQ}(t).$$

where we used that L_{AQ} is real.

- Notation: $\chi_{BA}(t) := \phi_{BA}(t)\,\theta(t)$

  i.e. $\phi_{BA}(t) = i\,\mathrm{Tr}\left([B(t), A]\rho_0\right)$

  and $\phi_{BA}(-t) = -\phi_{AB}(t)$

- Theorem (Callen-Welton fluctuation-dissipation theorem)

Let $\rho_0 = Z^{-1}(\beta) e^{-\beta H_0}$. Let $G_{BA}(t) = \frac{1}{2}\left(\omega_0(AB_t) + \omega_0(B_tA)\right)Z(\beta)$

Then:

$$\hat{G}_{BA}(\omega) = -\frac{i}{2}\coth\left(\frac{\beta\omega}{2}\right)\hat{\phi}_{BA}(\omega) \qquad (1)$$

and

$$\hat{G}_{AA}(\omega) = \coth\left(\frac{\beta\omega}{2}\right)\mathrm{Im}\,\hat{\chi}_{AA}(\omega) \qquad (2)$$

- Remarks: * If $\omega_0(A) = 0 = \omega_0(B)$, $G_{AA}(t)$ expresses fluctuations

  $\rightarrow$ (2) relates fluctuations of A to dissipation

  * Classical limit: reinstalling the $\hbar$'s:

$$\hat{G}_{AA}(\omega) = \hbar\coth\left(\frac{\beta\hbar\omega}{2}\right)\mathrm{Im}\,\hat{\chi}_{AA}(\omega)$$

$$\hbar\coth\frac{\beta\hbar\omega}{2} \simeq \frac{\hbar\omega}{k_BT}\,\frac{1+\left(1-\frac{\hbar\omega}{k_BT}\right)}{1-\left(1-\frac{\hbar\omega}{k_BT}\right)}\,\frac{k_BT}{\omega} = \frac{2k_BT}{\omega} \quad \left(\text{as } \frac{\hbar\omega}{k_BT}\to 0\right)$$

• Lemma (KMS-condition): (for finite systems) (true in a dense set of $\mathcal{A}$ in $\mathcal{H}_0$ is semi-bounded)
The function $t \mapsto f(t) = \mathrm{Tr}(B(t) A e^{-\beta H_0})$ has an analytic extension from $t \in \mathbb{R}$ to the strip $\underbrace{-\beta < \mathrm{Im}\, t < 0}_{e^{i(t-i\beta)H}}$, continuous up to the boundary with

$$f(t-i\beta) = \mathrm{Tr}\left(A B(t) e^{-\beta H_0}\right) \qquad = e^{i\mathrm{Re}\, t H} e^{-\underbrace{(\mathrm{Im}\, t+\beta)}_{>0} H}$$

$$\& \; e^{itH} = e^{i\mathrm{Re}\, t H} e^{-\underbrace{\mathrm{Im}\, t}_{<0} H} \text{ ch.}$$

In other words:

$$\cancel{\omega_0(B(t)A) = \omega_0}$$

$$\omega_0\left(B(t)A\right) = \omega_0\left(AB(t+i\beta)\right)$$

Proof: Simple in this case:

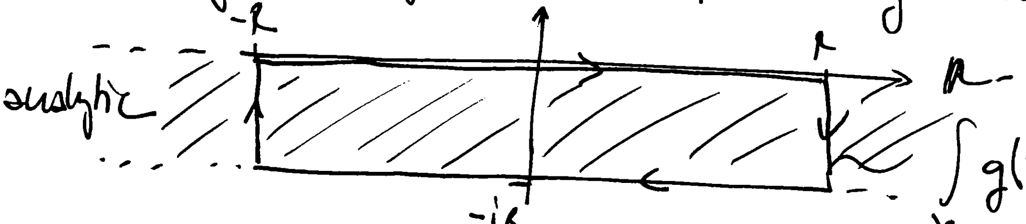
$$f(t-i\beta) = \mathrm{Tr}\left(e^{itH_0} e^{\beta H_0} B e^{-\beta H_0} e^{-itH_0} A e^{-\beta H_0}\right)$$

$$= \mathrm{Tr}\left(e^{-\beta H_0} A e^{itH_0} B e^{-itH_0}\right) = \mathrm{Tr}\left(AB(t) e^{-\beta H_0}\right)$$

by cyclicity. → More to discuss here.

• ~~Remark~~ of theorem:

Let $g(t) = f(t) e^{i\omega t}$. Then $\int_{-\infty}^{+\infty} g(t)\,dt = \int_{-\infty}^{+\infty} g(t-i\beta)\,dt$ since g is analytic in the strip and by contour deformation



$$\int_{\gamma_R} g(z)\,dz = 0.$$

Hence:

$$\hat{f}(\omega) = \int_{\mathbb{R}} f(t-i\beta)\, e^{i\omega(t-i\beta)}dt = e^{\omega\beta} \int_{\mathbb{R}} \mathrm{Tr}\left(AB(t)e^{-\beta H_0}\right) \overset{e^{i\omega t}}{} dt$$

so that

$$\hat{\phi}_{BA}(\omega) = i\int_{\mathbb{R}} f(t) e^{i\omega t} dt - i\int_{\mathbb{R}} \mathrm{Tr}\left(AB(t)e^{-\beta H_0}\right) e^{i\omega t} dt$$

$$= i\left(1 - e^{-\beta\omega}\right) \hat{f}(\omega)$$

and since $G_{BA}(t) = \frac{1}{2}\, \omega_0\left(\{A, B(t)\}\right) Z(\beta)$
$$= \frac{1}{2}\, \mathrm{Tr}\left(\{A, B(t)\} e^{-\beta H_0}\right) :$$
$$\hat{G}_{BA}(\omega) = \frac{1}{2}\left(1 + e^{-\beta\omega}\right) f(\omega).$$

All in all:
$$\hat{G}_{BA}(\omega) = -\frac{i}{2}\, \frac{(1+e^{-\beta\omega})}{1-e^{-\beta\omega}}\, \hat{\phi}_{BA}(\omega)$$

For (2), we note that
$$2i\, \mathrm{Im}\, \hat{\chi}_{AA}(\omega) = \hat{\chi}_{AA}(\omega) - \hat{\chi}_{AA}(-\omega) = \int_0^\infty \phi_{AA}(t)\left(e^{i\omega t} - e^{-i\omega t}\right)$$
$$= \int_0^\infty \phi_{AA}(t) e^{i\omega t} - \int_{-\infty}^0 \phi_{AA}(-t) e^{i\omega t}$$
$$= \int_{-\infty}^{+\infty} \phi_{AA}(t) e^{i\omega t}\, dt = \hat{\phi}_{AA}(\omega) \qquad \square$$

- Application : Brownian motion

1) Heuristic description:

Particles of size $\sim 10^{-6}$m in a liquid or gas perform random motion. $\rightsquigarrow$ diffusion : $*$ density $n(\vec{x}, t)$ of particles

~~Einstein:~~ + current density $j_{diff}(\vec{x}, t)$

for $\vec{x} \in \Omega \subset \mathbb{R}^3$.

Continuity equation : $\partial_t n + \mathrm{div}\, j_{diff} = 0$ (plus B.C)

Fick's law : $j_{diff} = -D \nabla n$, D const.

(linear response !)

$$\Rightarrow \partial_t n = -\mathrm{div}\, j_{diff} = D \Delta n \quad \to \text{Diffusion}.$$

Einstein's formula: $D = \mu k T$ (E)

where μ is the mobility : limiting velocity under a force F:

$$\vec{v} = \mu \vec{F} \qquad (*)$$

i.e. $\mu \sim$ inverse friction.
Note: $(*)$ is again a statement about linear response.
Important: D : "fluctuation"
μ : "dissipation"
In fact: (E) follows from Callen-Welton.

2) First: Einstein's thought experiment:
Apply external force $\vec{F}$ to the particles: $j_{diff} \neq j_{drift}$
and $j_{drift} = n\vec{v} = n\mu\vec{F}$

due to ∇n due to $\vec{F}$.

Assume: the force arises from a potential $\vec{F} = -\nabla U$.
Now: Total current vanishes at equilibrium, i.e. for
$$n(x) \propto \exp\left(-U(x)/kT\right) \qquad \text{(local equilibrium!)}.$$
$$0 = j_{diff} + j_{drift} \implies -D\nabla n = -n\mu F = n\mu \nabla U$$
$$\to \frac{D}{kT}\nabla U = \mu \nabla U$$
Thus $\quad D = \mu k T$

3) Second: from general theory: (1-d)
Setup: * $H_I(t) = -f(t)\,x$ $\quad$ i.e. $A = x$
* Observable: velocity $\quad$ i.e. $B = \dot{A} = \dot{x}$
* Response function: $\hat{\chi}_{BA}(\omega) = \mu(\omega)$:
$$\langle \dot{x} \rangle(\omega) = \mu(\omega) F(\omega)$$
The μ of Einstein's relation is the response to a constant driving: $\mu = \hat{\mu}(0)$.

Kubo: $\chi_{BA}(t) = \beta\,\left(\dot A(t), \dot A\right)_\beta\,\Theta(t)$ i.e.

$$\mu(\omega) = \beta \int_0^\infty \left(\dot x(t), \dot x\right)_\beta e^{i\omega t}\, dt$$

but $[\dot x, H_0] = 0$ (no drift before an external force is applied, only diffusion)

so that $\left(\dot x(t), \dot x\right)_\beta = \langle \dot x(t), \dot x\rangle_0 \left(= \langle \dot x, \dot x(t)\rangle_0\right)$

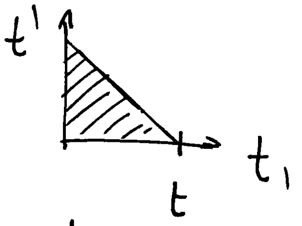
thermal expectation

On the other hand:

$$D := \lim_{t\to\infty} \frac{1}{2t} \left\langle (x(t) - x)^2 \right\rangle_0$$

$$= \lim_{t\to\infty} \frac{1}{2t} \int_0^t dt_1 \int_0^t dt_2 \, \langle \dot x(t_1)\dot x(t_2)\rangle_0$$

$$\overset{t_2 = t_1 + t'}{=} \lim_{t\to\infty} \frac{1}{t} \int_0^t dt_1 \int_0^{t-t_1} dt' \, \underbrace{\langle \dot x(t_1)\dot x(t_1+t')\rangle_0}_{\text{stationary process: } = \langle \dot x(0)\dot x(t')\rangle_0}$$



$$= \lim_{t\to\infty} \frac{1}{t} \int_0^t dt_1 \int_0^\infty dt' \, \langle \dot x(0)\dot x(t')\rangle = \int_0^\infty \langle \dot x(0)\dot x(t')\rangle$$

$\Rightarrow \quad \mu = \hat\mu(0) = \beta D \quad$ or $\quad D = \mu k T$

Kubo: $\chi_{BA}(t) = \beta \left(\dot{A}(t), \dot{A}\right)_\beta \Theta(t)$ i.e.

$$\mu(\omega) = \beta \int_0^\infty \left(\dot{x}(t), \dot{x}\right)_\beta e^{i\omega t}\, dt$$

but $[\dot{x}, H_0] = 0$ (no drift before an external force is applied, only diffusion)

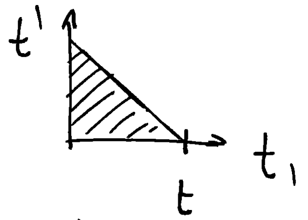
so that $\left(\dot{x}(t), \dot{x}\right)_\beta = \langle \dot{x}(t), \dot{x} \rangle_0 \left(= \langle \dot{x}, \dot{x}(t)\rangle_0 \right)$ ← thermal expectation

On the other hand:

$$D := \lim_{t\to\infty} \frac{1}{2t} \left\langle \left(x(t) - x\right)^2 \right\rangle_0$$

$$= \lim_{t\to\infty} \frac{1}{2t} \int_0^t dt_1 \int_0^t dt_2 \, \langle \dot{x}(t_1)\dot{x}(t_2)\rangle_0$$

$$\overset{t_2 = t_1 + t'}{=} \lim_{t\to\infty} \frac{1}{t} \underbrace{\int_0^t dt_1 \int_0^{t-t_1} dt'}\ \underbrace{\langle \dot{x}(t_1)\dot{x}(t_1+t')\rangle_0}_{\text{stationary process: } = \langle \dot{x}(0)\dot{x}(t')\rangle_0}$$



$$= \lim_{t\to\infty} \frac{1}{t} \int_0^t dt_1 \int_0^\infty dt' \, \langle \dot{x}(0)\dot{x}(t')\rangle = \int_0^\infty \langle \dot{x}(0)\, \dot{x}(t')\rangle$$

$$\Rightarrow \mu = \hat{\mu}(0) = \beta D \quad \text{or} \quad D = \mu k T$$

- Finally, we can derive everything from a <u>microscopic</u> model: Langevin's equation
  - * In Einstein's description: dynamics is in terms of velocities.
  - * In Langevin's: back to positions.
    - i) friction: averaged effect of collisions: $-\mu \dot{x}$
    - ii) fluctuating force: describes the deviation from average:

      $\xi(t)$: real random process s.t. : ξ is the <u>driving</u> here.

a) for all $t \geq 0$, the r.v. $\xi(t)$: $\langle \xi(t) \rangle = 0$.

b) correlation :

$$\langle \xi(t) \xi(t') \rangle = \alpha \, \delta(t-t') \quad , \quad \alpha \in \mathbb{R}.$$

Newton's law for the particle undergoing random motion:

$$m \frac{dv}{dt} = -\mu v + \xi(t) \qquad (v = \dot{x}), \quad t > 0. \qquad (*)$$

Initial condition: $\frac{1}{2} m \langle v^2(0) \rangle = \frac{3}{2} kT$ (equipartition).

Critical parameter: $\frac{m}{\mu}$ with dimension of a time

Finally: α will be determined by the condition $\langle v^2(t) \rangle = \langle v^2(0) \rangle$.

Solution : a) Assume $v(t)$ solves $(*)$. Then

Assume: $t \mapsto x(t)$ is continuous. $x(0), v(0)$ independent. $\langle v(0) \rangle = 0$. (isotropy)

$$\frac{d}{dt}\left(v(t) e^{\mu/m\, t}\right) = \left(\frac{dv}{dt} + \frac{\mu}{m} v\right) e^{\mu/m\, t} \overset{(*)}{=} \xi(t) e^{\mu/m\, t}$$

Therefore $v(t)$ ~~satisfies the integral equation~~ can be written:

$$v(t) = e^{-\mu/m\, t}\left(v(0) + \underbrace{\frac{1}{m}\int_0^t \xi(s) e^{\mu/m\, s} ds}_{\sim \text{ well-defined by continuous processes } s \mapsto \xi(s)} \right)$$

b) α: $$\langle v^2(t) \rangle = e^{-\frac{2\mu}{m} t} \Big(\langle v(0)^2 \rangle + \frac{2}{m} \langle v(0) \int \xi(s) e^{\frac{\mu}{m} s} ds \rangle + \frac{1}{m^2} \int_0^t ds_1 ds_2 \, \langle \xi(s_1) \xi(s_2) \rangle e^{\frac{\mu}{m}(s_1+s_2)} \Big)$$

+ $v(0)$ independent of $\{ \xi(s) : s \in [0,t] \}$

$\Rightarrow$ cross-term vanishes.

$$\Rightarrow \langle v^2(t) \rangle = e^{-\frac{2\mu}{m} t} \left(\langle v(0)^2 \rangle + \frac{1}{m^2} \alpha \int_0^t ds \, e^{\frac{2\mu}{m} s} \right)$$

$$= \frac{\alpha}{2\mu m} + e^{-\frac{2\mu}{m} t} \left(\langle v(0)^2 \rangle - \frac{\alpha}{2\mu m} \right)$$

Imposing $\langle v^2(t)\rangle = \langle v^2(0)\rangle$: in particular $\langle v^2(t)\rangle$ is independent of t, i.e.

$$\langle v^2(t)\rangle = \langle v^2(0)\rangle \Rightarrow \alpha = 2\mu m \langle v(0)^2\rangle$$

Fluctuations:

$$\frac{d^2}{dt^2}\langle x^2(t)\rangle = 2\left\langle\left(\frac{dx}{dt}\right)^2\right\rangle + 2\left\langle x\frac{d^2x}{dt^2}\right\rangle$$

but $\left\langle x\frac{d^2x}{dt^2}\right\rangle = -\frac{\mu}{m}\left\langle x\frac{dx}{dt}\right\rangle + \frac{1}{m}\langle x(t)\xi(t)\rangle$

and $\ast$ $x\frac{dx}{dt} = \frac{1}{2}\frac{d}{dt}x^2$

$\ast$ $\langle x(t)\xi(t)\rangle = \langle x(t)\rangle\langle\xi(t)\rangle$ since $x(t)$ depends only on $\{\xi(s) : 0 \leq s < t\}$, and $x(t)$ is continuous

Hence:

$$\frac{d^2}{dt^2}\langle x^2(t)\rangle + \frac{\mu}{m}\frac{d}{dt}\langle x^2(t)\rangle = 2\underbrace{\langle v^2\rangle}_{\text{fixed constant.}}$$

this can be solved for the variable $u(t) = \frac{d}{dt}\langle x^2(t)\rangle$ with initial condition

$$u(0) = 2\langle v(0)x(0)\rangle = 2\langle v(0)\rangle\langle x(0)\rangle = 0$$

$$u(t) = \frac{2m}{\mu}\langle v^2\rangle\left(1 - e^{-\frac{\mu}{m}t}\right)$$

$$\rightarrow \langle x^2(t)\rangle - \langle x^2(0)\rangle = \frac{2m}{\mu}\langle v^2\rangle\left(t - \frac{m}{\mu}\left(1 - e^{-\frac{\mu}{m}t}\right)\right)$$

<u>Now</u>: $\ast$ $\lim_{t\downarrow 0}\frac{\langle x^2(t)\rangle - \langle x^2(0)\rangle}{t^2} = \langle v^2\rangle$

in physical terms: for $t \ll \frac{m}{\mu}$:

$\langle x^2(t)\rangle - \langle x^2(0)\rangle \sim \langle v^2\rangle t^2$: ballistic motion!

so $$\lim_{t\nearrow\infty} \frac{\langle x^2(t)\rangle - \langle x^2(0)\rangle}{t} = \frac{2m\langle v^2\rangle}{\mu} = \frac{6kT}{\mu}$$

in other terms: for $t \gg \frac{m}{\mu}$:

$$\langle x^2(t)\rangle - \langle x^2(0)\rangle \sim 6Dt$$

Diffusive motion with $D = \frac{kT}{\mu}$, Einstein's relation.

2 Fluctuations, Irreversibility & the 2nd law of thermodynamics

- Consider two Hamiltonians $H^{(0)}$ & $H^{(1)}$, and imagine the system in contact with a heat bath: fixed β.

Let ΔF be the free energy difference at β

Note: ΔF is the work done along a quasi-static path $H^{(0)} \to H^{(1)}$ (changes are infinitely slow, temperature remains fixed at β at all times)

Recall: $dF = -SdT + \delta W$.

Now: We switch $H^{(0)} \to H^{(1)}$ in an arbitrary way, performing work W along the way, and let the system relax back to the equilibrium state of $H^{(1)}$

β-Eq. state of $H^{(0)}$ $\xrightarrow[\text{slowly}: \ \Delta F]{\text{infinitely}}$ β-Eq. state of $H^{(1)}$

β-Eq. state of $H^{(0)}$ $\rightsquigarrow$ (arbitrary W) State, Hamiltonian is $H^{(1)}$ $\nearrow$ relax to equilibrium, heat Q. (β-Eq. state of $H^{(1)}$)

Question: Can we compare W, ΔF ?

First: classical case. Let $H = H(x,\lambda)$: $x \in \Gamma$, the phase space
$\lambda \in \mathbb{R}$, a work parameter
s.t. $H(x,0) = H^{(0)}(x)$ and $H(x,1) = H^{(1)}(x)$
an arbitrary path is given by $t \mapsto \lambda(t)$:
$t \in [0,\tau]$; $\lambda(0) = 0$; $\lambda(\tau) = 1$.
assume for simplicity $\lambda'(\tau) > 0$.

<u>Theorem</u> (Jarzynski 97). Let $W, \Delta F$ be as above, and let $\omega_\beta^{(0)}$ be the thermal state at inverse temp. β of the system $H^{(0)}$. Then:

$$\omega_\beta^{(0)}\left(e^{-\beta W}\right) = e^{-\beta \Delta F} \qquad (*)$$

Before we prove this, we note that
<u>Corollary</u> 1: In the above setup: $\omega_\beta^{(0)}(W) \geq \Delta F$

Proof of corollary 1: Jensen's inequality and the convexity of $f(x) = e^{-\beta x}$ yield:

$$e^{-\beta \omega_\beta^{(0)}(W)} \leq \omega_\beta^{(1)}\left(e^{-\beta W}\right) \overset{(*)}{=} e^{-\beta \Delta F}$$

$\square$

Note: The difference $\omega_\beta^{(0)}(W) - \Delta F$ is the <u>dissipated work</u> associated with the increase of entropy (entropy production) during the irreversible process.

<u>Proof of theorem</u>: Let $\gamma_t : \Gamma \to \Gamma$ be the flow on phase space generated by $H(\cdot, \lambda(t))$. For any observable, let $A_t(x,t) = \cancel{A(x,t)}\ A(\gamma_t(x), t)$. Then

$$\frac{d}{dt} A_t(x,t) = \{H, A\} + \frac{\partial A}{\partial t}$$

In particular: $\frac{dH}{dt} = \{H, H\} + \frac{\partial H}{\partial t} = \frac{\partial H}{\partial t}$.

Let $W(x)$ be defined by

$$W(x) = \int_0^\tau \frac{\partial}{\partial t} H(\gamma_t(x), \lambda(t)) = \int_0^\tau \frac{d}{dt} H(\gamma_t(x), \lambda(t))$$

$$= H(x(\tau), \lambda(\tau)) - H(x(0), \lambda(0)) = H^{(1)}(x(\tau)) - H^{(0)}(x)$$

where $x(\tau) = \gamma_\tau(x)$.

Now:

$$\omega_\beta^{(0)}(e^{-\beta W}) = Z^{(0)}(\beta)^{-1} \int_\Gamma dx\, e^{-\beta H(x, \lambda(0))} e^{-\beta W(x)}$$

$$= Z^{(0)}(\beta)^{-1} \int_\Gamma dx\, e^{-\beta H(x(\tau), \lambda(\tau))}$$

$$= Z^{(0)}(\beta)^{-1} \int_\Gamma dy\, e^{-\beta H^{(1)}(y)} = \frac{Z^{(1)}(\beta)}{Z^{(0)}(\beta)}$$

where we used the symplectic change of variable $x \to y = x(\tau) = \gamma_\tau(x)$.
It remains to recall that $F_i = -\frac{1}{\beta} \log Z^{(i)}(\beta)$ to conclude □

- Corollary 2 : (Violation of the 2nd law).
  Assume that $\omega_\beta^{(0)}(W) > \Delta F$. Then there exist $B \in \Gamma$ s.t. $\mu_\beta^{(0)}(B) > 0$ (μ_β is the Gibbs measure $Z^{(0)}(\beta)^{-1} e^{-\beta H^{(0)}(x)} dx$) and

$$\omega_\beta^{(0)}(W(x)) < \Delta F$$

- In other words: The second law holds on average (Corollary 1) but it fails on "rare occasions" (Corollary 2).

Proof: Suppose otherwise : $\omega_\beta^{(0)}(W(x)) \geq \Delta F$ a.e.. Then the condition $\omega_\beta^{(0)}(W) > \Delta F$ implies that
$e^{-\beta W(x)} < e^{-\beta \Delta F}$ for $x \in B$, $\mu_\beta^{(0)}(B) > 0$. But then $\omega_\beta^{(0)}(W(x)) < e^{-\beta \Delta F} \omega_\beta^{(0)}(1) = e^{-\beta \Delta F}$ violates Jarzynski □

- Why violation of 2^{nd} law? Recall

  "There is no cyclic machine that draws heat from a single reservoir and produces work".

  Here: the cycle would be: $H^{(0)} \to H^{(1)}$ along an arbitrary path, then relax to eq. state $\omega_\beta^{(1)}$, and come back to $\omega_\beta^{(0)}$ along a quasi-static path. The total work done is $W_{tot} = W - \Delta F$. 2^{nd} law: $W - \Delta F \overset{!}{\geq} 0$

- Corollary 3: For any $\mu > 0$:

$$\mu_\beta^{(0)}\left(W(x) \leq \Delta F - \mu\right) \leq e^{-\beta\mu}.$$

This is the probability of violation of 2^{nd} law.

Proof: $\mu_\beta^{(0)}\left(W(x) \leq \Delta F - \mu\right) = \int \chi\left(W(x) \leq \Delta F - \mu\right) e^{-\beta H^{(0)}(x)} dx$

$$\leq \int e^{-\beta\left(W(x) - \Delta F + \mu\right)} e^{-\beta H_0^{(0)}(x)} dx$$

$$= e^{\beta(\Delta F - \mu)} \, \omega_\beta^{(0)}\left(e^{-\beta W}\right) = e^{-\beta\mu}$$

Note: In probability, Corollary 3 is called large deviation

- On path space:

Let $T : \Gamma \to \Gamma$, $x \mapsto Tx$ be defined as $T(p,q) = (-p,q)$.

T: "time reversal".

For a path: $(\tilde{T}\gamma)(t) = T\left(\gamma(\tau - t)\right)$ $t \in [0,\tau]$

Now: Assume $H(x,\lambda)$ is time-reversal invariant:

$$H(x,\lambda) = H(Tx,\lambda), \quad \text{for all } \lambda.$$

Then: if γ is a trajectory for $\lambda(t)$, then $\tilde{T}\gamma$ is a trajectory for $\lambda(\tau - t)$

indeed, eq. of motion: $\dot{q} = \frac{\partial H}{\partial p}$; $\dot{p} = -\frac{\partial H}{\partial q}$

Let $q^\dagger(t) = q(\tau - t)$; $p^\dagger(t) = -p(\tau - t)$. Then

$$\frac{\partial H(q^\dagger, p^\dagger, \lambda(\tau-t))}{\partial p^\dagger} = \frac{\partial H(q(\tau-t), p(\tau-t), \lambda(\tau-t))}{-\partial p(\tau-t)} = -\frac{d}{d(\tau-t)} q(\tau-t)$$

$$= \frac{d}{dt} q^\dagger$$

and similarly for $-\frac{\partial H^\dagger}{\partial q^\dagger}$.

The measure on phase space $d\mu_\beta^{(0)}(x) = Z^{(0)}(\beta)^{-1} e^{-\beta H^{(0)}(x)} dx$ lifts to a measure on paths $\mathbb{P}_\beta^{(0)}[\gamma]$.

- Theorem:

$$\frac{\mathbb{P}_\beta^{(0)}[\gamma]}{\mathbb{P}_\beta^{(1)}[\tilde{T}\gamma]} = e^{\beta(W[\gamma] - \Delta F)}$$

Proof:

$$\frac{\mathbb{P}_\beta^{(0)}[\gamma]}{\mathbb{P}_\beta^{(1)}[\tilde{T}\gamma]} = \frac{Z^{(1)}(\beta)}{Z^{(0)}(\beta)} e^{-\beta H^{(0)}(x_0) + \beta H^{(1)}(Tx_1)}$$

$$= e^{-\beta\Delta F} e^{-\beta H^{(0)}(x_0) + \beta H^{(1)}(x_1)}$$

$$= e^{-\beta\Delta F} e^{\beta W[\gamma]}$$

□

- Remark: Although both γ and $\tilde{T}\gamma$ satisfy the eq. of motion, (microscopic reversibility) the probability to see the path violating the second law is exponentially small compared to the prob. of seeing the path that satisfies it. (macroscopic irreversibility).

But: the breaking of symmetry occurs "by hand", by starting in the equilibrium state.

- Quantum Jarzynski:

Consider a similar situation as before:
Initial and final Hamiltonians $H^{(0)}, H^{(1)}$ on $\mathcal{H}$, Gibbs states given by density matrices $\rho_\beta^{(0)}$ and $\rho_\beta^{(1)}$, time evolution generated by $H(t)$, $t \in [0,1]$ s.t. $H(0) = H^{(0)}$, $H(1) = H^{(1)}$: $U(t)$.
Let $U := U(1)$

<u>Proposition</u>: Let
$$\langle W \rangle := \operatorname{tr}\left(U \rho_\beta^{(0)} U^+ H^{(1)}\right) - \operatorname{tr}\left(\rho_\beta^{(0)} H^{(0)}\right) \qquad (W)$$
Then
$$\langle W \rangle \geq \Delta F$$
where
$$\Delta F = -\frac{1}{\beta}\left(\log Z^{(1)}(\beta) - \log Z^{(0)}(\beta)\right)$$

<u>Proof</u>: Uses again Klein's inequality. Since $-\beta H^{(1)} = \log \rho_\beta^{(1)} + \log Z^{(1)}(\beta)$:
$$\begin{aligned}
\beta \langle W \rangle &= \operatorname{tr}\left(\rho_\beta^{(0)} \log \rho_\beta^{(0)}\right) + \log\left(Z^{(0)}(\beta)\right) \operatorname{tr}\left(\rho_\beta^{(0)}\right) \\
&\quad - \operatorname{tr}\left(U \rho_\beta^{(0)} U^+ \log \rho_\beta^{(1)}\right) - \log\left(Z^{(1)}(\beta)\right) \operatorname{tr}\left(\rho_\beta^{(1)}\right) \\
&= \operatorname{tr}\left(\rho_\beta^{(0)} \log \rho_\beta^{(0)}\right) - \operatorname{tr}\left(\rho_\beta^{(0)} \log U^+ \rho_\beta^{(1)} U\right) \\
&\quad + \log Z^{(0)}(\beta) - \log Z^{(1)}(\beta) \\
&\geq \operatorname{tr}\left(\rho_\beta^{(0)} - U^+ \rho_\beta^{(1)} U\right) + \beta \Delta F = \beta \Delta F
\end{aligned}$$
□

- Question: What is the statistics behind (W)?
  i) Measurement of $U^+ H^{(1)} U - H^{(0)}$?
  No: it would be an observable at different times.
  ii) Difference of two measurements?
  Yes: Assume: $H^{(0)} = \sum_\alpha E_\alpha^{(0)} P_\alpha^{(0)}$, $\sum_\alpha P_\alpha^{(0)} = 1$.
  1st measurement: outcome $E_i^{(0)}$
  state after measurement $\sum_\alpha P_\alpha^{(0)} \rho_\beta^{(0)} P_\alpha^{(0)}$
  with probability $\operatorname{Tr}\left(P_i^{(0)} \rho_\beta^{(0)} P_i^{(0)}\right)$

After evolution: state is $U \sum_\alpha P_\alpha^{(0)} \rho_\beta^{(0)} P_\alpha^{(0)} U^\dagger$

2^{nd} measurement: $\sum_{\alpha,\gamma} P_\gamma^{(1)} U P_\alpha^{(0)} \rho_\beta^{(0)} P_\alpha^{(0)} U^\dagger P_\gamma^{(1)}$

Work $W_{ij} = \cancel{E_{ij}}\ E_j^{(1)} - E_i^{(0)}$ with probability $\mathrm{Tr}(\cdots j \cdots i \cdots)$.

$\rightsquigarrow$ Expected work:

$$\langle W \rangle = \sum_{\alpha\gamma} (E_\gamma^{(1)} - E_\alpha^{(0)}) \mathrm{Tr}\left(P_\gamma^{(1)} U P_\alpha^{(0)} \rho_\beta^{(0)} P_\alpha^{(0)} U^\dagger P_\gamma^{(1)}\right)$$

$$= \sum_{\alpha\gamma} (E_\gamma^{(1)} - E_\alpha^{(0)}) \mathrm{Tr}\left(P_\gamma^{(1)} U P_\alpha^{(0)} \rho_\beta^{(0)} U^\dagger\right)$$

$$= \mathrm{Tr}\left(\left(\sum_\gamma E_\gamma^{(1)} P_\gamma^{(1)}\right) U \left(\sum_\alpha P_\alpha^{(0)}\right) \rho_\beta^{(0)} U^\dagger\right)$$

$$- \mathrm{Tr}\left(\left(\sum_\gamma P_\gamma^{(1)}\right) U \left(\sum_\alpha E_\alpha^{(0)} P_\alpha^{(0)}\right) \rho_\beta^{(0)} U^\dagger\right)$$

$$= \mathrm{Tr}\left(H^{(1)} U \rho_\beta^{(0)} U^\dagger\right) - \mathrm{Tr}\left(U H^{(0)} \rho_\beta^{(0)} U^\dagger\right)$$

- <u>Theorem</u>: quantum Jarzynski - Tasaki's identity (2000)

$$\langle e^{-\beta W} \rangle = e^{-\beta \Delta F}$$

Note again the meaning of $\langle \cdot \rangle$ (compared to classical case).

<u>Proof</u>: As above:

$$\langle e^{-\beta W} \rangle = \sum_{\alpha\gamma} e^{-\beta(E_\gamma^{(1)} - E_\alpha^{(0)})} \mathrm{Tr}\left(P_\gamma^{(1)} U P_\alpha^{(0)} \rho_\beta^{(0)} U^\dagger\right)$$

$$= \sum_{\alpha\gamma} e^{-\beta(E_\gamma^{(1)} - E_\alpha^{(0)})} \mathrm{Tr}\left(P_\gamma^{(1)} U P_\alpha^{(0)} Z^{(0)}(\beta)^{-1} e^{-\beta E_\alpha^{(0)}} U^\dagger\right)$$

$$= Z^{(0)}(\beta)^{-1} \mathrm{Tr}\left(e^{-\beta H^{(1)}} U \,\cancel{\cdot}\, \mathbb{1} U^\dagger\right) = \frac{Z^{(1)}(\beta)}{Z^{(0)}(\beta)}$$

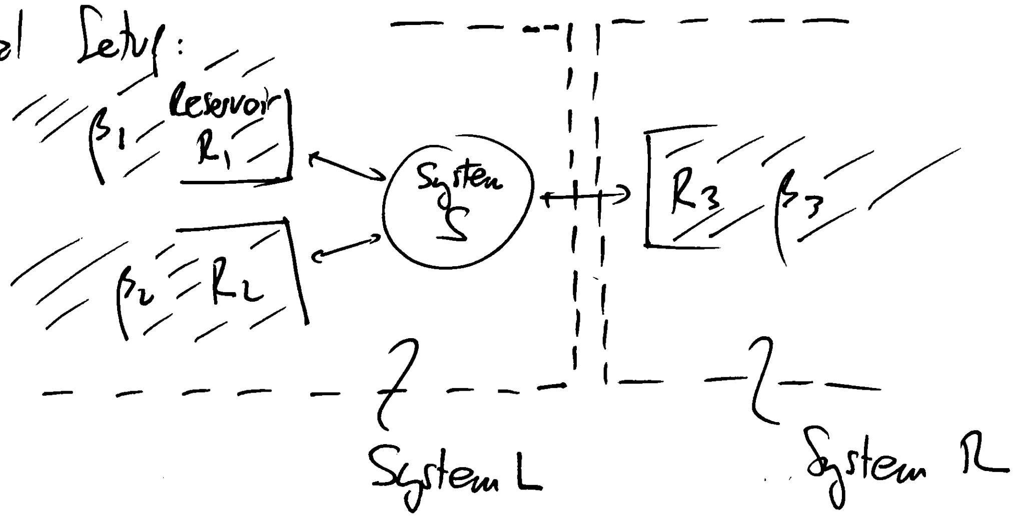
$$= e^{-\beta \Delta F}$$

$\square$

Part III: Open quantum systems and algebraic quantum statistical mechanics

VII. Open Quantum Systems: an algebraic approach

- General Setup:



"$\leftrightarrow$" exchanges of heat, but also of work and matter.
this will be our interest, mostly.

In general: Hamiltonian description fails:
- number of particles is ∞
- energy is ∞
- partition function does not exist
- ...

$\rightsquigarrow$ One way out:
- Switch from states on $\mathcal{H}$ to the algebra of observables, which exists indep. of a particular representation as (a subset) of $\mathcal{B}(\mathcal{H})$.
- Switch from the Hamiltonian and the Schrödinger picture to the dynamics and the Heisenberg picture.

$\Rightarrow$ Quantum dynamical systems: see e.g.
C.A. Pillet: 'Quantum dynamical systems' in
Open Quantum Systems I: The Hamiltonian Approach
Lecture Notes in Mathematics 1880, Springer

- The algebra of observables is a quasi-local algebra

Def: A directed set I has an orthogonality relation if there is a symmetric relation $\perp$ s.t.

i) $\alpha \in I \Rightarrow \exists \beta \in I : \alpha \perp \beta$

ii) $\alpha \leq \beta$ and $\beta \perp \gamma \Rightarrow \alpha \perp \gamma$

iii) $\alpha \perp \beta$ and $\alpha \perp \gamma \Rightarrow \exists \delta \in I$ s.t. $\alpha \perp \delta$ and $\delta \geq \beta$, $\delta \geq \gamma$.

Ex: I: bounded open subsets of $\mathbb{R}^4$. $\alpha \perp \beta$ if $\alpha \cap \beta = \phi$, and $\alpha \leq \beta$ is the inclusion.

Def: A quasi-local algebra is a C^*-algebra $\mathcal{A}$ and a net $\{\mathcal{A}_\alpha\}_{\alpha \in I}$ of C^*-subalgebras s.t. I has an orth. relation and:

i) $\alpha \geq \beta \Rightarrow \mathcal{A}_\alpha \supseteq \mathcal{A}_\beta$

ii) $\mathcal{A} = \overline{\bigcup_{\alpha \in I} \mathcal{A}_\alpha}^{\|\cdot\|}$

iii) The $\mathcal{A}_\alpha$ have a common identity.

iv) $\exists \sigma$, an automorphism of $\mathcal{A}$ s.t. $\sigma^2 = 1$, $\sigma(\mathcal{A}_\alpha) = \mathcal{A}_\alpha$ and, if $\alpha \perp \beta$:

$$[\mathcal{A}_\alpha^e, \mathcal{A}_\beta^e] = 0$$
$$[\mathcal{A}_\alpha^e, \mathcal{A}_\beta^o] = 0$$
$$\{\mathcal{A}_\alpha^o, \mathcal{A}_\beta^o\} = 0$$

where $\mathcal{A}_\alpha^o = \{A \in \mathcal{A}_\alpha : \sigma(A) = -A\}$

$\mathcal{A}_\alpha^e = \{A \in \mathcal{A}_\alpha : \sigma(A) = A\}$.

Ex. For bosons, take $\sigma = 1$ and (iv) simplifies to

$$[\mathcal{A}_\alpha, \mathcal{A}_\beta] = 0$$

i.e. observables located in (with support in) disjoint subsets of $\mathbb{R}^4$ commute.

- **Def**: A pair $(\mathcal{A}, \tau^t)$ is a C^*-dynamical system if $\mathcal{A}$ is a quasi-local algebra and τ^t is a strongly continuous group of $*$-automorphisms of $\mathcal{A}$.

Note: Strong continuity means: $t \mapsto \tau^t(A)$ is continuous in the $\|\cdot\|$ topology $\forall A \in \mathcal{A}$.

- Proposition: Let $\delta_t := -t^{-1}(1-\tau^t)$ and

$$D(\delta) := \{A \in \mathcal{A} : \lim_{t \to 0^+} \delta_t(A) \text{ exists}\}.$$

For $A \in D(\delta)$, let $\delta(A) := \lim_{t \to 0^+} \delta_t(A)$.

Then A is closed and densely defined.

We will write

$$\tau^t(A) = e^{+t\delta}(A),$$

since $\frac{d}{dt}\tau^t(A) = \delta(\tau^t(A))$ for $A \in D(\delta)$.

Proof: exercise.

- Properties: $*$ $\tau^t(1) = 1 \Rightarrow D(\delta) \ni 1$ and $\delta(1) = 0$
  - $*$ $\tau^t(AB) = \tau^t(A)\tau^t(B) \Rightarrow \delta(AB) = \delta(A)B + A\delta(B)$ for all $A, B \in D(\delta)$
  - $*$ $\tau^t(A^*) = \tau^t(A)^* \Rightarrow \delta(A^*) = \delta(A)^*$ for all $A \in D(A)$

An operator with these properties is called a *-derivation.

- For a finite quantum system: $\mathcal{A} = \mathcal{B}(\mathcal{H})$,

$\tau^t(A) = e^{itH} A e^{-itH}$ and $\delta(A) = i[H, A]$.

- In other words: the generator of a τ^t is a $*$-derivation; and reciprocally a (closed, densely defined) operator δ on $\mathcal{A}$ generates a τ^t iff (Hille-Yosida)
  i) δ is a $*$-derivation
  ii) $\mathrm{Ran}\,(1 + \lambda\delta) = \mathcal{A}$ $\forall \lambda \in \mathbb{R}$
  iii) $\|A + \lambda\delta(A)\| \geq \|A\|$ $\forall \lambda \in \mathbb{R}$, and $A \in D(\delta)$

- Def: $A \in \mathcal{A}$ is analytic for τ^t if the function $t \mapsto \tau^t(A)$ extends to an entire analytic function on $\mathbb{C}$.
- Def: A state on $\mathcal{A}$ is an element $\omega \in \mathcal{A}^*$ s.t.
  i) $\omega(A^*A) \geq 0$ (positive)
  ii) $\omega(1) = 1$ (normalized)
  It is faithful if $\omega(A^*A) = 0$ implies $A = 0$.

Lemma: (i), (ii) $\Rightarrow$ $\|\omega\| = 1$:

$$|\omega(A)| \leq \omega(1)^{1/2} |\omega(A^*A)|^{1/2} \leq \|A^*A\|^{1/2}\omega(1) \overset{C^*\text{-property}}{=} \|A\|\,\omega(1)$$

Cauchy Schwarz; (i) and $\|A^*A\| \cdot 1 - A^*A \geq 0$.

Therefore $\omega \in \mathcal{A}_1^*$, the unit ball of $\mathcal{A}^*$, and

$$\mathcal{E}(\mathcal{A}) = \{\omega \in \mathcal{A}_1^* : \omega(A^*A) \geq 0 \ \forall A \in \mathcal{A}\}$$

is a weak-$*$ compact subset of $\mathcal{A}^*$ by Banach-Alaoglu.

- Theorem: If $\mathcal{A}$ is a C^*-algebra with a unit, and $\omega \in \mathcal{E}(\mathcal{A})$, then there exists a Hilbert space $\mathcal{H}_\omega$, a representation $\pi_\omega : \mathcal{A} \to \mathcal{B}(\mathcal{H}_\omega)$ and $\Omega_\omega \in \mathcal{H}_\omega$, $\|\Omega_\omega\| = 1$ s.t.

$$\omega(A) = \langle \Omega_\omega, \pi_\omega(A)\Omega_\omega \rangle \quad A \in \mathcal{A},$$

and $\{\pi_\omega(A)\Omega_\omega : A \in \mathcal{A}\}$ is dense in $\mathcal{H}_\omega$.

We say that Ω_ω is a cyclic vector for $\pi_\omega(\mathcal{A})$.

Proof: Exercise.

- Def: Let $(\mathcal{A}, \tau^t)$ be a C^* dynamical system. $\omega \in \mathcal{E}(\mathcal{A})$ is called τ^t invariant if

$$\omega \circ \tau^t = \omega \qquad \forall t \in \mathbb{R}.$$

Denote the set of such states by $\mathcal{E}(\mathcal{A}, \tau^t)$.

- Theorem: Let $(\mathcal{A}, \tau^t)$ be as above. If $\exists\, \omega \in \mathcal{E}(\mathcal{A})$ s.t. $t \mapsto \omega(\tau^t(A))$ is continuous $\forall A \in \mathcal{A}$, then $\mathcal{E}(\mathcal{A}, \tau^t)$ is a non-empty, convex, weak-* compact subset of $\mathcal{A}^*$.

Proof: For $T > 0$, and $A \in \mathcal{A}$, let

$$\omega_T(A) := \frac{1}{T}\int_0^T \omega \circ \tau^s(A)\, ds,$$

where the integral is well-defined by the continuity assumption. We have $\omega_T \in \mathcal{E}(\mathcal{A})$. But compactness, the net $\{\omega_T\}_{T>0}$ has a weak*-convergent subnet. It remains to prove the accumulation point are τ^t-invariant. Since

$$\omega_T(\tau^t(A)) - \omega_T(A) = \frac{1}{T}\left[-\int_0^t \omega(\tau^s(A))\,ds + \int_T^{T+t} \omega(\tau^s(A))\,ds\right],$$

we have that

$$|\omega_T(\tau^t(A)) - \omega_T(A)| \le \frac{1}{T}\left(2|t|\,\|A\|\right) \xrightarrow{T\to\infty} 0 \qquad \square$$

- Def: The triple $(\mathcal{A}, \tau^t, \omega)$ is a <u>quantum dynamical system</u> if $(\mathcal{A}, \tau^t)$ is a C^*-dynamical system and $\omega \in \mathcal{E}(\mathcal{A}, \tau^t)$ ~~s.t.~~

- Now: In the GNS representation of the invariant state, there is always a good generator of the dynamics.

Proposition: Let $(\mathcal{A}, \tau^t, \omega)$ be a quantum dynamical system, with GNS representation $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$. Then there exists a unique self-adjoint operator L_ω on $\mathcal{H}_\omega$ s.t.

(i) $\pi_\omega(\tau^t(A)) = e^{itL_\omega}\pi_\omega(A)e^{-itL_\omega}$
for all $A \in \mathcal{A}$ and $t \in \mathbb{R}$.

(ii) $L_\omega\Omega_\omega = 0$.

In other words, the dynamics is unitarily implementable in the GNS Hilbert space of an invariant state.

Proof: * First, we show that the GNS representation for any μ is unique up to unitary equivalence. Let $(\mathcal{H}_\mu', \pi_\mu', \Omega_\mu')$ be another GNS rep. and define U through

$$U : \mathcal{H}_\mu \to \mathcal{H}_\mu' \quad ; \quad U\pi_\mu(A)\Omega_\mu = \pi_\mu'(A)\Omega_\mu'.$$

Then:

$$\langle U\pi_\mu(A)\Omega_\mu, U\pi_\mu(B)\Omega_\mu\rangle_{\mathcal{H}_\mu'} = \langle \pi_\mu'(A)\Omega_\mu', \pi_\mu'(B)\Omega_\mu'\rangle_{\mathcal{H}_\mu'}$$
$$= \mu(A^* B) = \langle \pi_\mu(A)\Omega_\mu, \pi_\mu(B)\Omega_\mu\rangle_{\mathcal{H}_\mu}$$

Hence U is a densely defined operator that preserves the scalar product, and is in particular bounded. It follows that its closure is a unitary operator s.th.

$$U^* \pi_\mu'(A) U = \pi_\mu(A) \qquad \forall A \in \mathcal{A}. \qquad (\diamond)$$

* We apply this uniqueness to the representation $(\mathcal{H}_\omega, \pi_\omega\circ\tau^t, \Omega_\omega)$ (also GNS for ω) for any fixed $t \in \mathbb{R}$, i.e. $\exists\ U_\omega^t$ s.t. $(\mathcal{H}_\omega', \pi_\omega', \Omega_\omega')$

$$U_\omega^t \pi_\omega(A)\Omega_\omega = \pi_\omega(\tau^t(A))\Omega_\omega \qquad (\diamond\diamond)$$

and $U_\omega^t\Omega_\omega = \Omega_\omega$.

* Now we claim that U_ω^t is a strongly continuous semi-group.

$$U_\omega^t U_\omega^s \pi_\omega(A)\Omega_\omega = U_\omega^t(\pi_\omega(\tau^s(A))\Omega_\omega) = \pi_\omega(\tau^t\circ\tau^s(A))\Omega_\omega$$
$$= \pi_\omega(\tau^{t+s}(A))\Omega_\omega = U_\omega^{t+s}\pi_\omega(A)\Omega_\omega.$$

The continuity of $t \mapsto \omega(B^*\tau^t(A))$ implies the continuity of $t \mapsto \langle \pi_\omega(B)\Omega_\omega, U_\omega^t\pi_\omega(A)\Omega_\omega\rangle$

so that U^t_ω is weakly continuous, and since it is unitary also strongly continuous.
By Stone's theorem, $U^t_\omega = \exp(itL_\omega)$ for a self-adjoint operator L_ω, with $U^t_\omega \Omega_\omega = \Omega_\omega \Rightarrow L_\omega \Omega_\omega = 0$,
~~and~~ ($\Diamond$) now reads:

$$e^{-itL_\omega}\, \Pi_\omega(\tau_t(A))\, e^{itL_\omega} = \Pi_\omega(A) \quad \text{, i.e. (1).}$$

Finally, uniqueness follows from ($\Diamond\Diamond$) $\square$

- In the context of open quantum systems, L_ω is called the ω-Liouvillean (usually defined on the algebra $\Pi_\omega(\mathcal{A})''$)
Warning: L_ω does not represent the energy of the system anymore
→ see exercise about finite quantum systems.

- Def: Let $(\mathcal{A}, \tau^t)$ be a C^*-dynamical system. A state ω is a <u>(τ^t, β)-KMS state</u> at $\beta > 0$ if for any $A, B \in \mathcal{A}$, there exists a function $F_\beta(A, B, z)$, analytic in the strip

$$S_\beta := \{ z \in \mathbb{C} : 0 < \operatorname{Im} z < \beta \},$$

continuous on its closure and s.t.

$$F_\beta(A, B; t) = \omega(A\tau^t(B))$$
$$F_\beta(A, B; t + i\beta) = \omega(\tau^t(B)A)$$

("KMS boundary condition")

- Lemma: Let ω be a (τ^t, β)-KMS state of $(\mathcal{A}, \tau^t)$ and let $A \in \mathcal{A}$, and $B \in \mathcal{A}$ be an analytic element of τ^t. Then:

$$\omega(A\tau^{i\beta}(B)) = \omega(BA) \qquad (*)$$

Proof: $z \mapsto \omega(A\tau^z(B))$ is entire analytic, and by definition $\omega(A\tau^t(B)) = F_\beta(A, B; t)$ for $t \in \mathbb{R}$. Thus, the function $\omega(A\tau^z(B)) - F_\beta(A, B; z)$ is :

* analytic on S_β
* continuous on $S_\beta \cup \mathbb{R}$
* vanishes on $\mathbb{R}$

Hence it extends to an analytic function on $\{-\beta < \mathrm{Im}\, z < \beta\}$ which vanishes on $\mathbb{R}$ and therefore on the entire strip, and by continuity $\overline{S_\beta}$, i.e. in particular

$$\omega(A\tau^{i\beta}(B)) - f_\beta(A,B;i\beta) = 0$$

$C=1$
KMS BC
$$\omega(A\tau^{i\beta}(B)) = \omega(BA)$$
$\square$

• <u>Theorem</u>: If ω is a (τ^t, β)-KMS state, then it is τ^t-invariant, i.e. $\omega \in \mathcal{E}(\mathcal{A}, \tau^t)$.

<u>Proof</u>: Let A be an analytic element of τ^t, and let $f_A(z) = \omega(\tau^z(A))$ so that $z \mapsto f(z)$ is analytic. By the above lemma,

$$f_A(t+i\beta) = \omega(1\,\tau^{i\beta}(\tau^t(A))) = \omega(\tau^t(A)\cdot \mathbb{1}) = f_A(t)$$

i.e. f_A is a periodic function. Moreover, on $\overline{S_\beta}$, $t \in \mathbb{R}$, $\alpha \in \mathbb{R}$.

$$|f_A(t+i\alpha)| \leq \|\tau^{t+i\alpha}(A)\| = \|\tau^{i\alpha}(A)\|$$
$$\leq \sup_{0 \leq \gamma \leq \beta} \|\tau^{i\gamma}(A)\| < \infty$$

since $[0,\beta]$ is compact and $z \mapsto \tau^z(A)$ is analytic. Altogether, $f_A(z)$ is bounded on $\mathbb{C}$, and since it is entire analytic it must be constant on $\mathbb{C}$. $\square$

Physically: KMS states play the role of thermodynamic <u>equilibrium</u> states in an abstract setting where the Gibbs states cannot be defined.

<u>Remark</u>: In fact, in the case of a C^*-dynamical system, eq. (✵) can be taken as the <u>definition</u> of a KMS-state: ω is a (τ^t,β)-KMS state iff there exists a dense, τ^t-invariant subalgebra D of analytic elements for τ^t s.t. (✵) holds for all $A, B \in D$.

- **Def**: Let $(\mathcal{A}, \tau_0^t)$ be a C^*-dynamical system, and let δ_0 be its generator. A local perturbation of δ_0 is
$$\delta_V = \delta + i[V, \cdot] \qquad \text{(note: } V \text{ is bounded)}$$
where $V = V^* \in \mathcal{A}$ and s.t. $D(\delta_V) = D(\delta_0)$

By Hille-Yosida, δ_V generates a strongly continuous group of $*$-automorphisms τ_V^t on $\mathcal{A}$.

- Interaction picture: Let Γ_V^t be the unique solution of
$$\begin{cases} \partial_t \Gamma_V^t = i \Gamma_V^t \tau_0^t(V) \\ \Gamma_V^0 = 1 \end{cases}$$

It follows that
$$\tau_V^t(A) = \Gamma_V^t \, \tau_0^t(A) \Gamma_V^{t\,*}$$
since, for both sides: $\frac{d}{dt}(\cdot)\Big|_{t=0} = \delta_0(A) + i[V, A]$

Consequences:

i) $\Gamma_V^{t+s} = \Gamma_V^t \tau_0^t(\Gamma_V^s) = \tau_V^t(\Gamma_V^s)\Gamma_V^t$

ii) Γ_V^t is a unitary element of $\mathcal{A}$.

iii) Γ_V^t has the convergent expansion: (Dyson)
$$\Gamma_V^t = 1 + \sum_{h=1}^{\infty} i^h \int_{0 \le t_1 \le \dots \le t_h \le t} dt_1 \cdots dt_h \; \tau_0^{t_1}(V) \cdots \tau_0^{t_h}(V)$$

- Perturbation theory: Let ω^0, resp. ω^V, be a (τ_0^t, β), resp. (τ_V^t, β)-KMS state. Then,
$$\omega^V(A) = \omega^0(\Gamma_V^{i\beta})^{-1} \omega^0(A \Gamma_V^{i\beta})$$
for all $A \in \mathcal{A}$.

Proof: it suffices to check condition $(*)$ for the state $\mu(A) := \omega^0(\Gamma_V^{i\beta})^{-1} \omega^0(A\Gamma_V^{i\beta})$.

$$\begin{aligned}\mu\left(A\tau_V^{i\beta}(B)\right) &= \omega^\circ(\Gamma_V^{i\beta})^{-1}\,\omega^\circ\left(A\tau_V^{i\beta}(B)\Gamma_V^{i\beta}\right)\\ &= \omega^\circ(\Gamma_V^{i\beta})^{-1}\,\omega^\circ\left(A\Gamma_V^{i\beta}\,\tau_0^{i\beta}(B)\right)\\ &= \omega^\circ(\Gamma_V^{i\beta})^{-1}\,\omega^\circ\left(BA\Gamma_V^{i\beta}\right)\\ &= \mu(BA)\end{aligned}$$

where we used the KMS-condition for ω° in the 3^{rd} equality.

The statement follows after checking that $\mu(1) = 1$ $\square$

- Now: we prove Green-Kubo formula and Onsager's reciprocal relations axiomatically, for thermal forces.

Setup: Two systems, initially at $\beta_L = \beta$ for the "left system" and β_R for the right system.

Thermal force:

$$X := \beta - \beta_R \quad , \quad X \in I \quad , \quad I \text{ neighbourhood of } 0.$$

Two quantum dynamical systems: $(\mathcal{A}_L, \tau_L, \omega_L)$ and $(\mathcal{A}_R, \tau_R, \omega_R)$ with

$$\tau_{L,R} = \exp(t\delta_{L,R})$$

Brought into contact : $\mathcal{A} := \mathcal{A}_L \otimes \mathcal{A}_R$

No coupling : $\tau_0 = \tau_L \otimes \tau_R$

$\delta_0 = \delta_L + \delta_R$

(i.e. $\delta_L \otimes 1 + 1 \otimes \delta_R$)

Interaction: $V \in \mathcal{A}$ which is a local perturbation, and $\delta_V = \delta_0 + i[V, \cdot]$ now generates τ.

<u>Def</u>: If $V \in D(\delta_R)$, then the observable

$$\Phi = \delta_R(V)$$

is the heat flux out of R.

Why? For Hamiltonian systems: $H_{tot} = H_L + H_R + V$

and $\Phi = -\frac{d}{dt} e^{itH_{tot}} H_R e^{-itH_{tot}}\Big|_{t=0}$

$= i[H_R, V]$ ⟶ hence the general definition.

- Assumptions I : (AI)

(i) States:

* ω_L is the unique (τ_L, β)-KMS state on $\mathcal{A}_L$.
* For $X \in I$, $\omega_{R,X}$ is the unique $(\tau_R, \beta - X)$-KMS state on $\mathcal{A}_R$.

(ii) Heat flux: $V \in D(\delta_R)$.

(iii) Time reversal: $\exists\ \Theta$ of $(\mathcal{A}, \tau_0)$ s.t.

$$\Theta \circ \tau_L^t = \tau_L^{-t} \circ \Theta \ ; \ \Theta \circ \tau_R^t = \tau_R^{-t} \circ \Theta \ ; \ \Theta(V) = V$$

Notations & consequences:

* $X \in I$: $\omega_X^{(0)} := \omega_L \otimes \omega_{R,X}$
* $X \in I$: C^*-dynamics on $\mathcal{A}$:

$\sigma_X^{(0)}$ generated by $\delta_X^{(0)} := \delta_0 - \frac{X}{\beta}\delta_R$

σ_X generated by $\delta_X := \delta_X^{(0)} + i[V, \cdot]$

* $X \in I$: $\omega_X^{(0)}$: unique $(\sigma_X^{(0)}, \beta)$-KMS state on $\mathcal{A}$.

ω_X : unique (σ_X, β)-KMS state on $\mathcal{A}$ (exists by perturbation theory)

* $\omega_X^{(0)}$ & ω_X are time-reversal invariant (see later)

- ~~Theorem~~ Proposition 1 : If (AI) hold, and for any $A \in D(\delta_R)$ s.t. $A = A^*$, $\Theta(A) = -A$, the function

$$X \longmapsto \omega_X(\tau^t(A))$$

is differentiable at $X = 0$, and

$$\frac{\partial}{\partial X}\omega_X(\tau^t(A))\Big|_{X=0} = \frac{1}{\beta}\int_0^t ds \int_0^\beta d\gamma\, \omega_0\left(\tau^s(A)\,\tau^{i\gamma}(\Phi)\right)$$

- Remark: * R.H.S is the expectation in the KMS-state of the interacting dynamics, ~~but~~ i.e. the equilibrium state of the system when both reservoirs are at the same temperature β : no thermal force X, no heat flux Φ.
  * L.H.S. : the state appearing here is not the decoupled state $\omega_X^{(0)}$. This choice is however natural and should not matter in the limit $t \to +\infty$ if "all" states converge to the same non-equilibrium steady state.
  $\to$ see later.

- First: a formal computation, assuming Hamiltonian systems

$$\rho_X = Z^{-1} \exp\left(-\beta H_{tot} + X H_R\right)$$

$$\left(\text{this is not } \tilde{Z}^{-1} \exp\left(-\beta H_L - (\beta - X) H_R\right)\right).$$

Now:

$$\omega_X(A_t) = Z^{-1} \operatorname{Tr}\left(e^{-\beta H_{tot} + X H_R} e^{itH_{tot}} A e^{-itH_{tot}}\right)$$

$$= Z^{-1} \operatorname{Tr}\left(e^{-\beta\left(H_{tot} - \frac{X}{\beta} H_R\right)} e^{-it\left(H_{tot} - \frac{X}{\beta} H_R\right)} e^{itH_{tot}} A e^{-itH_{tot}} \cdot e^{it\left(H_{tot} - \frac{X}{\beta} H_R\right)}\right)$$

$$= \omega_X\left(e^{-it\left(H_{tot} - \frac{X}{\beta} H_R\right)} A_t \, e^{it\left(H_{tot} - \frac{X}{\beta} H_R\right)}\right)$$

Hence:

$$\omega_X(A_t) - \omega_X(A) = \frac{X}{\beta} \int_0^t ds \, \omega_X\left(i [H_R, A_s]\right)$$

Moreover: $\omega_X(A) = 0$ since ω_X is T.R.I and $\Theta(A) = -A$. Hence,

$$\frac{\partial}{\partial X} \omega_X(A_t)\Big|_{X=0} = \frac{1}{\beta} \int_0^t ds \, \omega_0\left(i [H_R, A_s]\right)$$

Finally: $\omega_0([H_R, A_s]) = -Z^{-1} \operatorname{Tr}\left([H_R, e^{-\beta H}] A_s\right) =$

$$= +Z^{-1}\, \mathrm{Tr}\left(\left(e^{-\beta H} H_R e^{\beta H} - H_R\right) e^{-\beta H} A_S\right)$$
$$= -Z^{-1} \int_0^\beta \mathrm{Tr}\left(e^{-\gamma H} [V, H_R] e^{\gamma H} e^{-\beta H} A_S\right)$$

so that $\omega_0\left(i [H_R, A_S]\right) = \omega_0\left(A_S\, \tau^{i\gamma}(\Phi)\right)$

Now: Prop. 1 is the statement that this holds for abstract C^*-dynamical systems as a consequence of the KMS condition.

- A few technical lemmas:
- Lemma 1: i) Θ is a time-reversal of $(\mathcal{A}, \tau^t)$ and $(\mathcal{A}, \sigma_X^t)$
  ii) ω_X is time-reversal invariant for $X \in \mathcal{I}$.
  iii) $\Theta(\Phi) = -\Phi$

Proof: (i) follows from $\tau^t(A) = \Gamma^t \tau_0^t(A) \Gamma^{t*}$ with

$$\Gamma^t = 1 + \sum_{k\geq 1} (it)^k \int_{0\leq t_1 \leq \dots \leq t_k \leq 1} dt_1 \dots dt_k\, \tau_0^{tt_1}(V) \dots \tau_0^{tt_k}(V)$$

Use: * $\Theta(V) = V$
* $\Theta \circ \tau_0^t = \tau_0^{-t} \circ \Theta$
* Θ is antilinear

to obtain $\Theta(\Gamma^t) = \Gamma^{-t}$

$$\Theta(\tau^t(A)) = \Theta(\Gamma^t)\, \Theta(\tau_0^t(A))\, \Theta(\Gamma^t)^*$$
$$= \Gamma^{-t} \tau_0^{-t}(\Theta(A)) (\Gamma^{-t})^*$$
$$= \tau^{-t}(\Theta(A))$$

$\Rightarrow$ Θ is a time-reversal for $(\mathcal{A}, \tau^t)$.

Moreover: Θ is a T.R. for δ_L, δ_R, therefore also for δ_0 and also $\delta_X^{(0)}$, i.e. a T.R. for $\sigma_X^{(0)}$. Repeating above with

$\sigma_X^{(0)} \leftrightarrow \tau_0$; $\sigma_X \leftrightarrow \tau$

yields the claim.

(ii) Consider $\tilde{\omega}_X(A) := \omega_X(\Theta(A^*))$

$$\tilde{\omega}_X(A\sigma_X^{i\beta}(B)) = \omega_X\left(\Theta\left(\sigma_X^{i\beta}(B^*)A^*\right)\right)$$
$$\overset{(i)}{=} \omega_X\left(\sigma_X^{-i\beta}(\Theta(B)^*)\Theta(A)^*\right)$$
$$(\sigma^t(B^*) = \sigma^{\bar{t}}(B)^*) \to \text{KMS}, \quad = \omega_X\left(\Theta(A)^*\Theta(B^*)\right)$$
$$= \omega_X\left(\Theta((BA)^*)\right) = \tilde{\omega}_X(BA)$$

Hence $\tilde{\omega}_X$ is a (σ_X, β)-KMS state. Since ω_X is also one and by uniqueness, $\tilde{\omega}_X = \omega_X$. It remains to see that $\tilde{\omega}$ is TRI:

$$\tilde{\omega}(\Theta(A)) = \omega(\Theta(\Theta(A)^*)) = \omega(\Theta\circ\Theta(A)^*) = \omega(A^*) \quad \checkmark$$

(iii) $$-\delta_R(V) = \frac{d}{dt}\tau_R^{-t}(V)\Big|_{t=0} = \frac{d}{dt}\Theta(\tau_R^t(V))\Big|_{t=0}$$
$$= \Theta\left(\frac{d}{dt}\tau_R^t(V)\Big|_{t=0}\right) = \Theta(\delta_R(V))$$

$\square$

- Lemma 2: $D(\delta_R)$ is invariant under τ^t, and $\forall A \in D(\delta_R)$,
$$t \mapsto \delta_R(\tau^t(A)), \quad t \in \mathbb{R}$$
is norm-continuous.

Proof: First:
$$\left.\begin{array}{l} * \ \tau_0^t \text{ preserves } D(\delta_R) \\ * \ V \in D(\delta_R) \\ * \ \text{Dyson's expansion} \end{array}\right\} \Rightarrow \Gamma^t \in D(\delta_R)$$

Then:
$$\delta_R(\Gamma^t) = \sum_{n\geq 1}(it)^n \int dt_1 \dots dt_n \sum_{j=1}^{n} \tau_0^{tt_1}(V)\dots\tau_0^{tt_j}(\delta_R(V)) \dots \tau_0^{tt_n}(V)$$
is uniformly convergent on compact subsets of $\mathbb{R}$.
Hence $t \mapsto \delta_R(\Gamma^t)$ is norm continuous.

Finally,
$$\delta_R(\tau^t(A)) = \delta_R(\Gamma^t)\tau_0^t(A)\Gamma^{t*} + \Gamma^t\tau_0^t(\delta_R(A))\Gamma^{t*} + \Gamma^t\tau_0^t(A)\delta_R(\Gamma_t)^*$$
i.e. $A \in D(\delta_R) \Rightarrow \tau^t(A) \in D(\delta_R)$

$\square$

- Now: In order to tackle the problem of differentiability of $\omega_\chi(\tau^t(A))$, we first compare the dynamics τ^t and σ_χ^t, whose generator differ by $-\frac{\chi}{\beta}\delta_R$ (recall that ω_χ is a KMS state for σ_χ^t)

<u>Lemma 3</u>: For $A \in D(\delta_R)$:

$$\sigma_\chi^t(A) - \tau^t(A) = -\frac{\chi}{\beta}\int_0^t ds\ \sigma_\chi^{t-s}\left(\delta_R(\tau^s(A))\right).$$

<u>Proof</u>: We assume that $A \in D(\delta_R) \cap D(\delta)$. If $A \notin D(\delta)$, we would need to approximate it by analytic elements. Since

$$\sigma_\chi^{-(t+\varepsilon)} \circ \tau^{(t+\varepsilon)} - \sigma_\chi^{-t}\circ\tau^t = \sigma_\chi^{-(t+\varepsilon)} \circ \tau^t \circ (\tau^\varepsilon - 1) + \sigma_\chi^{-(t+\varepsilon)} \circ (1-\sigma_\chi^\varepsilon)\circ \tau^t,$$

we have:

$$\frac{d}{dt}\sigma_\chi^{-t}(\tau^t(A)) = \sigma_\chi^{-t}(\tau^t(\delta_V(A))) - \sigma_\chi^{-t}(\delta_\chi(\tau^t(A)))$$
$$= \sigma_\chi^{-t}\Big(\underbrace{(\delta_V - \delta_\chi)}_{=\frac{\chi}{\beta}\delta_R}(\tau^t(A))\Big)$$
$$= \frac{\chi}{\beta}\sigma_\chi^{-t}(\delta_R(\tau^t(A)))$$

so that

$$\sigma_\chi^t(A) - \tau^t(A) = -\sigma_\chi^{t-s}(\tau^s(A))\Big|_{s=0}^{s=t} = -\frac{\chi}{\beta}\int_0^t ds\ \sigma_\chi^{t-s}(\delta_R(\tau^s(A))) \qquad \square$$

- for $A \in D(\delta_R)$: $\lim_{\chi\to 0}\|\sigma_\chi^t(A) - \tau^t(A)\| = 0$ and this holds for $A \in \mathcal{A}$ by density of $D(\delta_R)$. In turn, we have the following weak continuity:

<u>Lemma 4</u>: For $A \in \mathcal{A}$: $\lim_{\chi\to 0}\omega_\chi(A) = \omega_0(A)$.

<u>Proof</u>: By compacity, there are limit points of ω_χ in the weak-* topology. Since

i) σ_X^t converges strongly to τ^t $(X \to 0)$

ii) ω_X are (σ_X, β)-KMS states for all X

(Bratteli-Robinson) Then: Any limiting point is a (τ, β)-KMS state

By assumption: there is a unique (τ, β)-KMS state, i.e.

$$\omega_X(A) \to \omega_0(A) \quad \forall A$$

□

- Central lemma:

<u>Lemma 5</u>: Let $A \in D(\delta_R)$ s.t. $\begin{cases} A = A^* \\ \Theta(A) = -A \end{cases}$. $\forall t \in \mathbb{R}$,

$$X \mapsto \omega_X(\tau^t(A)), \quad X \in I$$

is differentiable at $X = 0$, and

$$\frac{\partial}{\partial X} \omega_X(\tau^t(A))\Big|_{X=0} = \frac{1}{\beta} \int_0^t \omega_0(\delta_R(\tau^s(A)))\, ds .$$

Proof: Since ω_X is (σ_X, β)-KMS, it is σ_X-invariant. By Lemma 3:

$$\frac{1}{X}\left(\omega_X(\tau^t(A)) - \omega_X(A)\right) = \frac{1}{\beta} \int_0^t ds\, \omega_X(\delta_R(\tau^s(A)))$$

But: i) By Lemma 1: $\omega_X(A) = \omega_X(\Theta(A)) = -\omega_X(A)$

$\Rightarrow \omega_X(A) = 0$.

ii) Similarly: $0 = \omega_0(A)$ &

and $\omega_0(A) = \omega_0(\tau^t(A))$.

Hence:

$$\frac{1}{X}\left[\omega_X(\tau^t(A)) - \omega_0(\tau^t(A))\right] = \frac{1}{\beta} \int_0^t ds\, \omega_X(\delta_R(\tau^s(A)))$$

Now: a) pointwise convergence $\omega_X(\delta_R(\tau^s(A))) \to \omega_0(\delta_R(\tau^s(A)))$ by Lemma 4

b) $|\omega_X(\delta_R(\tau^t(A)))| \leq \|\delta_R(\tau^t(A))\|$

which is uniformly bounded on the compact $[0, t]$ by Lemma 2

Dominated convergence yields the Lemma □

- We are now ready to prove the proposition.

• <u>Proof of Proposition 1</u>: With Lemma 5, the only remaining claim to be proven is that

$$\int_0^t \omega_0\left(\delta_R(\tau^t(A))\right) ds = \int_0^t ds \int_0^\beta d\gamma\, \omega_0\left(\tau^s(A)\,\tau^{i\gamma}(\Phi)\right)$$

Here, we shall assume that A, V (both $\in D(\delta_R)$ by assumption) are also analytic elements of τ^t. If not, approximate.

We claim: $\omega_0(\delta_R(A)) = \int_0^\beta d\gamma\, \omega_0(A\tau^{i\gamma}(\Phi))$.

and prove this by perturbation theory.

Dyson's expansion yields an analytic continuation of $t \mapsto \Gamma^t$ to $z \mapsto \Gamma^z$, and similarly for $z \mapsto \Gamma^{\bar z *}$, $z \in \mathbb{C}$. Moreover:

$$\Gamma_{\bar z}^{*} \Gamma_z = 1 \quad ; \Gamma_z \Gamma_{\bar z}^{*} = 1 \tag{1}$$

Also:
$$\frac{d}{dt}\Gamma^z = i\Gamma^z\tau_0^z(V)$$
$$\frac{d}{dz}\Gamma^{\bar z *} = -i\tau_0^z(V)\Gamma^{\bar z *}$$

and as above $\Gamma^z, \Gamma^{\bar z *} \in D(\delta_R)$, with (Check!)

$$\frac{d}{dt}\delta_R(\Gamma^z) = i\delta_R(\Gamma^z)\tau_0^z(V) + i\Gamma_z\tau_0^z(\Phi)$$
$$\frac{d}{dt}\delta_R(\Gamma^{\bar z *}) = -i\tau_0^z(\Phi)\Gamma^{\bar z *} - i\tau_0^z(V)\delta_R(\Gamma^{\bar z *}).$$

Then:
$$\frac{d}{dt}\Gamma_z\delta_R(\Gamma^{\bar z *}) = i\Gamma^z\tau_0^z(V)\,\delta_R(\Gamma^{\bar z *})$$
$$-i\Gamma^z\tau_0^z(\Phi)\Gamma^{\bar z *} - i\Gamma^z\tau_0^z(V)\,\delta_R(\Gamma^{\bar z *})$$
$$= -i\tau^z(\Phi) \tag{2}$$

Perturbation:

$$\underset{\text{refers to } X=0}{\omega_0}\left(\delta_R(A)\right) = \overset{\text{refers to } V=0}{\omega_0^{(0)}}(\Gamma^{i\beta})^{-1}\,\omega_0^{(0)}\left(\delta_R(A)\Gamma^{i\beta}\right)$$

where $\omega_0^{(0)} = \omega_L \otimes \omega_R$ (decoupled thermal states at β).

Since $\omega_0^{(0)}$ is τ_R-invariant, $\omega_0^{(0)}(\delta_R(C)) = 0$, $C \in D(\delta_R)$.

Hence: $\omega_0^{(0)}\left(\delta_R(A)\Gamma^{i\beta}\right) = -\omega_0^{(0)}\left(A\,\delta_R(\Gamma^{i\beta})\right)$.

$$= -\omega_0^{(0)}\left(A\,\delta_R(\Gamma^{i\beta})\,\Gamma^{-i\beta\lambda}\,\Gamma^{i\beta}\right) = \omega_0^{(0)}\left(A\,\Gamma^{i\beta}\,\delta_R(\Gamma^{-i\beta\lambda})\,\Gamma^{i\beta}\right)$$

where we used $1 = \Gamma^{i\beta}\Gamma^{-i\beta\lambda} \Rightarrow \delta_R(\Gamma^{i\beta})\Gamma^{-i\beta\lambda} = -\Gamma^{i\beta}\,\delta_R(\Gamma^{-i\beta\lambda})$

Hence:

$$\omega_0(\delta_R(A)) = \omega_0^{(0)}(\Gamma^{i\beta})^{-1}\,\omega_0^{(0)}\left(\left[A\,\Gamma^{i\beta}\,\delta_R(\Gamma^{-i\beta\lambda})\right]\Gamma^{i\beta}\right)$$

$$\overset{!}{=} \omega_0\left(A\,\Gamma^{i\beta}\,\delta_R\left(\Gamma^{-i\beta\lambda}\right)\right). \qquad (3)$$

Now: (2) with $t = i\beta$:

$$\frac{d}{d\gamma}\left(\Gamma^{i\gamma}\,\delta_R\left(\Gamma^{-i\gamma\lambda}\right)\right) = \tau^{i\gamma}(\Phi)$$

and after integration:

$$\Gamma^{i\beta}\,\delta_R\left(\Gamma^{-i\beta\lambda}\right) = \int_0^\beta \tau^{i\gamma}(\Phi)\,d\gamma$$

with (3):

$$\omega_0(\delta_R(A)) = \int_0^\beta \omega_0\left(A\,\tau^{i\gamma}(\Phi)\right)d\gamma$$

$\square$

- Prop. 1 can be understood as a finite time Kubo formula. We now discuss the limit $t \nearrow \infty$.

<u>Assumptions I</u> (AII)

(i) Limiting state: $X \in I$, $\exists$ a state $\omega_{X,+}$ s.t. $\forall A \in \mathcal{A}$:

$$\lim_{t\to\infty} \omega_X(\tau^t(A)) = \omega_{X,+}(A)$$

(ii) Mixing property: $\forall A, B \in \mathcal{A}$:

$$\lim_{|t|\to\infty} \omega_0\left(\tau^t(A)B\right) = \omega_0(A)\,\omega_0(B)$$

Note: for $X = 0$, (i) holds with $\omega_{0,+} = \omega_0$ since ω_0 is a (τ^t, β)-KMS state.

The limit will be taken only for a particular set of observables.

Def: Let (AI) and (AII) hold. An $A \in \mathcal{A}$ s.t.

(i) $X \mapsto \omega_X(\tau^t(A))$ is differentiable at $X=0$ for all t

is called regular if

(ii) $X \mapsto \omega_{X,+}(A)$ is differentiable at $X=0$

and

(iii) $\lim_{t\to\infty} \frac{\partial}{\partial X}\omega_X(\tau^t(A))\Big|_{X=0} = \frac{\partial}{\partial X}\omega_{X,+}(A)\Big|_{X=0}$

Remark: Prop. I precisely established (i) under (AI). Regularity is about the limiting properties.

- Theorem I: Assume that (AI) & (AII) hold. Let $A \in D(\delta_R)$ be a regular observable s.t. $A = A^*$, $\Theta(A) = -A$. Then:

$$\frac{\partial}{\partial X}\omega_{X,+}(A)\Big|_{X=0} = \frac{1}{2}\int_{-\infty}^{+\infty} dt\, \omega_0(A\tau^t(\Phi))$$

- Proof: From Prop. I and the assumption that A is regular, we have

$$\frac{\partial}{\partial X}\omega_{X,+}(A)\Big|_{X=0} = \frac{1}{\beta}\int_0^\infty dt \int_0^\beta d\gamma\, \omega_0(\tau^t(A)\tau^{i\gamma}(\Phi)) \quad (*)$$

The rest of the proof is a piece of asymptotic analysis, using the KMS condition and the limiting assumption.

First: for $s,r \in \mathbb{R}$, and since $\Theta(A) = -A$, $\Theta(\Phi) = -\Phi$:

$$\begin{aligned}
\omega_0(\tau^s(A)\tau^r(\Phi)) &= \omega_0(\tau^s(\Theta(A))\tau^r(\Theta(\Phi))) \\
&= \omega_0(\Theta[\tau^{-s}(A)\tau^{-r}(\Phi)]) = \omega_0((\tau^{-s}(A)\tau^{-r}(\Phi))^*) \\
&= \omega_0(\tau^{-r}(\Phi)\tau^{-s}(A)) \\
&\overset{\text{KMS}}{=} \omega_0(\tau^{-s}(A)\tau^{-r+i\beta}(\Phi))
\end{aligned}$$

By def of the KMS state, it has an analytic continuation in

$(r+i\gamma)$, $r\in\mathbb{R}$, $\gamma\in(0,\beta)$, so that

$$\omega_0\big(\tau^s(A)\,\tau^{i\gamma}(\Phi)\big) = \omega_0\big(\tau^{-s}(A)\,\tau^{i(\beta-\gamma)}(\Phi)\big).$$

Therefore:

$$\int_0^\beta\int_{-t}^0 \omega_0\big(\tau^s(A)\,\tau^{i\gamma}(\Phi)\big) = \int_0^\beta\int_0^t \omega_0\big(\tau^{-s}(A)\,\tau^{i(\beta-\overset{\mu}{\cancel{\gamma}})}\big)$$

$$= \int_0^\beta\int_0^t \omega_0\big(\tau^s(A)\,\tau^{i\mu}(\Phi)\big)$$

and

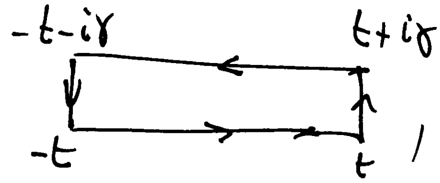
$$\frac{1}{\beta}\int_0^t ds\int_0^\beta d\gamma\,\omega_0\big(\tau^s(A)\,\tau^{i\gamma}(\Phi)\big)$$

$$= \frac{1}{2\beta}\int_0^\beta d\gamma\int_{-t}^t ds\,\omega_0\big(\tau^s(A)\,\tau^{i\gamma}(\Phi)\big)$$

$$= \frac{1}{2\beta}\int_0^\beta d\gamma\Big[\int_{-t}^t ds\,\omega_0\big(A\,\tau^{s+i\gamma}(\Phi)\big)\Big]$$

↑ $s\leadsto -s$ and τ-inv. of ω_0.

Compute $[\dots]$ by complex integration over



since $z\mapsto\omega_0(A\,\tau^z(\Phi))$ is analytic:

$$[\dots] = \int_{-t}^t \omega_0\big(A\,\tau^s(\Phi)\big)\,ds \qquad \text{(does not depend on } \gamma)$$

$$+\; i\int_0^\gamma dy\,\Big(\omega_0\big(A\,\tau^{t+iy}(\Phi)\big) - \omega_0\big(A\,\tau^{-t+iy}(\Phi)\big)\Big)$$

Carrying out the γ integration:

$$\frac{1}{\beta}\int_0^t ds\int_0^\beta d\gamma\,\omega_0\big(\tau^s(A)\,\tau^{i\gamma}(\Phi)\big) = \frac12\int_{-t}^t \omega_0\big(A\,\tau^s(\Phi)\big)\,ds$$

$$+\;\frac{i}{2\beta}\int_0^\beta d\gamma\int_0^\gamma dy\,(\dots)$$

Now, let $t\to\infty$, the first term is what we want. Moreover,

$$\omega_0\big(A\,\tau^{\pm t}(\tau^{iy}(\Phi))\big) \to \omega_0(A)\,\omega_0\big(\tau^{iy}(\Phi)\big)$$

$$= \omega_0(A)\,\omega_0(\Phi)$$

By dominated convergence:

$$\lim_{t\to\infty} |\mathrm{Re}\, I_t| \leq \frac{1}{2} \sup_{\gamma\in[0,\beta]} \lim_{t\to\infty} \left| \int_0^\gamma dy\, (\cdots) \right|$$

$$\leq \frac{1}{2} \sup_{\gamma\in[0,\beta]} \int_0^\gamma dy \lim_{t\to\infty} (\cdots) = 0$$

$\square$

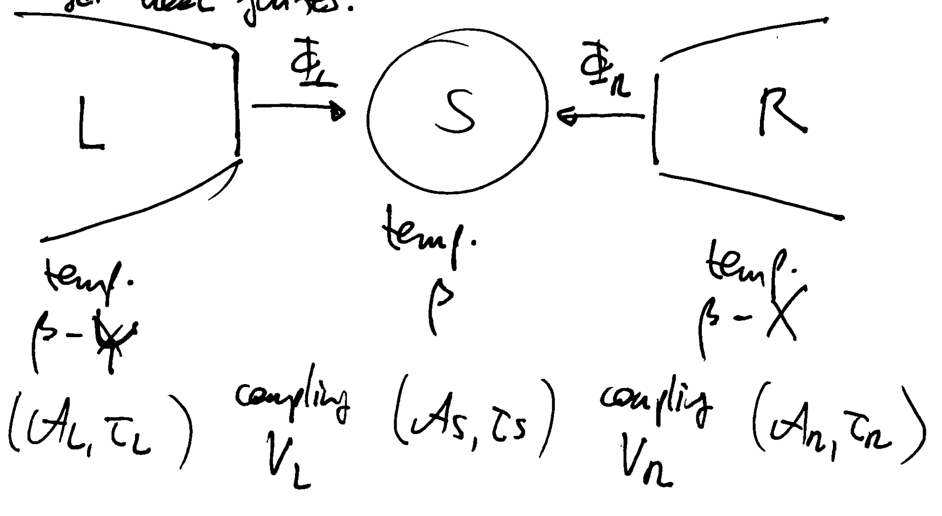
- Remarks: * in the statement of the theorem, $\int_{-\infty}^{+\infty}$ really means $\lim_{t\to\infty} \int_{-t}^{t}$
  * Kubo formula without mixing assumption holds in the form $(*)$
  * Also: without time-reversal assumption, i.e. under AI (i, ii) and AII (i):

$$\partial_X \omega_{X,+}(A)\big|_{X=0} = \partial_X \omega_X(A)\big|_{X=0} + \frac{1}{\beta}\int_0^\infty dt \int_0^\beta dy\, \omega_0\big(\tau^t(A)\tau^{iy}(\Phi)\big).$$

  * In applications to concrete models, (AI) is relatively easy to check, (AII) are the key assumptions/restrictions, and that for observables of physical interest, typically currents, the regularity assumption holds.

    Example: free Fermi gas reservoirs coupled to a finite quantum system, with observables being heat fluxes in the left system.

- To complete the discussion, we prove Onsager's reciprocal relations for heat fluxes. Picture:



Full dynamics τ^t generated by $\delta_L + \delta_S + \delta_R + i[V_L, \cdot] + i[V_R, \cdot]$

where $V_L \in \mathcal{A}_L \otimes \mathcal{A}_S$; $V_R \in \mathcal{A}_S \otimes \mathcal{A}_R$

and assume $V_L \in D(\delta_L)$; $V_R \in D(\delta_R)$

so that

$$\Phi_L := \delta_L(V_L) \quad ; \quad \Phi_R := \delta_R(V_R)$$

Define:

$$L_{LR} := \frac{\partial}{\partial X} \omega_{X,0,+}(\Phi_L)\Big|_{X=0}$$

$$L_{RL} := \frac{\partial}{\partial Y} \omega_{0,Y,+}(\Phi_R)\Big|_{Y=0}$$

Interpretation: if L & S are at the same temperature, there can be a heat flux Φ_L due to the temperature difference between S and R, and it will be given by

$$\omega_{X,+}(\Phi_L) = L_{LR} \cdot X + o(X)$$

Now: Assume (A1) and (A2) hold, and assume that Φ_L and Φ_R are regular observables. Then

$$L_{LR} = L_{RL} \qquad \text{(ORR)}$$

By theorem 1:

$$L_{LR} = \frac{1}{i}\int_{-\infty}^{+\infty} \omega_{0,0}(\Phi_L \tau^t(\Phi_R))\,dt$$

$$L_{RL} = \frac{1}{i}\int_{-\infty}^{+\infty} \omega_{0,0}(\Phi_R \tau^t(\Phi_L))\,dt = \frac{1}{i}\int_{-\infty}^{+\infty} \omega_{0,0}(\tau^t(\Phi_R)\Phi_L)\,dt$$

where $\omega_{0,0}$ is the KMS state of τ^t. Hence ORR follows from the following lemma:

<u>Lemma</u>: Assume that ω is a (τ^t, β)-KMS state that is mixing, i.e. $\lim_{|t|\to\infty} \omega(A\tau^t(B)) = \omega(A)\omega(B)$. Then

$$\lim_{T\to\infty} \int_{-T}^{+T} dt\, \omega([A, \tau_t(B)]) = 0$$

Proof: By the KMS condition,

$$\int_{-T}^{T} dt\, \omega([A, \tau^t(B)]) = \int_{-T}^{T} \omega\left(A\tau^t(B) - A\tau^{t+i\beta}(B)\right)$$

Once again, the analyticity of $z \mapsto \omega(A\tau^z(B))$ and the integration around a rectangle yields that

$$\int_{-T}^{T} dt\, \omega([A, \tau^t(B)]) = i\int_0^\beta d\gamma \left[\omega\left(A\tau^{-T+i\gamma}(B)\right) - \omega\left(A\tau^{T+i\gamma}\right)\right]$$

The conclusion follows by dominated convergence and the mixing condition. $\square$

- In the rest of this section: $(\mathcal{A}, \tau, \omega)$ is a quantum dynamical system

A state $\eta \in \mathcal{E}(\mathcal{A})$ is called <u>normal</u> w.r.t ω (ω-normal) if there is a density matrix ρ_η on the GNS Hilbert space $\mathcal{H}_\omega$ s.t.

$$\eta(A) = \mathrm{Tr}\left(\rho_\eta \pi_\omega(A)\right)$$

intuition: all ω-normal state have the same thermodynamics than ω

Notation: $\mathcal{N}_\omega$.

- Model in mind for the rest of this section:
  - System S: finite quantum system with Hilbert space $\mathcal{H}_S$ and Hamiltonian H_S
  - Reservoir $\mathcal{R}_k$, $k = 1, \dots, N$: Q.D.S. $(\mathcal{A}_k, \tau_k, \omega_k)$, where ω_k are (τ_k, β_k)-KMS states $\;\;\llcorner$ generator δ_k.
  - Decoupled dynamics: $\tau = \tau_S \otimes \tau_1 \otimes \dots \otimes \tau_N$

    Initial state (typically): $\omega = \underset{\uparrow}{\omega_S} \otimes \omega_1 \otimes \dots \otimes \omega_N$

    any τ_S-inv. state on $\mathcal{A}_S$.
  - Couplings: $V_k \in \mathcal{A}_S \otimes \mathcal{A}_k$.

    $\rightsquigarrow$ full interaction: $\lambda V := \lambda \sum_{k=1}^{N} V_k$

    Assumption: $V_k \in D(\delta_k)$

    i.e. $V \in \bigcap_{k=1}^{N} D(\delta_k)$

    Coupled dynamics generated by
    $$\delta_{\lambda V} = \sum_{k=1}^{N} \delta_k + i\,[H_S + \lambda V, \cdot\,].$$
    $\rightsquigarrow \tau_{\lambda V}$.
  - Heat flux out of $\mathcal{R}_k$: $\Phi_k = \lambda \delta_k(V) = \lambda \delta_k(V_k)$.

A) Non-equilibrium steady states.

- Def: a NESS is a weak-* limit point, $(T\to\infty)$, of
$$\omega_{\partial V}^{T} := \frac{1}{T}\int_0^T \omega\circ\tau_{\partial V}^{t}\,dt$$

Already seen: The set $\Sigma_{\partial V}^{+}(\omega)$ is non-empty, and
$$\mu\in\Sigma_{\partial V}^{+}(\omega) \Rightarrow \mu \text{ is } \tau_{\partial V}\text{-invariant}.$$

Note: Other useful definition: weak-* limit point, $\varepsilon\to 0$, of
$$\varepsilon\int_0^\infty e^{-\varepsilon t}\,\omega\circ\tau_{\partial V}^{t}\,dt$$

- Altough the set of NESS depends on the initial state in general, we have that if $\eta\in\mathcal{N}_\omega$ and
$$\lim_{T\to\infty}\frac{1}{T}\int_0^T \eta\left([\tau_{\partial V}^{t}(A), B]\right)dt = 0 \qquad (*)$$
then $$\Sigma_{\partial V}^{+}(\eta) = \Sigma_{\partial V}^{+}(\omega).$$
i.e. normal states converge in the long-time limit to the same asymptotic state(s).

Note: Condition $(*)$ can be checked for the situation described above.

- Now: In which case are the NESS in fact equilibrium states? This is the question of stability of thermal equilibrium, under small, local perturbation.

First: structural stability of KMS-states: if ω is a (τ,β)-KMS state, then for every local perturbation V, there is a (τ_V,β)-KMS state $\omega_V\in\mathcal{N}_\omega$ s.t.
$$\|\omega_V-\omega\| = O(\|V\|)$$
and $\omega\mapsto\omega_V$ is a bijection from the set of (τ,β)-KMS states to that of (τ_V,β)-KMS states

In particular, if there is a unique (τ, β)-KMS state, then there is a unique (τ_V, β)-KMS state.

Second: dynamical stability. Is the structural isomorphism $\omega \mapsto \omega_V$ also realized dynamically, i.e. do we have

$$\Sigma^+_{\lambda V}(\omega) = \{\omega_V\} \qquad (D)$$

i.e. start from the KMS state of the uncoupled system at β, run the coupled dynamics, then you end up in the β-KMS state of the coupled system

(Note: all reservoirs here at same β!).

The ~~answer~~ answer is yes under the "stability criterion":

$$\int_{-\infty}^{+\infty} \| [V, \tau^t_{\lambda V}(A)] \| \, dt < \infty \qquad (\ast)$$

for A in a dense subset of $\mathcal{A}$, and $|\lambda|$ small enough.

In fact: If $(\ast)$ holds, then (D) holds and $\|\omega_{\lambda V} - \omega\| \to 0$ if <u>and only if</u> ω is a (τ, β)-KMS state.

The above situation is usually referred to as "near equilibrium": Start in the equilibrium state, perturb it, run the perturbed dynamics $\to$ end up in the equilibrium state of the coupled system.

Different situation if $(\mathcal{A}, \tau, \omega)$ is not in thermal equilibrium. In general, it is hard even to prove that $\Sigma^+_{\lambda V}(\omega)$ contains a unique $\omega^+_{\lambda V}$ (which is no KMS state of course).

$\hookrightarrow$ has been proved for the small system coupled to reservoirs made of free fermi gases. Moreover, for any $\eta \in \mathcal{N}_\omega$:

$$\lim_{t \to \infty} \eta \circ \tau^t_{\lambda V}(A) = \omega^+_{\lambda V}(A).$$

in that case.

there, the map $\lambda \mapsto \omega^+_{\lambda V}(A)$ is even analytic for $|\lambda| < \Lambda$. Precisely, $\exists\ \omega^+_j$, linear functionals on $\mathcal{A}$ s.t.

$$\omega^+_{\lambda V}(A) = \sum_{j \geq 0} \lambda^j \omega^+_j(A)$$

and ω^+_0 is a product state

$$\omega^+_0 = \underbrace{\omega_{S,eq}}_{\tau_S\text{-invariant.}} \otimes \omega_1 \otimes \cdots \otimes \omega_N$$

B) <u>Entropy production</u>:

- Abstract thermodynamics: $\quad R_1 \xrightarrow{\Phi_1} S \xleftarrow{\Phi_2} R_2$

First law: energy conservation (no work done) : $\Phi_1 + \Phi_2 = 0$.

Second law: change of entropy : $\dfrac{\Phi_1}{T_1} + \dfrac{\Phi_2}{T_2} = -\Delta S_S \leq 0$

i.e. i) entropy S_S is not decreasing

ii) $\Phi_1 \leq -\dfrac{T_1}{T_2}\Phi_2$, with $\Phi_1 = -\Phi_2$:

$$\Phi_1\left(1 - \frac{T_1}{T_2}\right) \leq 0$$

i.e. $\Phi_1 \geq 0$ if $T_1 \geq T_2$

heat flows from hotter to colder reservoir through S.

In particular: if $T_1 = T_2$, then $\Delta S_S = 0$

or $\Delta S > 0$ indicates a non-equilibrium situation.

Now: from "first principles"?

Precisely: if μ is a NESS, does $\mu\left(-\sum_{k=1}^{N} \beta_k \Phi_k\right)$ have all the expected properties?

- Let $S(\eta|\omega)$ be the <u>relative entropy</u> of a state η with respect to ω, with $\eta \in \mathcal{N}_\omega$. For finite quantum systems:

$$S(\eta|\omega) = -\mathrm{Tr}(\eta \log \eta) + \mathrm{Tr}(\eta \log \omega)$$
$$= \mathrm{Tr}(\eta(\log \omega - \log \eta))$$

and there is a general definition using <u>modular theory</u>

Note: if $\eta \notin \mathcal{N}_\omega$, $S(\eta|\omega) = -\infty$.

Properties
 + $S(\eta|\omega) \leq 0$ and $= 0$ iff $\eta = \omega$
 + $S(\eta \circ \tau^t | \omega \circ \tau^t) = S(\eta|\omega)$

- In the following:
 + reference state: $\omega = \underbrace{\omega_S}_{\omega_0} \otimes \omega_1 \otimes \dots \otimes \omega_N$
 where $\omega_S, \omega_1, \dots, \omega_N$ are (τ_h, β_h)-KMS states
 $\Rightarrow$ Check: ω is a $\left(\otimes_h \tau_h^{\beta_h t}, -1\right)$-KMS state
 or a $\left(\otimes_h \tau_h^{\frac{\beta_h}{\beta} t}, \beta\right)$-KMS state.

 + let $\delta_\omega := -\sum_h \beta_h \delta_h$, where δ_h generates τ_h.
 i.e. δ_ω generates $\otimes \tau_h^{\beta_h t}$

- Entropy production observable: Let V be a local perturbation of the Q.D.S. $(\mathcal{A}, \tau, \omega)$, let

$$\sigma_V := \delta_\omega(V)$$

i.e. $$\sigma_V := -\sum_h \beta_h \Phi_h$$

Finally: for $\eta \in \mathcal{N}_\omega$: $Ep(\eta) := \eta(\sigma_V)$.

- <u>Theorem</u> : $\eta \in \mathcal{N}_\omega$

$$S(\eta \circ \tau_V^t | \omega) = S(\eta|\omega) - \int_0^t \eta\left(\tau_V^s(\sigma_V)\right) ds \qquad (*)$$

<u>Corollary</u> : For any $\mu \in \Sigma_V^+(\omega)$: $Ep(\mu) \geq 0$.

- Proof of Thm for finite systems:

$$S(\eta \circ \tau_V^t|\omega) = Tr\left(\eta_t \log \omega\right) - Tr\left(\eta \log \eta\right)$$ no t!

$$\Rightarrow \frac{d}{dt} S(\eta \circ \tau_V^t|\omega) = i\, Tr\left([\eta_t, H+V] \log \omega\right)$$
$$= -i\, Tr\left(\eta_t [\log\omega, H+V]\right)$$
$$= -i\, Tr\left(\eta_t [\log\omega, V]\right)$$

since $[\omega, H] = 0$ by τ-invariance of ω.

Now $\delta_\omega(V) = i[-\sum_k \beta_k H_k, V] = i[\log\omega, V]$, hence

$$\frac{d}{dt} S(\eta \circ \tau_V^t|\omega) = -Tr\left(\eta_t \delta_\omega(V)\right) = -\eta\left(\tau_V^t(\delta_\omega(V))\right).$$

□

Proof of corollary. Let $\mu \in \Sigma_V^+(\omega)$. Then $\exists (T_n)_{n\in\mathbb{N}}$ s.t. $\mu(A) = \lim_{n\to\infty} \omega^{T_n}(A)$, so that

$$\lim_{n\to\infty} \frac{1}{T_n} S(\omega \circ \tau_V^{T_n}|\omega) \overset{(*)}{=} -\lim_{n\to\infty} \frac{1}{T_n}\int_0^{T_n} \omega\left(\tau_V^t(\sigma_V)\right)dt$$
$$\overset{\text{def of } \mu}{=} -\mu(\sigma_V) = -Ep(\mu)$$

For for any η : $S(\omega \circ \tau_V^{T_n}|\omega) \leq 0$, being a relative entropy □

- $Ep(\mu)$ is the rate of decrease of the relative entropy along the trajectory $\omega \circ \tau_V^t$ (asymptotically)

Note ! μ is not necessarily in $\mathcal{N}_\omega$!

- Hard question : when is $Ep(\mu) > 0$ for $\mu \in \Sigma_V^+(\omega)$?

  1) The negative answer : if $\mu \in \Sigma_V^+(\omega)$ and $\mu \in \mathcal{N}_\omega$,

     then $Ep(\mu)$

  2) If $\mu \in \Sigma_V^+(\omega)$ and

  $$\sup_T \left| \int_0^T \left(\omega(\tau_V^t(\sigma_V)) - \mu(\sigma_V) \right) \right| < \infty$$

  Then $\mu \in \mathcal{N}_\omega \iff Ep(\mu) = 0$.

- In the concrete model : $Ep(\mu) = - \sum_k \beta_k \mu(\Phi_k)$

  i.e. $Ep(\mu) > 0$ is equivalent to the NESS carrying non-vanishing heat currents .