ADVANCED MATHEMATICAL STATISTICAL PHYSICS WS13/14
EXERCISE SET 1

DISCUSSION :

i. Review of thermodynamic potentials
ii. Representation theory of $su(2)$ (in physics textbooks : 'angular momentum')

EXERCISES :

i. Prove that
$$S = \frac{1}{T}(U + pV - \mu N)$$
(Hint. Use the homogeneity relation for the entropy)

ii. Let ω be a classical state on Γ : $\int_\Gamma \omega(x)dx = 1$ (a probability measure on Γ). Prove (no technicalities required) that the Gibbs state $\omega(x) = Z(\beta)^{-1}\exp(-\beta H(x))$ is a minimizer of the entropy $S(\omega) = \int_\Gamma \omega(x)\ln\omega(x)dx$ at fixed energy $U := \int_\Gamma \omega(x)H(x)dx$.
(Hint. Use two Lagrange multipliers, one of them turns out to be β)

iii. Prove Fekete's lemma : Let $\{a_n\}_{n\in\mathbb{N}}$ be a real sequence such that $a_n > 0$ and
$$a_{n+m} \le a_n + a_m.$$
for all $n, m \ge 1$. Then
$$\lim_{n\to\infty} \frac{a_n}{n} = \inf_{n\in\mathbb{N}} \frac{a_n}{n}.$$
(i.e the limit exists and is given by the right hand side)

iv. For $a \in \mathbb{R}^3$, let $U(a) = \exp(-\mathrm{i}\sum_{i=1}^3 a_i \cdot S^i)$ where $\{S^i\}_{i=1}^3$ is a representation of $su(2)$. For any $\Lambda \subset \Gamma$ finite, let $U_\Lambda(a) = \otimes_{x\in\Lambda} U_x(a)$ and for any $A \in \mathcal{A}_\Lambda$,
$$\gamma_\Lambda^a(A) = U_\Lambda(a)^* A U_\Lambda(a).$$
$\gamma_\Lambda^a(\cdot)$ is the quantum mechanical action of rotations by around a by an angle $\|a\|$. Prove that the Heisenberg interaction $\Phi_{xy,0} = S_x \cdot S_y$ is rotation invariant :
$$\gamma_{\{x,y\}}^a(\Phi_{xy,0}) = \Phi_{xy,0}$$
for all $a \in \mathbb{R}^3$. Prove that the addition of an external magnetic field, namely $\Phi_{xy,h} = S_x \cdot S_y + (h/2)(S_x^3 + S_y^3)$, with $h \neq 0$ breaks this invariance.

Übungen I Thermodynamic Potentials.

Thermodynamics: A system is characterized by its state variables,

$$z = (\underset{\text{energy}}{U}, \underset{\text{volume}}{V}) \qquad \left(\text{or} \quad (U, V, \underset{\text{\# of particles / mass}}{N})\right)$$

Entropy: $S(z)$. In a <u>closed</u> system (no exchange of heat or matter):

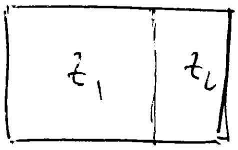
$$S(z_1) \leq S(z_2) \qquad (*)$$

for any process $z_1 \to z_2$.

Note: S defines the thermodynamics completely:

$$\left(\frac{\partial S}{\partial U}\right)_V =: \frac{1}{T}, \qquad \left(\frac{\partial S}{\partial V}\right)_U =: \frac{p}{T}$$

T: temperature. p: pressure

Extremal principle:  $(z_1 | z_2)$ vs $(z_1 + z_2)$ after removing the barrier

with closed barrier:

$$U(z_1|z_2) = U(z_1) + U(z_2)$$
$$S(z_1|z_2) = S(z_1) + S(z_2)$$

removing the barrier (no work, no heat):

$$U(z_1|z_2) = U(z_1 + z_2)$$
$$S(z_1|z_2) \leq S(z_1 + z_2) \qquad \text{by } (*)$$

$$\Rightarrow \quad S(z_1) + S(z_2) \leq S(z_1 + z_2)$$

with "=" ~~iff~~ whenever removing the barrier is reversible. z_1 & z_2 are in equilibrium.

$\Rightarrow$ **In a closed system, the entropy is maximized at equilibrium.**

Homogeneity: $U(\lambda z) = \lambda U(z)$
$S(\lambda z) = \lambda S(z)$.

chemical potential

Ex 1: Define $\left(\frac{\partial S}{\partial N}\right)_{U,V} =: -\frac{\mu}{T}$

Prove : $S = \frac{1}{T}(U + pV - \mu N)$.

Also: $S(\alpha z_1 + (1-\alpha) z_2) \geq \alpha S(z_1) + (1-\alpha) S(z_2)$

$\Rightarrow$ S is a <u>concave</u> function:

<u>Ex 2</u>: The following are equivalent:
(a) Equilibrium: $S(z_1 + z_2) = S(z_1) + S(z_2)$
(b) $S(z)$ is linear between z_1 and z_2.
(c) $T_1 = T_2$; $P_1 = P_2$; $\mu_1 = \mu_2$

Instead of $S(U,V,N)$: Consider $U(S,V,N)$

<u>Ex 3</u>: Prove that the map $S \to U$ is ~~bijective~~ well-defined at (V,N) fixed. (Hint: use concavity of S).

Note: U is convex in all variables.

<u>Now</u>: In a system that is not closed. Typically: fixed T or p.
→ extremal principle for the entropy fails.

→ Free energy : $F(T,V,N) = \inf_S \left[U(S,V,N) - TS\right] = U - TS$
where S is the solution of $\frac{\partial U}{\partial S} = T$

$(-F)$ is the Legendre transform of U w.r.t. S

Also: $F = U - TS = -pV + \mu N$.

$\Rightarrow$ At fixed (V, T), the free energy F is minimal at equilibrium.

follows from concavity in (V, N)

Ex 4 : $f : \mathbb{R}^n \supset D \to \mathbb{R}$. The Legendre transform :

$$f^*(p) := \sup_{x \in D} \left(\langle p, x \rangle - f(x) \right)$$

($p \in D^*$: the sup is $< \infty$)

Prove the following :

i) $f^* : D^* \to \mathbb{R}$ is convex

ii) If f is convex, then $f^{**} = f$ (and $D^{**} = D$)

In the case of 1-d :

Let p_0 be the slope of a tangent : $f(x) \geq f(x_0) + p_0(x - x_0)$

Then $f^*(p_0) = p_0 x_0 - f(x_0)$

as $p_0 x - f(x) \leq p_0 x - f(x) - p_0(x - x_0)$.

Further : if f is differentiable : $p_0 = f'(x_0)$ $(\Diamond)$

and if is strictly convex, $(\Diamond)$ is invertible and

$$f^*(p) = px - f(x) \quad \text{where} \quad x = (f')^{-1}(p).$$

Connection with stat. mech. (classical here)

Entropy : $S(x) = k \int_\Gamma \omega(x) \log \omega(x)\, dx$

for a state ω abs. cont. w.r.t. Lebesgue on phase space Γ.

Gibbs state : $\omega_\beta(x) = \frac{1}{Z(\beta)} e^{-\beta H(x)}$

partition function $Z(\beta) = \int_\Gamma dx\, e^{-\beta H(x)}$

Ex 5 : (Neglecting technical details), prove that the Gibbs state maximizes the entropy among all states with fixed energy $\langle H \rangle$

Hint: Two Lagrange multipliers, one of them is β.

Finally :
$$\begin{cases} S(\beta) = k\beta \langle H \rangle_\beta + k \log Z(\beta) \\ F(\beta) = -\frac{1}{\beta} \log Z(\beta) \end{cases} \qquad (\heartsuit)$$

Ex 6 : Prove the above relations.

Note : * From $(\heartsuit)$, $\boxed{Z(\beta) \text{ yields the full thermodynamics}}$

* Also : $U(\beta) = \langle H \rangle_\beta = -\frac{\partial}{\partial \beta} \log Z(\beta)$.

Elements of representation theory of su(2)

- Algebra generated by S^1, S^2, S^3: $\quad [S^\alpha, S^\beta] = i\varepsilon^{\alpha\beta\gamma} S^\gamma$.
- Note: $su(2) = so(3)$ the algebra of rotations in 3d.
- We consider finite-dimensional representations, $\dim \mathcal{H} < \infty$.
- Define $\quad S^\pm := S^1 \pm i S^2 \quad$ (raising & lowering operator)

Check: $\quad [S^3, S^\pm] = \pm S^\pm \quad ; \quad [S^+, S^-] = 2S^3$.

Let $\quad S^3\psi = \lambda\psi \quad , \quad \lambda \in \mathbb{C}$.

Then $\quad \lambda \pm 1$ is also an eigenvalue, as long as $S^\pm\psi \neq 0$!

$$S^3(S^\pm\psi) = S^\pm S^3\psi + [S^3, S^\pm]\psi = (\lambda\pm 1)(S^\pm\psi)$$

Since $\dim \mathcal{H} < \infty$, $\exists\, j \in \mathbb{C}$ with eigenvector ψ_j s.t.

$$S^3\psi_j = j\psi_j \quad , \quad S^+\psi_j = 0$$

and inductively $\quad S^-\psi_m =: \psi_{m-1} \quad$ for $m = j, j-1, \dots$

so that $\quad S^3\psi_m = m\psi_m$

Again, there must be a k s.t. $\psi_{j-k} \neq 0$ but $\underbrace{S^-\psi_{j-k} = 0}_{(*)}$.

Now assume that $\exists\, \mu_m$ s.t. $\quad S^+\psi_m = \mu_m \psi_{m+1}$

($\hookrightarrow$ this holds for $m = j$, with $\mu_j = 0$)

then

$$S^+\psi_{m-1} = S^+S^-\psi_m = [S^+, S^-]\psi_m + S^-S^+\psi_m$$

$$\underset{(\text{hyp.})}{=} (2m + \mu_m)\psi_m \overset{!}{=} \mu_{m-1}\psi_m$$

Solve recursion (with $\mu_j = 0$): $\quad \mu_m = j(j+1) - m(m+1) = (j-m)(j+1+m)$. $\left(\begin{array}{l} \text{vanishes} \\ = 0 \text{ for } j = m \\ \text{also } m = -(j+1) \end{array}\right)$

$(*)\quad \mu_{j-k-1} \overset{!}{=} 0. \quad \left(S^+\psi_{j-k-1} = S^+S^-\psi_{j-k} \overset{(*)}{=} 0\right)$

i.e. $\quad j-k-1 = -(j+1) \Rightarrow 2j = k, \quad$ with $k \in \mathbb{N}$

Hence : to every representation corresponds an $j \in \frac{1}{2}\mathbb{N}$.
the dimension is given by $2j+1$, with basis vectors
$\psi_j, \dots, \psi_{-j}$

Notes : * by explicit computation in that basis:

$$(S)^2 = (S^1)^2 + (S^2)^2 + (S^3)^2 = j(j+1)\mathbb{1}.$$

* clearly, we get a rep. by defining $S^3, S^\pm$ in a $(2j+1)$-dim. basis as above.

Theorem: The finite dimensional irreducible representations D_j of $su(2)$ are parametrized by $j \in \frac{1}{2}\mathbb{N}$, with $\dim D_j = 2j+1$.

(also: * eigenvalues of S^i are $-j, -(j-1), \dots, j$.
* in the eigenbasis of S^3; $\{|j,m\rangle\}_{m=-j}^{j}$

$$(S)^2 |j,m\rangle = j(j+1)\, |j,m\rangle$$
$$S^3 |j,m\rangle = m |j,m\rangle$$
$$S^\pm |j,m\rangle = \sqrt{j(j+1) - m(m\pm1)}\, |j, m\pm1\rangle$$
)

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EXERCISE SET 2

EXERCISES :

Let H_k denote the set of $k \times k$ hermitian matrices, and H_k^+ the positive matrices. Prove the following inequalities :

i. *Monotonicity of trace functions.* Let $f : \mathbb{R} \to \mathbb{R}$ be a monotone increasing, continuously differentiable function. Let $A, B \in H_k$. If $A \geq B$, then
$$\mathrm{Tr} f(A) \geq \mathrm{Tr} f(B).$$
Note : The requirement can be relaxed to f being continuous.

ii. *Peierls' inequality.* Let $f : \mathbb{R} \to \mathbb{R}$ be a convex function. Let $\{e_i\}_{i=1}^k$ be an arbitrary orthonormal basis of $\mathbb{C}^k$. Then
$$\sum_{i=1}^{k} f\left(\langle e_i, A e_i \rangle\right) \leq \mathrm{Tr} f(A).$$

iii. *Klein's inequality.* Let $f : \mathbb{R} \to \mathbb{R}$ be a convex, differentiable function. Let $A, B \in H_k$. For all $A, B \in H_k$,
$$\mathrm{Tr}\left(f(A) - f(B) - (A - B) f'(B)\right) \geq 0.$$
If f is strictly convex, there is equality iff $A = B$.

iv. *Relative entropy inequality.* Let $A, B \in H_k^+$. Then
$$\mathrm{Tr}\left(A \log A\right) - \mathrm{Tr}\left(A \log B\right) \geq \mathrm{Tr}\left(A - B\right).$$

v. *Peierls-Bogoliubov's inequality I.* For any $k \in \mathbb{N}$, the map
$$A \mapsto \log \mathrm{Tr}\left(\mathrm{e}^A\right)$$
is convex on H_k.

vi. *Peierls-Bogoliubov's inequality II.* For any $A, B \in H_k$,
$$\frac{\mathrm{Tr}\left(B \mathrm{e}^A\right)}{\mathrm{Tr}\left(\mathrm{e}^A\right)} \leq \log \frac{\mathrm{Tr}\left(\mathrm{e}^{A+B}\right)}{\mathrm{Tr}\left(\mathrm{e}^A\right)}.$$

Note : All these inequalities can be extended to infinite dimensional Hilbert spaces, as long as all quantities involved are a priori well-defined (*e.g.* trace class)

i) Let $B \in \mathcal{M}_n$, $C \in \mathcal{M}_n^+$:

$$\frac{d}{dt} \operatorname{Tr} f(B+tC)\Big|_{t=0} = \frac{d}{dt} \sum_i f(\lambda_i(t))\Big|_{t=0} \quad \left(\begin{array}{l}\text{spectral thm,}\\ \lambda_i(t): \text{ev of}\\ B+tC\end{array}\right)$$

$$= \sum_i f'(\lambda_i(0))\,\lambda_i'(0) = \sum_i f'(\lambda_i(0))\,\langle e_i, C e_i\rangle$$

by 1st order perturbation theory, i.e.

$$= \operatorname{Tr}\left(f'(B)\,C\right) = \operatorname{Tr}\left(C^{\frac12} f'(B)\, C^{\frac12}\right) \geq 0$$

as $f'(B) \geq 0$, by monotonicity. Now, $A \geq B$:

$$\operatorname{Tr} f(A) - \operatorname{Tr} f(B) = \int_0^1 \frac{d}{dt} \operatorname{Tr} f(B+t(A-B))\Big|_{t=s}\, ds$$

$$= \int_0^1 \frac{d}{dt} \operatorname{Tr} f\big(B+s(A-B)+(t-s)(A-B)\big)\Big|_{t=s}\, ds$$

$$= \int_0^1 \operatorname{Tr}\left((A-B)^{\frac12} f'(B+s(A-B))\,(A-B)^{\frac12}\right) ds \geq 0 \quad \square$$

ii) $$\operatorname{Tr} f(A) = \sum_{i=1}^n \Big\langle e_i, \Big(\sum_{j=1}^{\ell} f(\lambda_j) P_j\Big) e_i\Big\rangle \qquad \Big(A = \sum_j \lambda_j P_j\Big)$$

$$= \sum_{i=1}^n \sum_{j=1}^{\ell} f(\lambda_j)\,\|P_j e_i\|^2$$

$$\geq \sum_{i=1}^n f\Big(\sum_{j=1}^{\ell} \lambda_j \|P_j e_i\|^2\Big) = \sum_{i=1}^n f\big(\langle e_i, A e_i\rangle\big)$$

Jensen's inequality, as $\sum_{j=1}^{\ell} \|P_j e_i\|^2 = \|e_i\|^2 = 1$

$\square$

iii) Convexity: $\forall (x,y)$: $\dfrac{f(x)-f(y)}{x-y} \geq f'(y)$

Let $\{a_i\}$, $\{b_i\}$ be eigenbases of A, B with eigenvalues $\{\alpha_i\}$, $\{\beta_i\}$; let $c_{ij} = \langle a_i, b_j\rangle$

$$\langle a_i, (f(A) - f(B) - (A-B) f'(B))\, a_i\rangle$$

$$= f(a_i) - \sum_j |c_{ij}|^2 f(b_j) - \sum_j |c_{ij}|^2 (a_i - b_j)\, f'(b_j)$$

$$= \sum_j |c_{ij}|^2 \left[f(a_i) - f(b_j) - (a_i - b_j) f'(b_j)\right] \geq 0$$

$\square$

iv) Take $t\log t = f(t)$ in ~~Peierls~~ Klein:

$$\mathrm{Tr}(A\log A) - \mathrm{Tr}(B\log B) - \mathrm{Tr}\left[(A-B)(\log(B)+1)\right] \geq 0$$

$$\Leftrightarrow \mathrm{Tr}(A\log A) - \mathrm{Tr}(A\log B) - \mathrm{Tr}(A-B) \geq 0. \qquad \square$$

Note: From the proof of Klein's inequality, it follows that it holds for A, B s.t.

$$\mathrm{Spec}(A) \subset D(f)$$
$$\mathrm{Spec}(B) \subset D(f)$$

i.e. here $f: [0,\infty) \to \mathbb{R}$.

v) Let $\phi: \mathbb{R}^n \to \mathbb{R}$; $\phi(x) = \log\left(\sum_{k=1}^n e^{x_k}\right)$

$$\frac{\partial^2}{\partial x_i \partial x_j}\phi(x) = a_j\delta_{ij} - a_i a_j \quad ; \quad a_i = \frac{e^{x_i}}{\sum_k e^{x_k}}$$

and $y \in \mathbb{R}^n$: $\langle y, \frac{\partial^2}{\partial x_i \partial x_j}\phi(x)\, y\rangle = \sum a_j y_j^2 - \left(\sum a_j y_j\right)^2$

use Schwarz: $\left(\sum a_j y_j\right)^2 \leq \underbrace{\left(\sum_j a_j\right)}_{=1}\left(\sum_j a_j y_j^2\right) \quad (a_j \geq 0)$

$\Rightarrow$ The Hessian of ϕ is positive $\Rightarrow$ ϕ is a convex $\forall x \in \mathbb{R}^n$.

Let $\{e_i\}$ be an eigenbasis of $(A+B)$, $\langle e_i, Ae_i\rangle =: x_i$

$\langle e_i, Be_i\rangle =: y_i$.

(a) $\log \mathrm{Tr}\left(e^{\frac{A+B}{2}}\right) = \log\left(\sum_j e^{\langle e_j, \frac{A+B}{2} e_j\rangle}\right) = \phi\left(\frac{x+y}{2}\right)$

(b) $\mathrm{Tr}\, f(A) \geq \sum f(\langle e_i, Ae_i\rangle)$ for $f(t) = e^t$

and monotonicity of $\log$:

$\log \mathrm{Tr}\, e^A \geq \phi(x)$

(c) Similarly $\log \mathrm{Tr}\, e^B \geq \phi(y)$

$\Rightarrow \log \mathrm{Tr}\left(e^{\frac{A+B}{2}}\right) = \phi\left(\frac{x+y}{2}\right) \leq \frac{1}{2}\phi(x) + \frac{1}{2}\phi(y) \leq \frac{1}{2}\log \mathrm{Tr}\, e^A + \frac{1}{2}\log\mathrm{Tr}\, e^B$

convexity

(and midpoint convex $\Leftrightarrow$ convex
f continuous)

$\square$

Conclude the argument by using:

$$\begin{pmatrix}\text{midpoint convex}\\ \text{and continuous}\end{pmatrix} \Leftarrow, \ \left(\text{convex and continuous}\right).$$

(vi) Let $\psi : [0,1] \to \mathbb{R} : t \mapsto \psi(t) = \log \operatorname{Tr}\left(e^{A+tB}\right)$.

By P.-B : ψ is convex $\Rightarrow$

$$\psi(1) - \psi(0) \geq \frac{\psi(t) - \psi(0)}{t} \qquad \forall t.$$

Now: $\lim_{t \to 0^+}$ $\quad \psi(1) - \psi(0) \geq \psi'(0^+)$

i.e. $\log \operatorname{Tr} e^{A+B} - \log \operatorname{Tr} e^{A} \geq \dfrac{\operatorname{Tr}(Be^{A})}{\operatorname{Tr}(e^{A})}$ $\qquad \square$

ADVANCED MATHEMATICAL STATISTICAL PHYSICS WS13/14
EXERCISE SET 3

DISCUSSION :

Falk-Bruch inequality. By absorbing β in the definition of H, we assume $\beta = 1$. Let $\varphi(x) := \sqrt{x}\coth(1/\sqrt{x})$. Then

i. Falk-Bruch inequality :
$$\frac{2\omega(\{A^*, A\})}{\omega([A^*,[H,A]])} \le \varphi\left(\frac{4(A^*, A)}{\omega([A^*,[H,A]])}\right)$$

ii. Corollary :
$$(A^*, A) + \frac{1}{2}\left[(A^*, A)\cdot\omega([A^*,[H,A]])\right]^{1/2} \ge \frac{1}{2}\omega(\{A^*, A\}) \tag{1}$$

Note : An explicit lower bound is given by
$$(A^*, A) \ge \frac{1}{2}\omega(\{A^*, A\})\phi\left(\frac{\omega([A^*,[H,A]])}{2\omega(\{A^*, A\})}\right)$$
where $\phi(x\tanh(x)) = x^{-1}\tanh(x)$.

EXERCISES :

Let $A, B \in \mathcal{A}_\Lambda$. We consider Duhamel's two-point function
$$(A,B)_\beta := Z(\beta)^{-1}\int_0^1 \mathrm{Tr}\left(\mathrm{e}^{-s\beta H} A \mathrm{e}^{-(1-s)\beta H} B\right) ds.$$

i. *Basic properties.* Prove that $(A,B)_\beta = (B,A)_\beta$.
Is the thermal two-point function $\omega_\beta(A,B)$ also symmetric ?
Prove Schwarz's inequality,
$$|(A,B)_\beta|^2 \le (A^*, A)_\beta (B^*, B)_\beta$$

ii. *Relation to thermal expectations.* Compute the thermal expectation value $\omega_\beta(A)$ using Duhamel's two-point function.
Conversely, let $\tau_t^\Lambda(A) = \exp(\mathrm{i}tH_\Lambda)A\exp(-\mathrm{i}tH_\Lambda)$, and let τ_z be its analytic continuation in the strip $|\Im z| \le 1$. Observe that
$$(A,B)_\beta = \int_0^1 \omega_\beta(B\tau^\Lambda_{\mathrm{i}s\beta}(A))ds$$

iii. *Bogoliubov's inequality.* Use a convexity argument for the function
$$h_\beta(s) := \mathrm{Tr}\left(\mathrm{e}^{-s\beta H} A^* \mathrm{e}^{-(1-s)\beta H} A\right)$$
to show that
$$(A^*, A)_\beta \le \frac{1}{2}\omega_\beta(\{A^*, A\}) \tag{2}$$
Further, prove prove that
$$\omega_\beta([A,B]) = ([A,\beta H], B)_\beta$$
and conclude that
$$|\omega_\beta([A,B])|^2 \le \frac{\beta}{2}\omega_\beta([A^*,[H,A]])\omega_\beta(\{B^*, B\})$$

Exercises :

i) Symmetry follows from cyclicity of the trace and the change of variables $s \mapsto t = 1-s$

Clearly, $\omega_\beta(A,B) = Z(\beta)^{-1}\,\mathrm{Tr}\,(e^{-\beta H}AB)$ is not symmetric

In fact:

$(A^*, A)_\beta > 0 \quad \forall A \neq 0$:

Indeed $Z(\beta)\,(A^*, A)_\beta = \int_0^1 \mathrm{Tr}(C^* C)\,ds$

where $C = e^{-\left(\frac{1-s}{2}\right)\beta H} A\, e^{-\frac{s}{2}\beta H}$

Therefore, $A, B \mapsto (A^*, B)_\beta$ defines a non-degenerate symmetric bilinear form and satisfies the Cauchy-Schwarz inequality.

ii) Immediately, $\omega_\beta(A) = (A, 1)_\beta$.

The converse follows from $\omega_\beta(B\,\tau_{is\beta}(A)) =$

$= Z(\beta)^{-1}\,\mathrm{Tr}\,(e^{-\beta H} B e^{-s\beta H} A\, e^{s\beta H})$ and cyclicity.

iii) We compute

$$\frac{d^2}{ds^2} h_\beta(s) = -\beta^2\,\mathrm{Tr}\left(e^{-s\beta H}[H, A^*]\,e^{-(1-s)\beta H}\,[H,A]\right)$$

$$\cancel{\ge \beta^2 \text{ so that}} \quad = \beta^2\,\mathrm{Tr}\left(e^{-s\beta H}[H,A]^* e^{-(1-s)\beta H}[H,A]\right)$$

i.e. $h_\beta''(s) \geq 0$, so that

$$(A^*, A)_\beta = Z(\beta)^{-1}\int_0^1 ds\, h_\beta(s) \overset{\text{convexity}}{\leq} \frac{1}{2Z(\beta)}\left(h_\beta(1) + h_\beta(0)\right)$$

$$= \frac{1}{2}\omega_\beta(\{A^*, A\}). \qquad (*)$$

Further, we note that

$$Z(\beta)([A, \beta H], B)_\beta = \int_0^1 \frac{d}{ds}\,\mathrm{Tr}\left(e^{-s\beta H} A e^{-(1-s)\beta H} B\right) = Z(\beta)\,\omega_\beta(AB - BA)$$

Hence, $\left|\omega_\beta([A,B])\right|^2 = \left|([A,\beta H],B)_\beta\right|^2$

$$\overset{\text{C.-S.}}{\leq} (B^*,B)_\beta \Big([\beta H,A^*],[A,\beta H]\Big)_\beta$$

$$\overset{(2)}{\leq} \tfrac{1}{2}\omega_\beta(\{B^*,B\})\Big([A^*,\beta H],[\beta H,A]\Big)$$

$$= \tfrac{\beta}{2}\omega_\beta(\{B^*,B\})\,\omega_\beta\Big([A^*,[H,A]]\Big).$$

Falk-Bruch's inequality. $(\beta=1)$

We have $\omega_\beta(\{A^*,A\}) = h(1)+h(0)$

Moreover, $h'(s) = \mathrm{Tr}\left(e^{-(1-s)H}[H,A]e^{-sH}A^*\right)$

so that $\omega\big([A^*,[H,A]]\big) = h'(1)-h'(0)$

Now: in the eigenbasis ϕ_i of H,

$$h(s) = \sum_{n,m}|A_{nm}|^2 e^{-E_m}e^{s(E_m-E_n)}$$

so that h is the Laplace transform of a positive measure μ:

$$h(s) = \int_{-\infty}^{+\infty} e^{st}\,d\mu(t)$$

Now:

* $\int_0^1 h(s)\,ds = \int_{-\infty}^{+\infty}\frac{e^t-1}{t}\,d\mu(t)$
* $h(0)+h(1) = \int_{-\infty}^{+\infty}(1+e^t)\,d\mu(t)$
* $h'(1)-h'(0) = \int_{-\infty}^{+\infty} t(e^t-1)\,d\mu(t)$

We define a measure $d\nu(t) := t(e^t-1)\,d\mu(t)$. With this:

* $\int_0^1 h(s)\,ds = \int\frac{1}{t^2}\,d\nu(t)$
* $h(0)+h(1) = \int\frac{1}{t}\,\frac{e^t+1}{e^t-1}\,d\nu(t) = \int\frac{1}{t}\coth\left(\frac{t}{2}\right)d\nu(t)$
* $h'(1)-h'(0) = \int d\nu(t)$

Finally, we use Jensen's inequality for the probability measure $d\bar{\nu} = \left(\int d\nu(t)\right)^{-1} d\nu$:

$$\varphi\left(\frac{4(A^*,A)}{\omega([A^*,[H,A]])}\right) = \varphi\left(\frac{4\int_0^1 h(s)ds}{h'(1)-h'(0)}\right) = \varphi\left(\int \frac{4}{t^2} d\bar{\nu}(t)\right)$$

$$\geq \int \varphi\left(\frac{4}{t^2}\right) d\bar{\nu}(t) = \int \frac{2}{t}\coth\left(\frac{t}{2}\right) d\bar{\nu}(t)$$

$$= 2\,\frac{(h(1)+h(0))}{h'(1)-h'(0)}$$

$$= \frac{2\,\omega(\{A^*,A\})}{\omega([A^*,[H,A]])}$$

Note: φ is a concave function.

For $x>0$:
$$\coth(x) = 1 + \frac{2}{e^{2x}-1}, \quad \text{with } e^{2x}-1 \geq 2x,$$

$$\varphi(x) \leq \sqrt{x}\left(1+\frac{1}{(1/\sqrt{x})}\right) = \sqrt{x}+x$$

which yields (1) by using Falk-Bruch's inequality.

Note: the explicit lower bound for (A^*,A) is obtained similarly, see [Dyson-Lieb-Simon].

ADVANCED MATHEMATICAL STATISTICAL PHYSICS WS13/14
EXERCISE SET 4

DISCUSSION :

Reflection positivity and the Laplacian. The Coulomb interaction between two charge distributions $f, g \in C_0^\infty(\mathbb{R}^3)$ is given by

$$E(f,g) = \int_{\mathbb{R}^N} \int_{\mathbb{R}^N} f(x) \, |x-y|^{-1} \, g(y) dx dy.$$

For any reflection R of $\mathbb{R}^N$ across a hyperplane and any function h, we define $\theta_R h(x) := h(Rx)$. Let g be supported on a half-space. Then

$$E(\theta_R g, g) \geq 0.$$

Similarly, if f and g are supported on two opposite half-spaces separated by R, then

$$|E(f,g)|^2 \leq E(f, \theta_R f) E(\theta_R g, g).$$

Despite being a non-trivial mathematical statement, reflection positivity is the simple physical result that the interaction of a charge distribution and its mirror is attractive.

EXERCISES :

i. Let $\mathcal{H} = \mathcal{K} \otimes \mathcal{K}$ with $\dim \mathcal{K} < \infty$. For any *real* matices $A, B, C_1, \ldots, C_l$ and any real numbers $\rho_1, \ldots, \rho_l$,

$$\mathrm{Tr}\left[\mathrm{e}^{A\otimes 1 + 1\otimes B - \sum_{k=1}^{l}(C_k \otimes 1 - 1\otimes C_k - \rho_k)^2}\right]^2$$
$$\leq \mathrm{Tr}\left[\mathrm{e}^{A\otimes 1 + 1\otimes A - \sum_{k=1}^{l}(C_k \otimes 1 - 1\otimes C_k)^2}\right] \mathrm{Tr}\left[\mathrm{e}^{B\otimes 1 + 1\otimes B - \sum_{k=1}^{l}(C_k \otimes 1 - 1\otimes C_k)^2}\right]$$

ii. Let $H = \omega A^* A$, with $[A, A^*] = s \cdot 1$ for $s \in \mathbb{C}$. The Hilbert space is spanned by $\{(A^*)^n \Omega\}_{n\in\mathbb{N}}$ for the particular vector Ω satisfying $A\Omega = 0$. Let ψ_n be the orthonormal basis such that $H\psi_n = n\omega s \psi_n$;

(a) compute (A^*, A), where (A, B) is Duhamel's two-point function at $\beta = 1$
(b) compute $\omega_1(\{A^*, A\})$
(c) compute $[A^*, [H, A]]$
(d) show that Falk-Bruch's inequality is saturated in this example
(e) for which operator B is Bogoliubov's inequality also saturated ?

Reflection positivity for the Green's function of $-\Delta$:

- We consider $\frac{1}{|x|}$ as a distribution T on $C_0^\infty(\mathbb{R}^3)$ and first prove that it is the inverse Fourier transform of $\frac{1}{|k|^2}$.

Recall: $\hat{T}[f] := T[\hat{f}]$, $f \in C_0^\infty(\mathbb{R}^3)$.

$$\frac{1}{(2\pi)^{3/2}} \int d^3x \int d^3k \, \frac{1}{(2\pi)^{3/2}|k|^2} e^{ikx} f(x)$$

$$= \frac{1}{(2\pi)^2} \int d^3x \underbrace{\int_0^\infty dr \, 2 \frac{\sin r|x|}{r|x|}}_{} f(x) = \frac{1}{(2\pi)^2} \int d^3x \, \frac{\pi}{|x|} f(x)$$

i.e. $\frac{1}{4\pi|x|} = \frac{1}{(2\pi)^{3/2}|k|^2}$

- W.l.o.g., we assume that R is the reflection $(x,y,z) \mapsto (-x,y,z)$, so that

$$E(\Theta_R g, g) = \int d^3x d^3y \, g(x_1,x_2,x_3)\left((x_1+y_1)^2+(x_2-y_2)^2+(x_3-y_3)^2\right)^{-1/2} g(y_1,y_2,y_3)$$

$$= \frac{1}{2\pi^2} \int d^3x d^3y dp dq dr \, g(\vec{x}) g(\vec{y}) \left(p^2+q^2+r^2\right)^{-1} e^{i[p(x_1+y_1)+q(x_2-y_2)+r(x_3-y_3)]}$$

Carrying out the p-integration:

[Using contour integrals: $\int_{-\infty}^{+\infty} \frac{1}{x^2+a^2} e^{ipx} dx = \frac{e^{-|p|a}}{\pi a}$]

$$E(\Theta_R g, g) = \frac{1}{2\pi^3} \int d^3x d^3y dq dr \, \frac{g(\vec{x}) g(\vec{y})}{(q^2+r^2)^{1/2}} e^{-|x_1+y_1|(q^2+r^2)^{1/2} + iq(x_2-y_2) + ir(x_3-y_3)}$$

and we note that both $x_1, y_1 > 0$ (on supp(g)), so that $|x_1+y_1| = (x_1+y_1) > 0$. Hence,

$$E(\Theta_R g, g) = \frac{1}{2\pi^3} \int dq dr \left| \int_0^\infty ds \, e^{-s(q^2+r^2)^{1/2}} \varphi_g(s) \right|^2 \frac{1}{(q^2+r^2)^{1/2}} \geq 0.$$

where $\varphi_g(s) := \int dx_2 dx_3 \, g(s,x_2,x_3) e^{iqx_2 + irx_3}$

- Now if f, g are supported on either side of the reflection plane, $E(\Theta f, g) = E(g, \Theta f)$ by a simple change of variables.
  Hence, the positivity of the form $E(\lambda f - \Theta_R g, \lambda \Theta_R f - g)$ yields
  $$\left(E(f,g)\right)^2 \leq E(f, \Theta_R f)\, E(\Theta_R g, g)$$
- Defining $\tilde{\Theta}_R f = -\Theta_R f$ corresponds to putting a mirror charge density across R, and the reflection positivity reads
  $$E(\tilde{\Theta}_R f, f) \leq 0 ,$$
  namely: mirror charges attract each other (that is not new!).
- Discussion of both exercises can be found in [Dyson-Lieb-Simon Lemma 4.1 & Appendix B.

ADVANCED MATHEMATICAL STATISTICAL PHYSICS WS13/14
EXERCISE SET 5

DISCUSSION :

More on $su(2)$: Clebsch-Gordon series

EXERCISES :

i. *Spin waves for the antiferromagnet.* Consider the spin s Heisenberg antiferromagnet H_L^{AF} on the chain of length L with unique ground state Ω_L, $\|\Omega_L\| = 1$. Let

$$U_L := \mathrm{e}^{\mathrm{i}A}, \qquad A = \frac{2\pi}{L}\sum_{x=1}^{L} x S_x^3,$$

and $\Psi_L := U_L \Omega_L$.

(a) Compute the energy gap $\delta_L := \langle \Psi_L, H_L^{AF} \Psi_L \rangle - \langle \Omega_L, H_L^{AF} \Omega_L \rangle$;

(b) If $s \in (1/2)\mathbb{N}$, show that $\langle \Psi_L, \Omega_L \rangle = 0$ (Hint : in this case, $\exp(2\pi \mathrm{i} S_x^3) = -1$) ;

(c) Conclude that δ_L is an upper bound for the spectral gap above the ground state energy.

ii. *Spin waves for the ferromagnet.* Consider the spin $1/2$ Heisenberg ferromagnet H_L^F on the chain of length L with periodic boundary conditions. Its ground state space is spanned by vectors of highest spin S_{max}. Let $\mathcal{H}^{S_{max}-1}$ be the eigenspace of S_{tot}^2 corresponding to $S_{max} - 1$. Compute the spectrum of $H_L^F \restriction_{\mathcal{H}^{S_{max}-1}}$ and conclude again that the spectral gap above the ground state energy vanishes in the thermodynamic limit.

Clebsch-Gordon series

- Recall: All finite dimensional irreducible representations of $su(2) = so(3)$ are parametrized by $j \in \frac{1}{2}\mathbb{N}$ (up to unitary equivalence). $\dim \mathcal{D}_j = 2j+1$

Unitary representation: $S_i = S_i^\dagger$, and so $S_\pm^\dagger = S_\mp$.
Basis of $\mathcal{D}_j$: $\{|j,m\rangle\}_{m=-j}^{j}$ s.t.

$$\begin{cases} S^2|j,m\rangle = j(j+1)\,|j,m\rangle \\ S_3|j,m\rangle = m\,|j,m\rangle \\ S_\pm|j,m\rangle = \sqrt{j(j+1)-m(m\pm1)}\;|j,m\pm1\rangle \end{cases}$$

- Now: consider two systems with Hilbert spaces $\mathcal{H}^{(1)}$ & $\mathcal{H}^{(2)}$, carrying representations of $SO(3)$ $U^{(1)}(R)$, $U^{(2)}(R)$, a global rotation is given by the tensor product representation

$$U(R) = U^{(1)}(R) \otimes U^{(2)}(R) \quad , \quad R \in SO(3)$$

or for the algebra $su(2) = so(3)$:

$$S_i = S_i^{(1)} \otimes \mathbb{1} + \mathbb{1} \otimes S_i^{(2)}$$

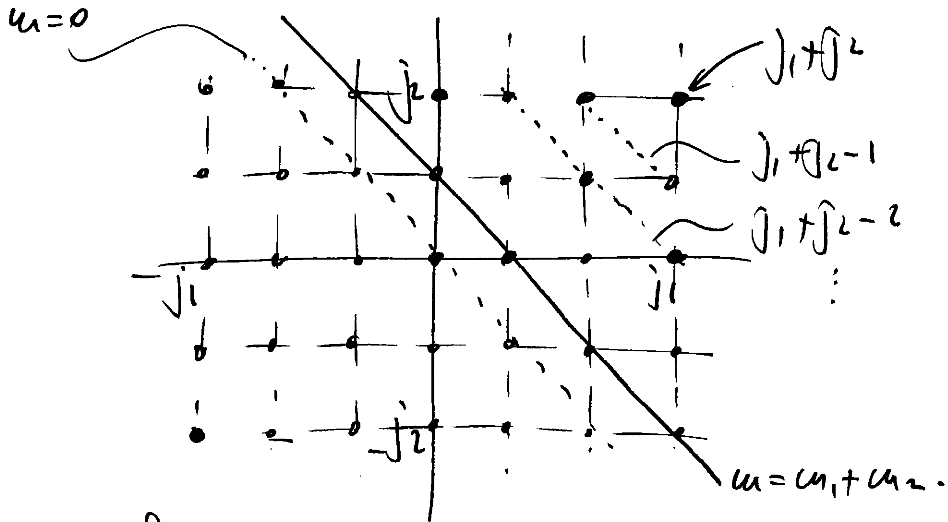
- Lemma (Clebsch-Gordon series)

$$\mathcal{D}_{j_1} \otimes \mathcal{D}_{j_2} = \mathcal{D}_{j_1+j_2} \oplus \mathcal{D}_{j_1+j_2-1} \oplus \cdots \oplus \mathcal{D}_{|j_1-j_2|}$$

Proof: Vectors in the product basis of $\mathcal{D}_{j_1} \otimes \mathcal{D}_{j_2}$ are eigenvectors of S_3:

$$\begin{aligned} S_3\big(|j_1,m_1\rangle \otimes |j_2,m_2\rangle\big) &= S_3^{(1)}|j_1,m_1\rangle \otimes 1\,|j_2,m_2\rangle \\ &\quad + 1\,|j_1,m_1\rangle \otimes S_3^{(2)}|j_2,m_2\rangle \\ &= (m_1+m_2)\big(|j_1,m_1\rangle \otimes |j_2,m_2\rangle\big) \end{aligned}$$

Ues.2



From the figure: the degeneracy of the eigenvalue $m=m_1+m_2$ is given by:

$m=j_1+j_2$: 1
$m=j_1+j_2-1$: 2
⋮ ⋮
$m=|j_1-j_2|$: $2\min(j_1,j_2)+1$ (diagonal of the rectangle).
$m=|j_1-j_2|-1$: $2\min(j_1,j_2)+1$
⋮ ⋮
$m=0$ $2\min(j_1,j_2)+1$

and similarly for $m\to -m$.
Moreover, there are a total of $(2j_1+1)(2j_2+1)$ eigenvectors of S_3
$\Rightarrow$ the tensor product vectors are a basis of $\mathcal{D}_{j_1}\otimes\mathcal{D}_{j_2}$.
Hence: (i) No eigenvector of S^2 with eigenvalue $j>j_1+j_2$ exists in $\mathcal{D}_{j_1}\otimes\mathcal{D}_{j_2}$

(ii) The eigenvectors for j_1+j_2 exist; $\mathcal{D}_{j_1+j_2}$ comes in only once, and (of course) contains one eigenvector for each $m=-j,\dots,j$. (by acting on $|j_1,j_1\rangle\otimes|j_2,j_2\rangle$ with S_-)

(iii) The remaining eigenvector for $m=j_1+j_2-1$ must therefore belong to $\mathcal{D}_{j_1+j_2-1}$

(iv) Continue inductively until all eigenvectors are arranged into $\mathcal{D}_j$'s, namely when $j=|j_1-j_2|$

The orthogonality of $\mathcal{D}_j$, $\mathcal{D}_k$ for $j\neq k$ follows from their definition as eigenspaces of S^2 for different eigenvalues.

□

Note: the proof allows for a recursive construction of the eigenvectors:

1) Start with $|j_1, j_1\rangle \otimes |j_2, j_2\rangle$
2) Generate $D_{j_1+j_2}$ by $\{(\Pi_-)^\ell |j_1,j_1\rangle \otimes |j_2,j_2\rangle \mid \ell = 0, \dots 2(j_1+j_2)\}$
3) Repeat, starting with a vector in
$$\mathrm{span}\{|j_1, j_1-1\rangle \otimes |j_2, j_2\rangle, |j_1,j_1\rangle \otimes |j_2, j_2-1\rangle\} \ominus \Pi_- |j_1,j_1\rangle \otimes |j_2,j_2\rangle .$$

Classic example: $D_{1/2} \otimes D_{1/2}$

Note $\Pi_- = (\Pi_-^{(1)} \otimes 1) + (1 \otimes \Pi_-^{(2)})$

$$\begin{cases} |1,1\rangle := |\tfrac{1}{2}, \tfrac{1}{2}\rangle \otimes |\tfrac{1}{2}, \tfrac{1}{2}\rangle \\ |1,0\rangle := \Pi_- |1,1\rangle = |\tfrac{1}{2}, -\tfrac{1}{2}\rangle \otimes |\tfrac{1}{2}, \tfrac{1}{2}\rangle + |\tfrac{1}{2}, \tfrac{1}{2}\rangle \otimes |\tfrac{1}{2}, -\tfrac{1}{2}\rangle \\ |1,-1\rangle := \Pi_-^2 |1,1\rangle = 2 |\tfrac{1}{2}, -\tfrac{1}{2}\rangle \otimes |\tfrac{1}{2}, -\tfrac{1}{2}\rangle . \end{cases}$$

"spin-1 triplet".

and

$$|0,0\rangle \in \mathrm{span}\left(|\tfrac{1}{2}, -\tfrac{1}{2}\rangle \otimes |\tfrac{1}{2}, \tfrac{1}{2}\rangle, |\tfrac{1}{2}, \tfrac{1}{2}\rangle \otimes |\tfrac{1}{2}, -\tfrac{1}{2}\rangle \right)$$
$$\text{s.t.} \quad \langle 0,0 | 1,0\rangle = 0$$
$$\Rightarrow |0,0\rangle = |\tfrac{1}{2}, -\tfrac{1}{2}\rangle \otimes |\tfrac{1}{2}, \tfrac{1}{2}\rangle - |\tfrac{1}{2}, \tfrac{1}{2}\rangle \otimes |\tfrac{1}{2}, -\tfrac{1}{2}\rangle$$

"spin-0 singlet".

in more classic notations: (and normalized)

$$\begin{cases} |1,1\rangle = |++\rangle \\ |1,0\rangle = \tfrac{1}{\sqrt{2}}(|-+\rangle + |+,-\rangle) \\ |1,-1\rangle = |--\rangle \end{cases}$$
$$\{ |0,0\rangle = \tfrac{1}{\sqrt{2}}(|-+\rangle - |+-\rangle) .$$

- ~~Lemma~~: If $j_1 = j_2 = j$, we can define a transposition T:
$$T(\psi_1 \otimes \psi_2) = (\psi_2 \otimes \psi_1) \quad \text{on} \quad D_j \otimes D_j .$$
- Lemma: $T\psi = \psi$ if $\psi \in D_{2j-2n}$
$$T\psi = -\psi \text{ if } \psi \in D_{2j-(2n+1)}$$

Remark: check this in the above example.

Proof: This follows from $|j,j\rangle \otimes |j,j\rangle \in \mathcal{D}_{2j}$ is symmetric and

$$[T, \Pi_-] = 0$$

so that all vectors in $\mathcal{D}_{2j}$ are symmetric.

Now: at fixed m: $\mathcal{H}^{(m)} = \mathcal{H}_s^{(m)} \oplus \mathcal{H}_a^{(m)}$

where $\Pi_3 \mathcal{H}^{(m)} = m \mathcal{H}^{(m)}$

and $T \mathcal{H}_s^{(m)} = \mathcal{H}_s^{(m)}$; $T\mathcal{H}_a^{(m)} = -\mathcal{H}_a^{(m)}$.

but $m = 2j - k = (j-\ell) + (j - (k-\ell))$

which gives rise to $\lceil \frac{k}{2} \rceil$ symmetric vectors and $\lfloor \frac{k}{2} \rfloor$ antisymmetric ones. (or from figures)

hence: while $m \to m-1$, the dimensions of the symmetric, resp. antisymmetric spaces grow by one alternatively.

$\to$ $\mathcal{D}_{2j}$ is symmetric

Hence: from $m = 2j-1$: $\mathcal{D}_{2j-1}$ is antisymmetric

and again inductively so until $m = |j_1 - j_2| = 0$ $\square$

In particular, if j is half-integer, then $\mathcal{D}_0$ corresponds to the antisymmetric vector.

<u>Spin waves for the antiferromagnet.</u> (sorry $N = L$)

- $U^* S_j^1 U = S_j^1 \cos \frac{2\pi j}{N} + S_j^2 \sin \frac{2\pi j}{L}$

  $U^* S_j^2 U = -S_j^1 \sin \frac{2\pi j}{N} + S_j^2 \cos \frac{2\pi j}{N}$

  $U^* S_j^3 U = S_j^3$

$$\Rightarrow U^* H_L^{AF} U = H_L^{AF} + \left(\cos \frac{2\pi}{N} - 1\right) \sum \left(S_j^1 S_{j+1}^1 + S_j^2 S_{j+1}^2\right) + \left(\sin \frac{2\pi}{N}\right) \sum \left(S_j^1 S_{j+1}^2 - S_j^2 S_{j+1}^1\right)$$

Note that $\sum (S^1_j S^2_{j+1} - S^2_j S^1_{j+1})$

$= [\sum j S^3_j , H^{AF}_L](-i)$ by the su(2)-relations

hence, $\langle \Omega_L , \sum (S^1_j S^2_{j+1} - S^2_j S^1_{j+1}) \Omega_L \rangle = 0$

for ~~the~~ the ground state Ω_L (in fact for any eigenvector of H).

Therefore:

$$\delta_L = \langle \Omega_L , (U^* H^{AF}_L U - H^{AF}_L)\Omega_L \rangle$$

$$= \underbrace{\left(\cos \frac{2\pi}{N} - 1\right)}_{O(\frac{1}{L^2})} \underbrace{\langle \Omega_L , \sum (S^1_j S^1_{j+1} + S^2_j S^2_{j+1}) \Omega_L \rangle}_{= O(L)}$$

$$= O\left(\frac{1}{L}\right)$$

- We now consider the chain on the circle and define the shift operator R:

$$R S^i_j R^{-1} = S^i_{j+1}$$

with the convention $L+1 = 1$.

Clearly: $R H^{AF}_L R^{-1} = H^{AF}_L$ (again $S_{L+1} = S_1$)

and since the ground state is unique, $R^{-1}\Omega_L = e^{i\alpha}\Omega_L$ for some $\alpha \in \mathbb{R}$.

$$\langle \Omega_L , \Psi_L \rangle = \langle \Omega_L , U \Omega_L \rangle = \langle \Omega_L , R U R^{-1} \Omega_L \rangle$$

$$= \langle \Omega_L , e^{\frac{2\pi i}{L} \sum_x x S^3_{x+1}} \Omega_L \rangle$$

$$= \langle \Omega_L , U e^{2\pi i S^3_1} e^{\frac{2\pi i}{L} \sum_x S^3_x} \Omega_L \rangle$$

$$= \langle \Omega_L , U e^{2\pi i S^3_1} \Omega_L \rangle$$

$\uparrow$ $S^3_{tot} \Omega_L = 0$.

For a half integer spin: all eigenvalues of S^3 are of the form $\frac{h}{2}$, $h \in \mathbb{Z}$ so that $e^{2\pi i S_1^3} = -\mathbb{1}$.

$$\Rightarrow \langle \Omega_L, U\Omega_L \rangle = -\langle \Omega_L, U\Omega_L \rangle$$

$$\Rightarrow \langle \Omega_L, \Psi_L \rangle = 0.$$

Now: by the variational principle:

$$\text{Gap} = \inf_{\substack{\|\Psi\|=1 \\ \Psi \perp \Omega_L}} \left(\langle \Psi, H_L^{AF} \Psi \rangle - \langle \Omega_L, H_L^{AF} \Omega_L \rangle \right)$$

$$\leq \langle \Psi_L, H_L^{AF} \Psi_L \rangle - \langle \Omega_L, H_L^{AF} \Omega_L \rangle = \delta_L = O\left(\frac{1}{L}\right)$$

$\rightarrow$ the spectral gap above the ground state energy vanishes (at least as $\frac{1}{L}$) as $L \to \infty$.

ADVANCED MATHEMATICAL STATISTICAL PHYSICS WS13/14
EXERCISE SET 6

DISCUSSION :

Theorem of Perron-Frobenius

EXERCISES :

i. Using Duhamel's formula, identify an exact expansion of $\exp(A+\lambda B)$ to order N in $\lambda \in \mathbb{R}$. Prove the convergence of the series for all λ if B is a bounded operator.

ii. Show that the pressure (free energy per unit volume) of the free, spinless Bose / Fermi gas of mass m in $\mathbb{R}^3$ is given by
$$p(\beta,\mu) = \mp\frac{1}{\beta}\frac{1}{(2\pi)^3}\int d^3k \log\left(1 \mp z\mathrm{e}^{-\frac{k^2}{2m}}\right)$$
where $z = \exp(\beta\mu)$, provided $\mu < 0$.

Note : The Hamiltonian is
$$H_\Lambda = \sum_{i=1}^{N} \frac{-\Delta}{2m}.$$
It is convenient to choose $\Lambda = [-L/2, L/2]^3$ and consider the self-adjoint Laplacian given by periodic boundary conditions. The pressure is given by
$$p(\beta,\mu) = \frac{1}{|\Lambda|}\log\Theta_\Lambda(\beta,\mu),$$
where $\Theta_\Lambda(\beta,\mu)$ is the grand canonical partition function at inverse temperature $\beta > 0$ and chemical potential $\mu \in \mathbb{R}$,
$$\Theta_\Lambda(\beta,\mu) = \mathrm{Tr}\left(\mathrm{e}^{-\beta(H_\Lambda-\mu N_\Lambda)}\right)$$
where N_Λ is the number operator.

Duhamel's series

- Recall: For any two bounded operators A, B, we have
$$e^{s(A+B)} = e^{sA} + \int_0^s e^{tA} B e^{(s-t)(A+B)} dt \qquad (*)$$
We prove by recursion that
$$e^{A+\lambda B} = \sum_{k=0}^{N-1} \lambda^k \int_{0 \le t_1 \le \dots \le t_k \le 1} dt_1 \dots dt_k \, e^{t_1 A} B e^{(t_2-t_1)A} B \dots B e^{(1-t_k)(A)}$$
$$+ \lambda^N \int_{0 \le t_1 \le \dots \le t_N \le 1} dt_1 \dots dt_N \, e^{t_1 A} B \dots e^{(1-t_N)(A+\lambda B)}$$
for $N \geq 1$, and the term $k=0$ being e^A.
  - $N=1$ is $(*)$
  - Assume the formula holds for N. Then insert $(*)$ into the remainder to get
$$\lambda^N \int dt_1 \dots dt_N \, e^{t_1 A} B \dots \Big[\underbrace{e^{(1-t_N)A}}_{\text{becomes the } k=N\text{th summand}} + \underbrace{\lambda \int_0^{1-t_N} ds \, e^{sA} B e^{(1-t_N-s)(A+\lambda B)}}_{\text{set } s = t_{N+1} - t_N \text{ and conclude.}} \Big]$$

- Convergence: The volume of the domain of integration is $\frac{1}{k!}$. Use $\|e^{tA}\| \le e^{t\|A\|}$ to get
$$\Big\| \sum_{k=0}^{N-1} \lambda^k \int dt_1 \dots dt_k \, e^{t_1 A} B \dots B e^{(1-t_k)A} \Big\| \le \sum_{k=0}^{N-1} \frac{\lambda^k}{k!} e^{\|A\|} \|B\|^k$$
$$\xrightarrow{N \to \infty} e^{\|A\| + \lambda \|B\|} \quad \text{for any } \lambda \in \mathbb{R}.$$
Moreover, $e^{A+\lambda B} = \sum_{k=0}^{\infty} (\dots)$ as, similarly
$$\Big\| \lambda^N \int dt_1 \dots dt_N \, e^{t_1 A} B \dots B e^{(1-t_N)(A+\lambda B)} \Big\| \le \frac{\lambda^N}{N!} e^{\|A\| t_N} \|B\|^N e^{(1-t_N)\|A+\lambda B\|}$$
$$\to 0 \quad (N \to \infty)$$

- <u>Ideal quantum gases.</u>

Consider Fermions/Bosons that evolve independently and with 1-particle energies $\{\varepsilon_\alpha\}_{\alpha\in\mathbb{N}}$ s.t.

$$-\infty < \varepsilon_0 \le \varepsilon_1 \dots \le \varepsilon_\alpha \le \dots \quad : \varepsilon_\alpha \to \infty \quad \alpha \to \infty.$$

Corresponding basis of Fock space: $|n_0, n_1, \dots, n_\alpha\rangle$, where

$$n_\alpha = \begin{cases} 0, 1 & F. \\ 0, 1, 2, \dots & B. \end{cases}$$

are the number of particles in the eigenstate α corresponding to ε_α

Number operator : $N|n_0,\dots\rangle = \left(\sum_\alpha n_\alpha\right)|n_0,\dots\rangle$

Hamiltonian : $H|n_0,\dots\rangle = \left(\sum_\alpha n_\alpha \varepsilon_\alpha\right)|n_0,\dots\rangle$

And the (grand canonical) partition function is given by

$$\Theta(\beta,\mu) = \mathrm{Tr}\left(e^{-\beta(H-\mu N)}\right) = \sum_{n_0,n_1,\dots\in\mathbb{N}} \prod_\alpha e^{\beta(\mu-\varepsilon_\alpha)n_\alpha}$$

$$= \prod_\alpha \sum_{n\in\mathbb{N}} e^{\beta(\mu-\varepsilon_\alpha)n}$$

$$= \prod_\alpha \left(1 \pm e^{\beta(\mu-\varepsilon_\alpha)}\right)^{\pm 1} \qquad \begin{pmatrix} + : F \\ - : B \end{pmatrix}$$

while for bosons $\mu - \varepsilon_\alpha < 0 \ \forall\alpha$ i.e. $\mu < \varepsilon_0$ so that the series converges.

Hence:

$$\log\Theta(\beta,\mu) = \pm\sum_\alpha \log\left(1 \pm e^{\beta(\mu-\varepsilon_\alpha)}\right)$$

Specializing to the case of a free gas in a box, the eigenfunctions are plane waves with energies

$$\varepsilon_{\vec{k}} = \frac{k^2}{2m}$$

Letting $z := e^{\beta\mu}$:

$$\frac{1}{V}\log \Theta_V(\beta,\mu) = \frac{1}{(2\pi)^3}\,\frac{(2\pi)^3}{L^3}\sum_{\vec{k}} \pm \log\left(1 \pm z e^{-\beta\frac{\vec{k}^2}{2m}}\right)$$

$$\xrightarrow{L\to\infty} \pm \frac{1}{(2\pi)^3}\int d^3k \,\log\left(1 \pm z e^{-\beta\frac{\vec{k}^2}{2m}}\right)$$

and since $\beta > 0$, we can rescale $\vec{k}$ to get

$$p(\beta,\mu) = \pm\frac{1}{\beta}\frac{1}{(2\pi)^3}\int d^3k\,\log\left(1 \pm z e^{-\cancel{\beta}\frac{\vec{k}^2}{2m}}\right)$$

$$\left(\begin{array}{l} + : \text{fermions} \\ - : \text{Bosons, with } \mu < \varepsilon_0 = 0 \end{array}\right).$$

- Perron-Frobenius : see attached booklet Gantmacher: "The theory of Matrices", vol 2, chap. XIII.

ADVANCED MATHEMATICAL STATISTICAL PHYSICS WS13/14
EXERCISE SET 8

DISCUSSION :

Non-equilibrium thermodynamics, part I : Fluctuations, fluxes and affinities

EXERCISES :

Perturbation theory : Consider two self-adjoint operators H, V on the Hilbert space $\mathcal{H}$, such that $V \in \mathcal{L}(\mathcal{H})$ and $\exp(-H)$ is trace-class. Let τ_V^t , $t \in \mathbb{R}$, be the automorphism of the observable algebra $\mathcal{A} = \mathcal{L}(\mathcal{H})$ defined by

$$\tau_V^t(A) = \mathrm{e}^{\mathrm{i}t(H+V)} A \mathrm{e}^{-\mathrm{i}t(H+V)}.$$

Similarly, one defines the thermal state $\omega_{\beta,V}$, $\beta \in (0, \infty)$ by

$$\omega_{\beta,V}(A) = \mathrm{Tr}\left(\mathrm{e}^{-\beta(H+V)}\right)^{-1} \mathrm{Tr}\left(A\mathrm{e}^{-\beta(H+V)}\right).$$

The goal of this exercise is to derive a rigorous expansion of $\omega_{\beta,V}$ with respect to V,

$$\omega_{\beta,V}(A) = \sum_{n=0}^{\infty} \nu_n(A), \qquad \beta\|V\| < \ln 2, \tag{1}$$

using the interaction picture propagator

$$U_V(t) = \mathrm{e}^{\mathrm{i}t(H+V)}\mathrm{e}^{-\mathrm{i}tH}.$$

Check the following basic relations :

$$\mathrm{e}^{\mathrm{i}t(H+V)} = U_V(t)\mathrm{e}^{\mathrm{i}tH}; \tag{2}$$

$$\tau_V^t(A) = U_V(t)\tau_0^t(A)U_V(t)^{-1}; \tag{3}$$

$$U_V(t)^{-1} = U_V(t)^* = \tau_0^t(U_V(-t)); \tag{4}$$

$$U_V(t+s) = U_V(s)\tau_0^s(U_V(t)); \tag{5}$$

$$\partial_t U_V(t) = \mathrm{i}U_V(t)\tau_0^t(V), \quad U_V(0) = 1. \tag{6}$$

Since $z \mapsto \tau_V^z(A)$ is an entire analytic function, show that *Dyson's expansion* is uniformly convergent on compact sets of $\mathbb{C}$:

$$U_V(t) = 1 + \sum_{k=1}^{\infty} (\mathrm{i}t)^k \int_{0\leq s_1 \leq \ldots \leq s_k \leq 1} \tau^{ts_1}(V) \cdots \tau^{ts_k}(V)\, ds_1 \cdots ds_k. \tag{7}$$

In particular, $U_V(\mathrm{i}\beta)$ is well-defined for all $\beta \in \mathbb{R}$. Use this and (2) to express $\omega_{\beta,V}$ in terms of $\omega_{\beta,0}$.

Now, with *Golden-Thomson's inequality*

$$\mathrm{Tr}\left(\mathrm{e}^{A+B}\right) \leq \mathrm{Tr}\left(\mathrm{e}^{A}\mathrm{e}^{B}\right)$$

and Trotter's product formula, show the following lemma :

Lemma 1. *For any β, V as above and $\alpha \in \mathbb{C}$,*

$$|\omega_{\beta,0}(U_{\alpha V}(\mathrm{i}\beta)) - 1| \leq \mathrm{e}^{|\alpha\beta|\|V\|} - 1. \tag{8}$$

Finally, use (7) and (8) to derive the expansion (1). In particular, show that

$$\nu_0(A) = \omega_{\beta,0}(A),$$
$$\nu_1(A) = -\beta\big(V, A - \omega_{\beta,0}(A)\big)_{\beta},$$

where $(\cdot,\cdot)_\beta$ is Duhamel's two-point function.

Non-equilibrium thermodynamics – part 1

- Setup: Thermodynamic system described by its entropy function:

  $S = S(X_1, \dots, X_n)$,

  where $X_1, \dots, X_n$ are extensive variables. (macroscopic)

  Intensive variables $F_1, \dots, F_n$ are given by

  $F_i = F_i(X_1, \dots, X_n) = \frac{\partial S}{\partial X_i}$.

Ex: $X_1 = U$ energy $\qquad F_1 = \frac{1}{T}$

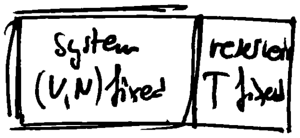
$X_2 = V$ volume $\qquad F_2 = -\frac{p}{T}$

$X_3 = N$ particle number $\qquad F_3 = -\frac{\mu}{T}$

$dS = \frac{1}{T} dU - \frac{p}{T} dV - \frac{\mu}{T} dN$ i.e.

Note. Often: some of the F_i are fixed, say $i = 1, \dots, r$.

and similarly for complementary X_j's:



$(r = 1)$

- ⟹ Postulate: Probability distribution of $X_1, \dots, X_r$ is the density

$$W(X_1, \dots, X_r) = \exp\left(\frac{1}{k} \left(S(X_1, \dots, X_r) - \sum_{i=1}^{r} F_i X_i - \hat{S}(F_1, \dots, F_r) \right) \right)$$

where $e^{-\frac{\hat{S}}{k}}$ is introduced so as to normalize W to make it a probability density.

Ex: (as above): $W(x)dx = Z^{-1} e^{-\beta H(x)}$ (classical)

in terms of the energy:

$$W(U) = \int \delta(H(x) - U) W(x) dx = Z^{-1} \underbrace{\int \delta(H(x) - U) e^{-\beta H(x)} dx}$$

$$= \frac{e^{-\beta U}}{Z} \int \delta(H(x) - U)\, dx = \frac{e^{-\beta U}}{Z} e^{\frac{1}{h} S(U)}$$

i.e. $W(U) = e^{\frac{1}{h}\left(S(U) - \frac{1}{T} U - \hat{S}\left(\frac{1}{T}\right)\right)}$

with $\hat{S}(T)$ given by $Z^{-1} \stackrel{!}{=} e^{-\frac{1}{h}\hat{S}\left(\frac{1}{T}\right)}$

i.e. $\log Z = \frac{1}{h}\hat{S}\left(\frac{1}{T}\right)$

but also $\log Z = \frac{1}{hT} \hat{F}$ ← free energy

$\Rightarrow \quad \hat{S} = \frac{\hat{F}}{T}$ in this case.

- Averages & fluctuations:
  - Average: $\langle X_i \rangle = -\frac{\partial \hat{S}}{\partial f_i}$ (*)

    indeed: $\int W = 1 \Rightarrow \quad 0 = \int \frac{1}{h}\left(-X_i - \frac{\partial \hat{S}}{\partial f_i}\right) W\, dX_1 \cdots dX_r$
  - fluctuations: Let $\delta X_i = X_i - \langle X_i \rangle$.

    then:

$$\langle \delta X_i \delta X_j \rangle = h\left(\frac{\partial^2 \hat{S}}{\partial f_i \partial f_j}\right) \qquad (**)$$

indeed. From: $e^{\frac{1}{h}\hat{S}} = \int e^{\frac{1}{h}\left(S - \sum_i f_i X_i\right)} dX_1 \cdots dX_r$

we get:

$$\frac{\partial^2 \hat{S}}{\partial f_i \partial f_j} + \frac{\partial \hat{S}}{\partial f_i}\frac{\partial \hat{S}}{\partial f_j} = \int X_i X_j\, e^{\frac{1}{h}\left(S(X_1 \ldots X_r) - \sum_i f_i X_i\right)} \cdot e^{-\frac{1}{h}\hat{S}(f_1, \ldots, f_r)} dX_1 \ldots dX_r.$$

$$\Rightarrow \frac{\partial^2 \hat{S}}{\partial f_i \partial f_j} \stackrel{(*)}{=} \langle X_i X_j \rangle - \langle X_i \rangle \langle X_j \rangle = \left\langle (X_i - \langle X_i \rangle)(X_j - \langle X_j \rangle) \right\rangle$$

$$= \langle \delta X_i \delta X_j \rangle$$

- Proposition. Let $Z(\lambda_1, \dots, \lambda_r)$ be defined for $\lambda_i \in \mathbb{C}$ by

$$Z(\lambda_1, \dots, \lambda_r) = e^{\frac{1}{\hbar}\left(\hat{S}(f_1-\lambda_1, \dots, f_r-\lambda_r) - \hat{S}(f_1, \dots, f_r)\right)}$$

Then:

$$\left\langle \prod_{i=1}^{n} X_{j_i} \right\rangle = \frac{\hbar^n}{Z(0, \dots, 0)} \left(\prod_{i=1}^{n} \frac{\partial}{\partial \lambda_{j_i}} \right) Z(\lambda_1, \dots, \lambda_r) \Big|_{\lambda=0}$$

Note. $Z(\lambda_1 \dots \lambda_r)$ is the generating function of the moments

Proof: $\left\langle \prod_i X_{j_i} \right\rangle = \hbar^n \int dX_1 \dots dX_n \left(\prod_i \frac{\partial}{\partial \lambda_{j_i}} \right) e^{\frac{1}{\hbar}(S - \Sigma(f-\lambda)X - \hat{S})} \Big|_{\lambda=0}.$

- Proposition. Let $\left\langle\!\left\langle \prod_{i=1}^{n} X_{j_i} \right\rangle\!\right\rangle$ be defined recursively by

$$\left\langle \prod_{i=1}^{n} X_{j_i} \right\rangle =: \sum_{P} \prod_{C \in P} \left\langle\!\left\langle \prod_{i \in C} X_{j_i} \right\rangle\!\right\rangle$$

where $P = (C_1, \dots)$ runs over all partitions of $\{1, \dots, n\}$.

Then:

$$\left\langle\!\left\langle \prod_{i=1}^{n} X_{j_i} \right\rangle\!\right\rangle = \hbar^{n-1} \left(\prod_{i=1}^{n} \frac{\partial}{\partial \lambda_{j_i}} \right) \left(\hat{S}(f_1-\lambda_1, \dots, f_r-\lambda_r) - \hat{S}(f_1, \dots, f_r) \right) \Big|_{\lambda=0}$$

$$= \hbar^n \left(\prod_{i=1}^{n} \frac{\partial}{\partial \lambda_{j_i}} \right) \log Z(\lambda_1, \dots, \lambda_r) \Big|_{\lambda=0}$$

Notes:
- $\langle\langle X_i \rangle\rangle = \langle X_i \rangle$
- $\langle\langle X_i X_j \rangle\rangle = \langle \delta X_i \, \delta X_j \rangle$
- From $(*)$ and $(**)$

$$\frac{\partial \langle X_i \rangle}{\partial f_j} = -\frac{1}{\hbar} \langle \delta X_i \, \delta X_j \rangle$$

* In the example above..

$$\langle (\delta U)^2 \rangle = -k \left(\frac{\partial \langle U \rangle}{\partial \left(\frac{1}{T}\right)} \right) = kT^2 \left(\frac{\partial \langle U \rangle}{\partial T} \right)$$

$$= kT^2 N \underbrace{c_V}_{}$$

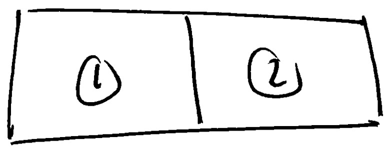
specific heat per molecule/mole.

Observation: $\begin{cases} \langle U \rangle \sim O(N) \\ \text{but } \langle (\delta U)^2 \rangle^{1/2} \sim O(N^{1/2}) \end{cases}$

Fluctuations are <u>subleading</u> in the limit $N \to \infty$, <u>except</u> when $c_V \to \infty$, i.e. at <u>phase transitions</u>.

- <u>Affinities & Fluxes</u>

(A) Discontinuous system:



Two TD systems, each of them at equilibrium, but not mutually. They can exchange X_i, $i=1,\dots,r$.
Now: drop indices and denote X^1, X^2 for subsystems.

$X^1 + X^2$ is fixed.

Define. <u>Flux</u> $J = \frac{\partial X_2}{\partial t} = -\frac{\partial X_1}{\partial t}$.

<u>Affinity</u>: $\frac{\partial}{\partial X_2} \left(S_1(X_1) + S_2(X_2) \right)$

$$= \frac{\partial}{\partial X_2} \left(S_1(X_0 - X_2) + S_2(X_2) \right)$$

$$= \tilde{F}_2 - \tilde{F}_1 .$$

where $\tilde{F}_i = \frac{\partial S_t}{\partial X_i}$ is the value for F_i s.t. the exponent in W is maximal,

i.e. $\tilde{F}_i$'s correspond to the most probable values for $\bar{X}_i$'s.

interpretation: $\tilde{F}_i$ are the prescribed values for F_i (temperature, ...)

Now: Entropy production:

$$\dot{S} = \frac{d}{dt}\left(S_1(X_1) + S_2(X_2)\right) = (F_2 - F_1)\, J .$$

and we see:

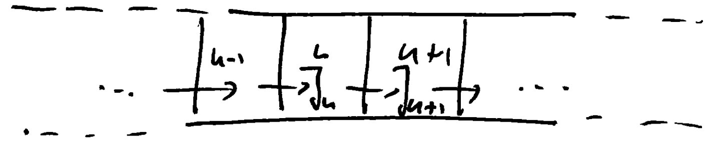
Equilibrium $\Leftrightarrow$ maximal entropy $\Leftrightarrow$ $(F_2 - F_1) = 0$

Equilibrium $\Leftrightarrow$ $\dot{S} = 0$

In the example: $X = U$, $F = \frac{1}{T}$, J: energy flux.

$$\dot{S} = \left(\frac{1}{T_2} - \frac{1}{T_1}\right) J$$

(B) Continuum limit:



* in cell n: $\frac{dX_n}{dt} = J_n - J_{n+1}$. (1)

no production of X: is the complete rate of change of X_n.

+ Entropy: i) in cell n: (transport)

$$\frac{dS_n}{dt} = \frac{\partial S}{\partial X_n}(J_n - J_{n+1}) = \tilde{F}_n (J_n - J_{n+1})$$

ii) at boundary (production)

$$\dot{S}_n = \left(\frac{\partial S}{\partial X_n} - \frac{\partial S}{\partial X_{n-1}}\right) J_n = (\tilde{F}_n - \tilde{F}_{n-1})\, J_n \quad (2)$$

$\rightarrow$ Entropy flux through cell n: $J_{S,n} = \tilde{F}_n J_n$.

All in all: $\frac{dS_n}{dt} = (F_{n+1} - F_n) J_{n+1} - F_{n+1} J_{n+1} + F_n J_n$

$$= \dot{S}_{n+1} - (J_{s,n+1} - J_{s,n}) \qquad (3)$$

+ Limit: $n \mapsto x$; $(n+1) - n \mapsto dx$; ...

(1) becomes: $\frac{\partial X}{\partial t} = -\nabla J$ (continuity equation)

(3) becomes: $\dot{S} = \frac{\partial S}{\partial t} + \nabla J_s$ (continuity with source)

(2) becomes: $\dot{S} = \nabla \tilde{F} \cdot J$ (entropy production rate)

Moreover: $\frac{\partial S}{\partial t} = -F \nabla J$

and $J_s = F \cdot J$ (entropy flux)

Note: current $\cancel{\frac{\partial X}{\partial t}}$ J.

affinity ∇F (~ thermodynamic forces: eg. temperature gradient)

+ Reinsert indices:

Entropy flux: $J_s = \sum_{n=1}^{r} \tilde{F}_n \cdot J_n$.

Entropy production: $\dot{S} = \sum_{n=1}^{r} \nabla \tilde{F}_n \cdot J_n$

Rate of change of entropy: $\frac{\partial S}{\partial t} = \dot{S} - \nabla J_s = -\sum_{n=1}^{r} \tilde{F}_n \cdot \nabla J_n$

+ Notes: i) In the steady state: $\frac{\partial X_i}{\partial t} = 0$; $\frac{\partial S}{\partial t} = 0$ but $\dot{S} \neq 0$!

ii) Heat flux: $J_Q := T J_s$. In steady state:

$$\dot{S} = \nabla J_s = \nabla\left(\frac{J_Q}{T}\right) = \underbrace{\nabla\left(\frac{1}{T}\right) J_Q}_{\mathrm{I}} + \underbrace{\frac{1}{T}\nabla J_Q}_{\mathrm{II}} \quad ;$$

I: heat transfer
II: heat source at temperature T.

- A priori: no relation between Fluxes and Affinities.

Now: Markov process assumption:

$$J_k = J_k(\mathcal{F}_1, \dots, \mathcal{F}_r, \tilde{f}_1, \dots, \tilde{f}_r)$$

where $\mathcal{F}_i = \nabla \tilde{f}_i$

and the relation is a <u>fixed time</u>

Even further: linear response:

$$J_k = \sum_{j=1}^{r} L_{kj} \mathcal{F}_j \qquad L_{kj} = L_{kj}(\tilde{f}_1, \dots, \tilde{f}_r)$$

Again in the example: $X = U$; $f = \frac{1}{T}$.

Fourier's law: $J_U = -\kappa \nabla T$.

this can be rewritten: $J_U = \kappa T^2 \nabla\left(\frac{1}{T}\right)$

i.e. $L_{UU} = \kappa T^2$

<u>Onsager's relation</u>: (heuristically derived)

$$L_{kj}(\tilde{F}_1, \dots, \tilde{F}_r) = \pm L_{kj}(\tilde{F}_1^{+}, \dots, \tilde{F}_r^{+})$$

where $\tilde{F}_i^{+}$ are the time-reversed F_i, which can be $\pm f_i$.

Exercise: Perturbation theory for $e^{-\beta(H+V)}$

- Check: (2): $U_V(t)e^{itH} = e^{it(H+V)}e^{-itH}e^{itH} = e^{it(H+V)}$ ✓

(3) $U_V(t)\tau_0^t(A)U_V(t)^{-1} = U_V(t)e^{itH}A(e^{+itH})^{-1}U_V(t)^{-1}$

$\overset{(2)}{=} e^{it(H+V)}A(e^{it(H+V)})^{-1} = \tau_V^t(A)$ ✓

(4) $U_V(t)^* U_V(t) = e^{itH}e^{-it(H+V)}e^{it(H+V)}e^{-itH} = 1 = U_V(t)U_V(t)^*$ ✓

~~$\tau_0^t(U_V(-t)) = e^{itH}$~~ $\tau_0^t(U_V(-t)) = e^{itH}e^{-it(H+V)} = U_V(t)^*$ ✓

~~$U_V(-t)U_V(t) =$~~

(5) $U_V(s)\tau_0^s(U_V(t)) = e^{is(H+V)}e^{-isH}e^{isH}e^{it(H+V)}e^{+itH}e^{-isH}$

$= e^{i(s+t)(H+V)}e^{-i(s+t)H} = U_V(s+t)$ ✓

(6) $\partial_t U_V(t) = ie^{it(H+V)}[(H+V)-H]e^{-itH}$

$= e^{it(H+V)}e^{-itH}e^{itH}Ve^{-itH}$ ✓

- Note: the condition $\exp(-H) \in \mathcal{C}_1$ implies that $\exp(-H)$ is in particular bounded, which implies that H is semi-bounded below.

- Iterating (6), we get

$$U_V(t) = 1 + i\int_0^t U_V(s_1)\tau_0^{s_1}(V)\,ds_1$$

$$= 1 + i\int_0^t ds_1\,\tau_0^{s_1}(V) - \int_0^t ds_1\int_0^{s_1} ds_2\,U_V(s_2)\tau_0^{s_2}(V)\tau_0^{s_1}(V)$$

$$= 1 + \sum_{h=1}^{N} i^h \int_{0\le s_1\le\dots\le s_h\le t} ds_1\dots ds_h\,\tau^{s_1}(V)\dots\tau^{s_h}(V)$$

$$+ i^{h+1}\int_{0\le s_1\le\dots\le s_{h+1}\le t} ds_1\dots ds_{h+1}\,U_V(s_1)\tau_0^{s_1}(V)\dots\tau_0^{s_{h+1}}(V)$$

Since $U_V(t)$ is unitary, the norm of the remainder is
$$\|\cdot\| \leq \frac{|t|^{k+1}}{(k+1)!}\|V\|^{k+1} \longrightarrow 0 \quad (k\to\infty) \text{ for all } t\in\mathbb{R}.$$
and similarly:
$$\left\|\sum_{k=1}^{N}(\dots)\right\| \leq \sum_{k=1}^{N}\frac{(|t|\|V\|)^{k+1}}{(k+1)!} \longrightarrow e^{|t|\|V\|} < \infty. \quad (N\to\infty).$$
Hence, the series converges to $U_V(t)$, for all fixed $t\in\mathbb{R}$, pointwise. This implies uniform convergence on compact sets of $\mathbb{R}$. Moreover, since τ_V^t has an analytic extension to $t\in\mathbb{C}$, the estimates above show the absolute convergence of the series pointwise for $t\in\mathbb{C}$, and hence uniformly on compacts.

- Now:
$$\omega_{\beta,V}(A) = \frac{\mathrm{Tr}\left(e^{-\beta(H+V)}A\right)}{\mathrm{Tr}\left(e^{-\beta(H+V)}\right)} = \frac{\mathrm{Tr}\left(U_V(i\beta)e^{-\beta H}A\right)}{\mathrm{Tr}\left(U_V(i\beta)e^{-\beta H}\right)}$$
$$= \frac{\omega_{\beta,0}\left(A\,U_V(i\beta)\right)}{\omega_{\beta,0}\left(U_V(i\beta)\right)} \qquad (*)$$
This and Dyson's expansion allows for the expansion of $\omega_{\beta,V}(A)$.

- First, we prove the lemma: (with $\omega_{\beta,0}$ instead of $\omega_{\beta,V}$!!!)
$$\omega_{\beta,0}\left(U_{\alpha V}(i\beta)\right) - 1 = \int_0^1 \frac{d}{ds}\omega_{\beta,0}\left(U_{s\alpha V}(i\beta)\right)ds$$
$$= -\alpha\beta\int_0^1 f(s)\,ds$$
where $f(s) = \dfrac{\mathrm{Tr}\left(Ve^{-\beta(H+s\alpha V)}\right)}{\mathrm{Tr}\left(e^{-\beta H}\right)}$ arising from Duhamel's formula applied to $e^{-\beta(H+\alpha sV)}$, and cyclicity.

Now: $$|f(s)| \leq \|V\| \frac{\|e^{-\beta(H+s\alpha V)}\|_1}{\mathrm{Tr}(e^{-\beta H})} = \frac{\|V\|\,\mathrm{Tr}(e^{-\beta(H+s\alpha V)})}{\mathrm{Tr}(e^{-\beta H})}$$

where we used that $\exp(-\beta(H+s\alpha V)) > 0$. By Golden-Thomson's inequality:

$$|f(s)| \leq \|V\| \frac{\mathrm{Tr}(e^{-\beta H} e^{-s\alpha\beta V})}{\mathrm{Tr}(e^{-\beta H})} = \|V\|\, \omega_{\beta,0}(e^{-s\alpha\beta V}) \leq \|V\| e^{s|\alpha\beta|\|V\|}$$

ω is a state

Integrating this bound yields

$$|\omega_{\beta,0}(U_{\alpha V}(i\beta)) - 1| \leq |\alpha\beta|\|V\| \left(e^{|\alpha\beta|\|V\|} - 1\right)\frac{1}{|\alpha\beta|\|V\|} \qquad \square$$

- Using Dyson's expansion at $t = i\beta$, and with $V \mapsto \alpha V$, we obtain

$$\omega_{\beta,0}(A\,U_V(i\beta)) = \sum_{n=0}^{\infty} \alpha^n c_n(A), \quad c_0(A) = \omega_{\beta,0}(A) \qquad (**)$$

where $$c_n(A) = (-\beta)^n \int_{0\leq s_1\leq\ldots\leq s_n\leq 1} ds_1\ldots ds_n\, \omega_{\beta,0}(A\,\tau^{i\beta s_1}(V)\ldots\tau^{i\beta s_n}(V))$$

$n \geq 1$.

- From Lemma 1, the function $\alpha \mapsto \omega_{\beta,0}(U_{\alpha V}(i\beta))$ does not have any zeros in the disk given by

$$e^{|\alpha||\beta|\|V\|} - 1 < 1 \quad \text{i.e.} \quad |\alpha| < \frac{\ln 2}{|\beta|\|V\|}$$

which in turn implies that $\alpha \mapsto \omega_{\beta,\alpha V}(A)$ is analytic in the disk by $(*)$ on page 9. Hence, it has an expansion

$$\omega_{\beta\alpha V}(A) = \sum_{n=0}^{\infty} \alpha^n\, \cancel{\omega_n(A)}\, v_n(A)$$

and $v_n(A)$ can be determined recursively from $(**)$:

$$\sum_{n=0}^{\infty} \alpha^n c_n(A) \stackrel{!}{=} \left(\sum_{n=0}^{\infty} \alpha^n v_n(A)\right)\left(\sum_{n=0}^{\infty} \alpha^n c_n(\mathbb{1})\right)$$

So that:
$$c_m(A) = \sum_{n=0}^{m} v_n(A)\, c_{m-n}(\mathbb{1})$$

All in all:

$$v_0(A) = c_0(A) = \omega_{\beta,0}(A) \quad \text{and}$$
$$v_n(A) = c_n(A) - \sum_{k=0}^{n-1} v_k(A)\, c_{n-k}(\mathbb{1})$$

and
$$\omega_{\beta,V}(A) = \sum_{n=0}^{\infty} v_n(A) \quad \text{in} \quad |\beta|\,\|V\| < \ln 2$$

In particular:

$$\begin{aligned}
v_1(A) &= c_1(A) - v_0(A)\, c_1(\mathbb{1}) \\
&= \underbrace{-\beta \int_0^1 ds\, \omega_{\beta,0}(A\,\tau^{i\beta s}(V))}_{=(V,A)_\beta \text{ (see Exercise set 3)}} - \omega_{\beta,0}(A)(-\beta)\int_0^1 ds\, \underbrace{\omega_{\beta,0}(\tau^{i\beta s}(V))}_{=(V,1)_\beta} \\
&= -\beta\left[(V,A)_\beta - (V, \omega_{\beta,0}(A))_\beta\right] \\
&= -\beta\left(V, (A - \omega_{\beta,0}(A))\right)_\beta .
\end{aligned}$$

$\square$

ADVANCED MATHEMATICAL STATISTICAL PHYSICS WS13/14
EXERCISE SET 9

DISCUSSION :

Non-equilibrium thermodynamics, part II :
Entropy production and Priorgine's variational principle

Non-equilibrium thermodynamics - part II.

- Recall: entropy production $\dot{S} = \sum_k DF_k \cdot J_k$

  affinities fluxes

  For a linear Markov process: $J_k = \sum_j L_{kj} DF_j$.

  $\leadsto$ $\dot{S} = \sum_{kj} DF_k L_{kj} DF_j = \langle DF, L DF \rangle$

  2nd law: $\dot{S} \geq 0$ i.e. L is a non-negative definite matrix.

  (and symmetric by Onsager)

- Recall: at equilibrium: Gibbs's variational principle:

  The equilibrium state is the maximizer of the entropy functional (under constraints: + fixed energy → microcanonical ensemble
  + fixed average energy → Gibbs' state
  + ...)

  Out of equilibrium: Prigogine's variational principle: minimal entropy production.

Theorem: Consider a time-reversal invariant classical system with configuration space $\Omega \subset \mathbb{R}^n$. Let $f_i(x)$ be the fields of intensive quantities. Assume:

(i) $L_{kj}(f_1, \dots, f_r) = L_{kj}$ (constant coefficients)

(ii) $L_{kj} = L_{jk}$ (Onsager)

(iii) either of (a) $f_j(x)$ fixed $\forall x \in \partial\Omega$ (prescribed boundary fields)

(b) $J_k \cdot d\sigma = 0$ on $\partial\Omega$ (no flux through boundary)

Then: the total entropy production

$$P[F] := \int_\Omega \dot{S}\, d^n x = \sum_k \int_\Omega (\nabla F_k \cdot J_k)\, d^n x$$

is minimal iff $F_i(x)$ is such that $\frac{\partial X_i}{\partial t} = 0$

(stationary state)

- In other words: the stationary state is characterized by its being the state with minimal total entropy production among all non-equilibrium states.

- Proof: First, we note that

$$\frac{\partial X_k}{\partial t} = -\operatorname{div} J_k = -\sum_j L_{kj} \operatorname{div}(\operatorname{grad} f_j) = -\sum_j L_{kj} \Delta f_j$$

We now compute a variation of $P[F]$:

$$\delta P = \delta \sum_{k,j} \int_\Omega \nabla f_k L_{kj} \nabla f_j\, d^n x = \sum_{kj} \int_\Omega (\nabla \delta f_k L_{kj} \nabla f_j + \nabla f_k L_{kj} \nabla \delta f_j)\, d^n x$$

$$\overset{(\text{Onsager})}{=} 2 \sum_{kj} \int_\Omega \nabla \delta f_k L_{kj} \nabla f_j\, d^n x$$

$$\overset{(\text{Green})}{=} 2 \sum_{kj} \left[\int_{\partial\Omega} \delta f_k L_{kj} D_\nu f_j\, d\sigma - \int_\Omega \delta f_k L_{kj} \Delta f_j\, d^n x \right]$$

$$\overset{(iii)}{=} 2 \sum_{k} \int_\Omega \delta f_k \frac{\partial X_k}{\partial t}\, d^n x .$$

Hence: $\delta P = 0$ for all variations $(\delta f_k)_{k=1}^r \iff \frac{\partial X_k}{\partial t} = 0$.

Moreover, the second variation gives

$$\delta^2 P = 2 \sum_{k,j} \int_\Omega (\nabla \delta f_k L_{kj} \nabla \delta f_j)\, d^n x \geq 0$$ since L is non-negative.

Hence the extremum is a minimum. $\square$

- Remarks: * The non-negativity also implied the existence of minimizers, a priori.
  * (i) is a problematic assumption. Recall the case of Fourier's law: $X = U$, $f = \frac{1}{T}$.
  $J_U = \kappa T^2 D\left(\frac{1}{T}\right)$, i.e. $L_{UU} = \kappa T^2$ (even $\kappa = \kappa(T)$!).

ADVANCED MATHEMATICAL STATISTICAL PHYSICS WS13/14
EXERCISE SET 10

DISCUSSION :

The GNS representation : Proof of the general theorem.

EXERCISES :

Finite quantum systems. Consider a quantum system defined on a Hilbert space $\mathcal{H}$ and whose dynamics is generated by a Hamiltonian H. Let $\mathcal{A} = \mathcal{B}(\mathcal{H})$ be the algebra of observables, and

$$\tau^t(A) = \mathrm{e}^{\mathrm{i}Ht} A \mathrm{e}^{-\mathrm{i}Ht}.$$

i. Show that the pair $(\mathcal{A}, \tau^t)$ is a C*-dynamical system if and only if H is a bounded operator.
Hint : The only non-trivial property to check is the strong continuity ;
Note : This example shows that the notion of a C*-dynamical system is in fact too restrictive for quantum mechanics, and that in many cases, W*-dynamical systems are more suited since continuity of the dynamics there is in a weaker topology ;

ii. Show that if $(\mathcal{A}, \tau^t)$ is a C*-dynamical system, then τ^t is in fact uniformly continuous ;

iii. A state is given by a density matrix ρ on $\mathcal{H}$. Show that $(\mathcal{A}, \tau^t, \rho)$ is a quantum dynamical system if $[\rho, H] = 0$;

iv. Prove that if H has purely continuous spectrum, then there is no trace-class operator $\rho \neq 0$ commuting with H, and hence no invariant state ;
Note : In other words, invariant states are given by convex combinations of projections on eigenstates ;

v. Assume that ρ is an invariant state. Construct its GNS representation ;
Hint : Let $\mathcal{K} = \mathrm{Ran}(\rho)$ and consider the Hilbert space $\mathcal{H}_\rho$ to be the set of Hilbert-Schmidt operators from $\mathcal{K}$ to $\mathcal{H}$;

vi. Show that the Liouvillean L_ρ is given by

$$\mathrm{e}^{\mathrm{i}tL_\rho} X = \mathrm{e}^{\mathrm{i}tH} X \mathrm{e}^{-\mathrm{i}tH\restriction_{\mathcal{K}}}$$

for any $X \in \mathcal{H}_\rho$;
Note : Clearly, the spectrum of the Liouvillean does not represent the energy of the system anymore.

Theorem: Let $\mathcal{A}$ be a C^*-algebra with a unit, $\omega \in \Sigma(\mathcal{A})$. Then, there exists a Hilbert space $\mathcal{H}_\omega$, a representation π_ω of $\mathcal{A}$ in $\mathcal{B}(\mathcal{H}_\omega)$ and a unit vector Ω_ω s.t.

$$\omega(A) = \langle \Omega_\omega, \pi_\omega(A)\Omega_\omega\rangle \qquad \forall A \in \mathcal{A}.$$

$\{\pi_\omega(A)\Omega_\omega : A \in \mathcal{A}\}$ is dense in $\mathcal{H}_\omega$.

Note: we have already proved uniqueness up to unitary equivalence in class.

Note: if $(\mathcal{H}, \pi)$ is a representation of $\mathcal{A}$ and Ω is a unit vector in $\mathcal{H}$, then

$$A \mapsto \langle \Omega, \pi(A)\Omega\rangle \quad , A \in \mathcal{A}.$$

defines a state on $\mathcal{A}$.

Proof: • Let $K_\omega := \{A \in \mathcal{A} : \omega(A^*A) = 0\}$. Since, $B \in \mathcal{A}$.

$$0 \le \omega((AB)^*(AB)) \le \|B\|^2 \omega(A^*A) = 0$$

K_ω is a left ideal. Let $h_\omega := \mathcal{A}/K_\omega$. Equip h_ω with the scalar product

$$\langle [A], [B]\rangle_\omega = \omega(B^*A)$$

+ well-defined: $\omega((B+I)^*(A+J))$

$= \omega(B^*A) + \omega(B^*J) + \omega(A^*I) + \omega(I^*J)$

$= \omega(B^*A)$

for any $I, J \in K_\omega$ by the ideal property.

+ if $\langle [A], [A]\rangle_\omega = 0$, then $A \in K_\omega$ i.e. $[A] = 0$.

+ positive.

$\Rightarrow$ h_ω is a pre-Hilbert space, $\mathcal{H}_\omega := \overline{h_\omega}$

• Let, for $A \in \mathcal{A}$: $L_A : h_\omega \to h_\omega$

$$[B] \mapsto [AB]$$

L_A is bounded:

$$\langle L_A[B], L_A[B]\rangle_\omega = \omega(B^*A^*AB) \le \|A\|^2 \omega(B^*B)$$
$$\le \|A\|^2 \langle [B],[B]\rangle_\omega$$

i.e. $\|L_A\| \le \|A\| < \infty$

hence L_A extends to a bounded operator on $\mathcal{H}_\omega$.
We call it $\pi_\omega(A)$.
We call $[I] =: \Omega_\omega$. Now check:

$$\langle \Omega_\omega, \pi_\omega(A)\Omega_\omega\rangle_\omega = \langle [I], L_A[I]\rangle_\omega = \langle [I],[AI]\rangle_\omega$$
$$= \omega(A)$$

and

$$\langle L_A[B],[C]\rangle_\omega = \langle [AB],[C]\rangle_\omega = \omega(B^*A^*C)$$
$$= \langle [B],[A^*C]\rangle_\omega = \langle [B], L_{A^*}[C]\rangle_\omega$$

i.e. $\pi_\omega(A)^* = \pi_\omega(A^*)$: π_ω is a $*$-automorphism. $\square$

Finite quantum systems.

- i) • if $H \in \mathcal{B}(\mathcal{H})$, then the Taylor expansion of e^{itH} converges in norm, and

$$(\lozenge) \quad \|e^{itH}Ae^{-itH} - A\| \le t\|[H,A]\| + O(t^2) \to 0 \quad (t\to 0).$$

• if τ^t is strongly continuous, then it is generated by $i[H,\cdot] =: \delta$

but $(\lambda+\delta)^{-1} = -\int_0^\infty e^{-\lambda t} e^{-t\delta}\, dt$ so that, $\lambda \in \mathbb{R}_+$

$$\|\lambda(\lambda+\delta)^{-1}\| \le \lambda \left|\int_0^\infty e^{-\lambda t}\, dt\right| = 1$$

$$\|e^{-t\delta}\| = 1.$$

which implies that $\|(\lambda+\delta)^{-1}\| \le \lambda^{-1}$, $\lambda > 0$.
But this is a contradiction if H – and therefore δ – is unbounded.

ii) This follows immediately from $(\diamond)$ and $\|[H,A]\| \le \|H\|\,\|A\|\,2$.

(iii) We need to show that ρ is invariant, i.e.

$$\operatorname{tr}\left(\rho\tau^t(A)\right) = \operatorname{tr}(\rho(A)) \qquad \forall A \in \mathcal{A}.$$

i.e. $\quad e^{-itH}\rho e^{itH} \overset{!}{=} \rho \qquad$ by duality.

and this clearly holds if $[\rho, H] = 0$.

iv) Fact: (see Reed-Simon Vol. 3, XV.3, Lemma 2)

If $\varphi \in P_{ac}(H)$, then $e^{-itH}\varphi \to 0$ weakly as $|t| \to \infty$.

Now assume $\exists \rho$, trace class and invariant. Then it is in particular compact so that

$$\rho = \sum_n \rho_n |\psi_n\rangle\langle\phi_n| \quad \Big(\text{or if you prefer } \sum_n \rho_n \langle\phi_n, \cdot\rangle\psi_n\Big)$$

Then, for any $\chi, \xi \in \mathcal{H}$:

$$\langle\chi, \rho\xi\rangle = \langle\chi, e^{-itH}\rho e^{itH}\xi\rangle$$
$$= \sum_n \rho_n \langle\chi, e^{-itH}\psi_n\rangle\langle\phi_n, e^{itH}\xi\rangle$$
$$\to 0 \quad \text{as } t \nearrow \infty. \quad \text{Hence } \rho = 0,$$

which contradicts $\operatorname{Tr}(\rho) = 1$

v) Let $i : \mathcal{K} \to \mathcal{H}$ be the canonical embedding and $\perp$.
Let $\mathcal{H}_\rho$ be the set of HS operators from $\mathcal{K}$ to $\mathcal{H}$, with inner product $\langle A, B\rangle_\rho := \operatorname{Tr}(A^*B)$

Define : $\Omega_\rho := \rho^{1/2} i$

and $\pi_\rho(A)$ by $\pi_\rho(A)B = AB$, for $B \in \mathcal{H}_\rho$.

$\Rightarrow \|\Omega_\rho\|_\rho^2 = \operatorname{Tr}\left(i^* \rho^{1/2}\rho^{1/2} i\right) = \operatorname{Tr}(\rho\, i i^*) = \operatorname{Tr}(\rho 1_{\mathcal{K}}) = 1$

so Ω_ρ is a unit vector.

$$\& \langle \Omega_\rho, \Pi_\rho(A)\Omega_\rho \rangle = \mathrm{Tr}\left(i^* \rho^{1/2} A \rho^{1/2} i \right)$$
$$= \mathrm{Tr}\left(\rho^{1/2} i i^* \rho^{1/2} A \right)$$
$$= \mathrm{Tr}\left(\rho A \right) = \rho(A)$$

Hence, $(\mathcal{H}_\rho, \Pi_\rho, \Omega_\rho)$ is the GNS representation of $(\mathcal{A}, \rho)$.

Moreover, $0 = \langle X, \Pi_\rho(A)\Omega_\rho \rangle = \mathrm{Tr}\left(X^* A \rho^{1/2} i \right)$
$$= \mathrm{Tr}\left((\rho^{1/2} i X^*) A \right) \quad \forall A \Rightarrow X = 0$$
hence $\Pi_\rho(\mathcal{A})\Omega_\rho$ is dense in $\mathcal{H}_\rho$.

vi) By definition, the Liouvillean is the generator of U_t s.t.
$$U_t \Pi_\rho(A)\Omega_\rho \stackrel{!}{=} \Pi_\rho\left(e^{itH} A e^{-itH}\right)\Omega_\rho$$
i.e.
$$U_t A \rho^{1/2} i \stackrel{!}{=} e^{itH} A e^{-itH} \rho^{1/2} i$$
and by assumption, $\rho^{1/2} i$ is invertible on $\mathcal{K}$, i.e.
$$U_t A i i^* = e^{itH} A e^{-itH} i i^*$$
and in particular for $X \in \mathcal{H}_\rho$:
$$U_t X = e^{itH} X e^{-itH}\restriction_{\mathcal{K}}$$

ADVANCED MATHEMATICAL STATISTICAL PHYSICS WS13/14
EXERCISE SET 11

DISCUSSION :

A few words about the Weyl algebra

EXERCISES :

Density of analytic elements. Let $(\mathcal{A}, \tau^t)$ be a C*-dynamical system, and let

$$\mathcal{A}_\tau := \{A \in \mathcal{A} : z \mapsto \tau^z(A) \text{ extends to an analytic function on } \mathbb{C}\}$$

be the set of analytic elements.

i. Show that $\tau^z(A^*) = \tau^{\bar{z}}(A)^*$;
ii. For any $A \in \mathcal{A}$, let

$$A_n := \sqrt{\frac{n}{\pi}} \int_{\mathbb{R}} \tau^t(A) \mathrm{e}^{-nt^2} dt$$

where the integral is in the Riemann sense with respect to the norm topology ;
Show that $A_n \in \mathcal{A}_\tau$;
iii. Use the definition above to prove that $\mathcal{A}_\tau$ is dense in $\mathcal{A}$.

Density of analytic elements

(i) Let A be fixed and define $f(z) = \tau^z(A)$, for $\operatorname{Im} z \geq 0$.
Since $\tau^t, t \in \mathbb{R}$ is a $*$-automorphism, $\tau^t(A)^* = \tau^t(A^*)$,
i.e. $\lim_{n\to\infty} \left[\tau^{t+i\gamma_n}(A) - \tau^{t+i\gamma_n}(A)^*\right] = 0$
for any sequence $\gamma_n \geq 0$, $\gamma_n \to 0$ $(n \to \infty)$.
By Schwarz's reflection principle, the extension of f to $\operatorname{Im} z < 0$ is such that

$$f(\bar{z}) = f(z)^* \quad \text{i.e.} \quad \tau^{\bar{z}}(A) = \tau^t(A^*)$$

(ii) First, we check that the integral converges, since

$$\|\tau^t(A) e^{-nt^2}\| = \|A\| e^{-nt^2} \subset L^1(\mathbb{R}) \quad \text{for } n > 0.$$

Now:

$$\tau^r(A_n) = \sqrt{\frac{n}{\pi}} \int_{-\infty}^{+\infty} \tau^{r+t}(A) e^{-nt^2} dt$$

$$= \sqrt{\frac{n}{\pi}} \int_{-\infty}^{+\infty} \tau^t(A) e^{-n(t-r)^2} dt$$

The r.h.s. is hence well-defined for all $z \in \mathbb{C}$, with

$$\|\text{r.h.s}\| \leq \|A\| e^{n(\operatorname{Im} z)^2}$$

and $A_n \in \mathcal{A}_\tau$.

(iii) We write $A = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{+\infty} e^{-t^2} A \, dt$ and

$$A_n = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-t^2} \tau^{t/\sqrt{n}}(A) dt \quad \text{to get}$$

$$A_n - A = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{+\infty} \left(\tau^{t/\sqrt{n}}(A) - A\right) e^{-t^2} dt$$

* Pointwise : $\| \tau^{t/\sqrt{n}}(A) - A \| \to 0 \quad (n \to \infty)$
by the strong continuity of $t \mapsto \tau^t$.

+ $\|$ integrand $\| \leq 2\|A\| e^{-t^2} \in L^1(\mathbb{R})$

Hence, by dominated convergence:

$$\lim_{n\to\infty} \|A_n - A\| \leq \lim_{n\to\infty} \frac{1}{\sqrt{\pi}} \int_{-\infty}^{+\infty} \| \tau^{t/\sqrt{n}}(A) - A \| e^{-t^2} dt$$

$$= \frac{1}{\sqrt{\pi}} \int \lim_{n\to\infty} \| \tau^{t/\sqrt{n}}(A) - A \| e^{-t^2} dt = 0.$$

• <u>On the Weyl algebra</u>

• Let $\mathcal{H}$ be a Hilbert space : the state space of a particle.
The <u>Weyl algebra</u> over $\mathcal{H}$ is the C^*-algebra generated by the elements $W(f)$, $f \in \mathcal{H}$ under the relation

$$W(f)W(g) = e^{-i\frac{1}{2}\mathrm{Im}\langle f, g\rangle} W(f+g) \;;\; W(-f) = W(f)^*$$

• It follows that
+ $W(0) = \mathbb{1}$
+ $W(f)$ is unitary, in particular $\mathrm{Spec}(W(f)) \subset S^1$

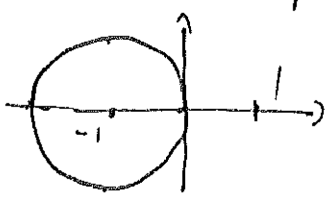
• Moreover:

$$W(g)^* W(f) W(g) = e^{-\frac{i}{2}\mathrm{Im}\langle f, g\rangle} W(-g) W(f+g)$$
$$= e^{i\,\mathrm{Im}\langle g, f\rangle} W(f)$$

Since $W(g)$ is unitary, this means that $\mathrm{Spec}(W(f))$ is invariant under rotations, i.e.

$$\mathrm{Spec}(W(f)) = S^1$$

Now: $(W(f) - \mathbb{1})$ is a normal operator with spectrum is :



in particular, its spectral radius is $+2$, so that
$$\| W(f) - \mathbb{1} \| = 2 \qquad \forall f \in \mathcal{H}.$$

- If U_t is the free one-particle dynamics, we define
$$\tau_t(W(f)) := W(U_t f) \qquad t \in \mathbb{R}$$

Then:
$$\begin{aligned}
\| \tau_t(W(f)) - W(f) \| &= \| W(U_t f) W(-f) - 1 \| \\
&= \| e^{-\frac{i}{2} \operatorname{Im} \langle U_t f, f \rangle} W(U_t f - f) - 1 \| \\
&= 2 \quad \text{for all } t \in \mathbb{R},\ U_t f \neq f.
\end{aligned}$$

hence: the free dynamics implemented on the Weyl algebra is not strongly continuous.
$\rightsquigarrow$ $(W(\mathcal{H}), \tau_t)$ is no C^*-dynamical system.

- On Fock space: Let $\mathcal{F}(\mathcal{H})$ be the bosonic Fock space over $\mathcal{H}$, with creation & annihilation operators $a(f)$, $a^*(f)$. Then
$$\tilde{W}(f) := \exp\left(\frac{i}{\sqrt{2}} \left(a(f) + a^*(f) \right) \right), \qquad f \in \mathcal{H}$$
extends to a unitary operator on $\mathcal{F}(\mathcal{H})$ and $\tilde{W}(f), \tilde{W}(g)$ satisfy the Weyl relations, as a consequence of the canonical commutation relations for $a(f), a^*(g)$.

Hence: $\tilde{W}(f)$ form a representation of the Weyl algebra

Now: $t \mapsto \tilde{W}(tf) = \exp\left(it \left(\frac{1}{\sqrt{2}} (a(f) + a^*(f)) \right) \right)$ is strongly continuous on Fock space, i.e.
$$\lim_{t \to 0} \tilde{W}(tf) \Psi = \Psi \qquad \Psi \in \mathcal{F}(\mathcal{H}).$$
(called a regular representation of the Weyl algebra).

- On Fock space let $\mathcal{U}_t$ be the extension of $U_t^{\otimes N}$ defined on each N-particle spaces. Then:

$$\mathcal{U}_t \tilde{W}(f) \mathcal{U}_t^* = \tilde{W}(U_t f)$$

i.e. $\mathcal{U}_t \cdot \mathcal{U}_t^*$ is a unitary implementation of τ_t on Fock space. But then, $\Phi, \Psi \in \mathcal{F}(\mathcal{H})$:

$$\langle \Phi, \mathcal{U}_t \tilde{W}(f) \mathcal{U}_t \Psi \rangle = \langle \mathcal{U}_t \Phi, \tilde{W}(f) \mathcal{U}_t \Psi \rangle$$

is continuous for $t \in \mathbb{R}$,

$\Rightarrow$ $t \mapsto \tilde{W}(U_t f)$ is weakly continuous on $\mathcal{F}(\mathcal{H})$ and $(\tilde{W}(\mathcal{H}), \tau_t)$ is called a W^*-dynamical system.

$$\tau_t = \mathcal{U}_t \cdot \mathcal{U}_t^* .$$

Note: the weak topology does not exist at the level of the abstract algebra, a W^*-dynamical system needs a representation of the C^*-algebra as a (subset of) $\mathcal{B}(\mathcal{H})$, the bounded operators on some Hilbert space.