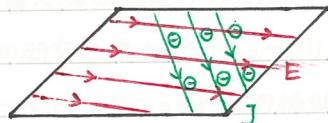


Introduction to an Analytic-Algebraic Approach to Linear Response Theory

1. Heuristic introduction

- Ohm's Law: $R = \frac{U}{I} \Leftrightarrow \vec{J} = \sigma \vec{E} + O(|E|^2)$

\hookrightarrow conductivity



- External parameters, e.g. temperature, magn. field ...
- Heuristically σ is very robust against perturbation \rightsquigarrow macroscopic quantity

Goal of LRT

- derive conductivity laws from microscopic model

$$\cdot J_{E,n}(f, T, B, \dots) = J_{\text{per}, E, n}(f, T, B) - J_{\text{eq}, n}(f, T, B)$$

$$(\text{taylor}) = \underbrace{J_{E,n}|_{E=0}}_0 + \sum_{k=1}^n E_k \underbrace{\frac{\partial}{\partial E_k} J_{E,n}|_{E=0}}_{\sigma_{nk}} + O(|E|)$$

$$= \sum_{k=1}^n \sigma_{nk} E_k + \underbrace{O(|E|)}_{\text{vanishes as } E \rightarrow 0}$$

1.1 Microscopic model

- provides an explicit expression for J_E
- quantum mechanics

Unperturbed systems

- $H = H^*$ on a Hilbert space \mathcal{H}

$\rightsquigarrow H$ is periodic or "periodic on average"

(disorder) $\curvearrowleft p$



- equilibrium state $\rightsquigarrow S$ density operator: $[S, H] = 0$

\rightsquigarrow e.g. $S = P_F$ (Fermi projection) $= \mathbb{1}_{(-\infty, E_F]}(H)$,

$$S = f_T(H), \quad f_T(E) = (1 + e^{-\frac{1}{k}(H - E_F)})^{-1}$$

(Fermi-Dirac distribution)

- \rightsquigarrow Dynamical equation: Liouville eq.

$$\frac{d}{dt} S(t) = -i[H, S(t)], \quad S(t_0) = S \quad (k = 1)$$

- here: $S(t) = S = \text{const}$

- trace-per-unit-volume

$$\mathcal{T}(A) := \lim_{\substack{\Lambda \nearrow \mathbb{R}^d, \mathbb{Z}^d}} \frac{1}{\text{Vol}(\Lambda)} \cdot \text{Tr}(\mathbb{1}_\Lambda(x) A \mathbb{1}_\Lambda(x))$$

$$\mathbb{1}_\Lambda(x) := \begin{cases} 1, & x \in \Lambda \\ 0, & x \notin \Lambda \end{cases}$$

- current observable

$$\frac{d}{dt} X_k = i [H, X_k] =: j_k$$

\uparrow position operator

$$\rightsquigarrow J_{eq,n} := \mathcal{T}(j_k S)$$

Perturbed system

- morally: $H_E = H + E \cdot X$

- Liouville eq.

$$\frac{\partial}{\partial t} S_E(t) = -i [H_E, S_E(t)], S_E(t_0) = S$$

- current operator:

$$\frac{d}{dt} X_k = i [H_E, X_k] =: j_{E,k} \stackrel{\downarrow}{=} j_k$$

here

Net current current density

$$J_E = \underbrace{j_E S_E(t)}_{\substack{\text{current in} \\ \text{perturbed system}}} - \underbrace{\mathcal{T}(j_S)}_{\substack{\text{current in equilibr system} \\ \text{often } = 0}}$$

$$= \sigma E + o(|E|)$$

Kubo formula

- equilibrium state $\rho = P_F$

$$\Rightarrow \sigma_{jn} = -i \mathcal{T}(P_F [\partial_j P_F, \partial_n P_F]) ; \partial_j P_F = i [X_k, P_F]$$

1.2 Why involve algebras

Our motivation

- provide general framework

- works on the continuum and discrete today only
discrete case

$$H = -\frac{1}{2m} (-i \nabla_x)^2 + V$$

\uparrow \uparrow
on $L^2(\mathbb{R}^d)$ on $\ell^2(\mathbb{Z}^d) \otimes \mathbb{C}^N$
unbounded

H bounded operator

$$L^2(\mathbb{R}^d) := \{ \psi: \mathbb{R}^d \mapsto \mathbb{C} \mid \int_{\mathbb{R}^d} dx |\psi(x)|^2 < \infty \}$$

$$\ell^2(\mathbb{Z}^d) := \{ \psi: \mathbb{Z}^d \mapsto \mathbb{C} \mid \sum_{j \in \mathbb{Z}^d} |\psi(j)|^2 < \infty \}$$

- can deal with disorder

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Date

Periodic case

- $H \cong \int_{\mathbb{T}^d} dk \underbrace{H(k)}_{\text{periodic}}$ $H(k) f_n(k) = E_n(k) \varphi_n(k)$

$N \times N$ matrix (tight-binding)

- \downarrow
- $\mathcal{T}(A) = \int_{\mathbb{T}^d} dk \operatorname{Tr}_{\mathbb{C}^N} (A(k))$

- $\sigma_{jn} = -i \int_{\mathbb{T}^d} dk \operatorname{Tr}_{\mathbb{C}^N} (P_F(k) [\partial_{k_j} P_F(k), \partial_{k_n} P_F(k)])$

Random case

- $H = (H_\omega)_{\omega \in \Omega}$, probability space (Ω, P) , covariance

$$T_\gamma H_\omega T_\gamma^{-1} = H_{\omega + \gamma}$$

\uparrow translation by γ

- Assumptions on P (e.g. P is ergodic)

$$\Rightarrow \mathcal{T}(A) = \int_{\Omega} dP(m) \langle \psi_0, A_\omega \psi_0 \rangle = \langle \psi_0, A_\omega \psi_0 \rangle$$

\uparrow with probability 1

$$\psi_0 = (\delta_{y_0}) \in L^2(\mathbb{Z}^d); \psi_0(\gamma) = \begin{cases} 1, & \gamma = 0 \\ 0, & \text{else} \end{cases}$$

\Rightarrow also here: same trace-per-unit-volume

$$\psi_\gamma = T_\gamma \psi_0$$

Both cases

- tons of similarities, common mathematical structures

- $\int \leftrightarrow \mathcal{T}$

- $\partial_{k_j} \leftrightarrow i [X_j, \cdot]$

$\mathcal{T}(j\beta)$ is well-defined $\hat{=} j\beta$ integrable

2 Primer on non-commutative L^p -spaces

- operator algebras with integrability properties

$$L^p(\mathbb{R}^d) = \{f: \mathbb{R}^d \mapsto \mathbb{C} \text{ measurable} \mid \|f\|_p := \left(\int_{\mathbb{R}^d} dx |f(x)|^p \right)^{1/p} < \infty\} / \sim$$

- operator algebra (von Neumann) A

$$\mathcal{L}^1(A) = \{A \in M(A) \mid \|A\|_p := (\mathcal{T}(|A|^p))^{1/p} < \infty\}$$

Derivatives via commutators

Hypothesis

$\{X_1, \dots, X_d\}$ is a collection of self-adjoint operators

(i) Compatible with A : $\forall A \in A : e^{itX_k} A e^{-itX_k} \in A$

(ii) Compatible with \mathcal{T} : $\mathcal{T}(e^{itX_k} A e^{-itX_k}) = \mathcal{T}(A)$

(iii) The X_k strongly commute ($e^{itX_j} e^{isX_k} = e^{isX_k} e^{itX_j}$)

Derivatives ∂_j on A :

$$\partial_j A = \lim_{t \rightarrow 0} \frac{e^{itX_j} A e^{-itX_j} - A}{t}$$

gives rise to

$$\mathcal{C}^n(A) = \{A \in A \mid \partial_1^{k_1} \circ \dots \circ \partial_d^{k_d} A \in A, \text{ for all } |k_1| + \dots + |k_d| \leq n\}$$

ditto on $L^p(A)$

$$\sim \omega^{L^p}(A) := \{A \in L^p(A) \mid \partial_{j_1, \dots, j_d} A \in L^p(A), \text{ for all } j_1, \dots, j_d \text{ such that } \text{limit exists}\}$$

3 LRT the analytic-algebraic way

Hypothesis 1

von Neumann algebra A with finite trace ($\mathcal{T}(1) < \infty$)

3.1 unperturbed system

Hypothesis 2

$H = H^* \in A$ (bounded)

$e^{-itH} \in A \Rightarrow \alpha_t^\circ(A) := e^{-itH} A e^{itH}$ is $*$ -isomorphism on $A, L^p(A)$

~ Solution to Liouville eq: $\rho(t) = \alpha_{t-t_0}^\circ(\rho)$

solves $\frac{d}{dt} \rho(t) = -i[H, \rho(H)], \rho(t_0) = \rho \in L^p(A)$

~ $L_H^{(p)} = -i[H, \cdot]$ on $L^p(A)$

3.2 perturbed case

Hypothesis 3 $\{X_1, \dots, X_d\}$

(i) Compatible with A ; (ii) Compatible with \mathcal{T} ; (iii) Strongly commute

· naively: $\tilde{H}_E := H + E \cdot X$

· better: $H_E := e^{+itE \cdot X} H e^{-itE \cdot X} \in A$

} are weakly equivalent in sense of expectation

if $\tilde{\psi}(t)$ is a weak solution of $i\partial_t \tilde{\psi}(t) = \tilde{H}_E \tilde{\psi}(t), \tilde{\psi}(0) = \phi$,

then $\psi(t) = e^{+itE \cdot X} \tilde{\psi}(t)$ solves $i\partial_t \psi(t) = H_E \psi(t), \psi(0) = \phi$

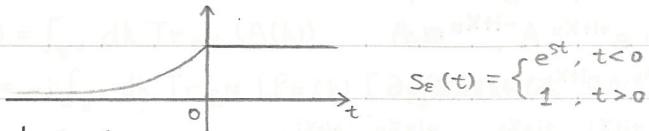
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Adiabatic switching

- slowly switch on perturbation, ramp speed $\sim \epsilon$

$$E \cdot X \rightsquigarrow S_\epsilon(t) E \cdot X$$



Hypothesis 4

$$H_E(t) = G_{\epsilon, E}(t) H G_{\epsilon, E}(t)^*$$

$$G_{\epsilon, E}(t) = e^{+i \int_{-\infty}^t dt S_\epsilon(t)} E \cdot X$$

- at $t = -\infty$: system is at equilibrium

- $t > T > 0$: system is fully perturbed

Current operators

$$j_n = +i [H, X_t] = -i [X_t, H] = -\partial_t H$$

Hypothesis 5

$$H \in C^n(A), n \geq 1 \Rightarrow j_n \in A$$

$$\begin{aligned} j_{\epsilon, E, k}(t) &= -i [H_{\epsilon, E}(t), X_k] = G_{\epsilon, E}(t) (-i [H, X_k]) G_{\epsilon, E}(t)^* \\ &=: \gamma_{\text{int}}^t(j_k) \end{aligned}$$

Perturbed dynamics

$$\frac{d}{dt} \rho_E(t) = -i [H_{\epsilon, E}(t), \rho_E(t)], \rho_E(t_0) = \rho$$

$$\rightsquigarrow \rho_E(t) = \alpha_{t, t_0}^{\epsilon, E}(\rho) := U_{\epsilon, E}(t, t_0) \rho U_{\epsilon, E}(t, t_0)^*$$

Hypothesis 6

$$(i) \rho \in A^+ \cap W^{1,1}(A) \cap W^{1,2}(A)$$

$$(ii) [H, \rho] = 0 \text{ (equilibrium)}$$

3.4 Putting all the pieces together

$$J_{\epsilon, E}(t) = J(j_{\epsilon, E}(t) \rho_{\text{full}}(t)) - J(j\rho); \rho_{\text{full}}(t) = \lim_{s \rightarrow -\infty} \alpha_{t, s}^{\epsilon, E}(\rho) \in A, \mathcal{L}^1(A)$$

$\Rightarrow J_{\epsilon, E}(t)$ well-defined

$$\phi = (\omega) \Psi \quad (\omega) \nabla \phi H = (\omega) \nabla \Psi \quad \text{so value } (\omega) \tilde{\Psi} \quad X \cdot \nabla \tilde{\Psi} \quad \phi = (\omega) \tilde{\Psi}$$