From the 2nd Law to AC–Conductivity Measures of Interacting Fermions in Disordered Media

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Based on:

"Heat Production of Non-Interacting Fermions Subjected to Electric Fields" (Comm. Pure Appl. Math. 2014)
"Microscopic Conductivity of Lattice Fermions at Equilibrium – Part I: Non–Interacting Particles" (J. Math. Phys. 2015)
"AC-Conductivity Measure from Heat Production of Free Fermions in Disordered Media" (Arch. Rat. Mech. Anal. 2015)
"Macroscopic Conductivity of Free Fermions in Disordered Media" (Rev. Math. Phys. 2014)
"Lieb–Robinson Bounds for Multi–Commutators and Applications to Response Theory" (preprint mp-arc 15-118)
"Microscopic Conductivity of Lattice Fermions at Equilibrium – Part II: Interacting Particles" (Lett. Math. Phys. 2015)
"From the 2nd Law to AC–Conductivity Measures of Interacting Fermions in Disordered Media" (M3AS, 2015)
"Microscopic Foundations of Ohm and Joule's Laws" (Proceedings of QMATH12)

Preliminary Remarks

- Ohm-Joule's laws are among the most resilient laws of (classical) electricity theory.
- Their microscopic origin is still not completely understood (at least from a mathematical perspective).
- Indeed, Ohm's law is not only valid at macroscopic scales, but also at the atomic scale for purely quantum systems (2012). Such a behavior was unexpected:

> "...In the 1920s and 1930s, it was expected that classical behavior would operate at macroscopic scales but would break down at the microscopic scale, where it would be replaced by the new quantum mechanics. The pointlike electron motion of the classical world would be replaced by the spread out quantum waves. These quantum waves would lead to very different behavior. ... Ohm's law remains valid, even at very low temperatures, a surprising result that reveals classical behavior in the **quantum** regime."
>
> [D.K. Ferry, *Science* **335**(6064), 45 (2012)]

Preliminary Remarks

- This work is inspired by [1] (see also [2,3]) where an AC–conductivity measure has been introduced for the first time in 2007:

For the Anderson model in presence of electric field $E(t)$ constant in space, there exists, with probability 1, a "conductivity measure" μ such that, if $\hat{E}$ is compactly supported, then the expected (in–phase) component of the velocity $v(t)$ of the electron obeys:

$$v(t) = \int \hat{E}(\nu) e^{i\nu t} \mathrm{d}\mu(\nu),$$

at leading order in E. Initial condition: Fermi-Dirac "density matrix" at $t = -\infty$.

[1] A. Klein, O. Lenoble, P. Müller, *Annals of Mathematics* (2007).

[2] A. Klein, P. Müller, *J. of Mathematical Physics, Analysis, Geometry* (2008).

[3] J.-M. Bouclet, F. Germinet, A. Klein, J.H. Schenker, *J. of Funct. Anal.* (2005).

Preliminary Remarks

- [4] is another example on free fermions proving Ohm's law for graphene–like materials subjected to space–homogeneous and time–periodic electric fields. See also works of V. Jakšić, Y. Ogata and C.-A. Pillet on linear response theory.

- We propose a different approach to the conductivity measure based on the 2nd law of thermodynamics saying that systems at equilibrium are unable to perform mechanical work in cyclic processes.

  It is related to Joule's law for the heat production of conducting media in presence of currents.

- We use the second quantized setting such that interacting systems can also be considered.

[4] M.H. Brynildsen, H.D. Cornean, Rev. Math. Phys. 25(4) (2013) 1350007.

Algebraic Formulation of Quantum Mechanics

- Let $\mathcal{U}$ be some C^*–algebra. Observables are self–adjoint elements of $\mathcal{U}$.
- States on $\mathcal{U}$ are $\rho \in \mathcal{U}^*$ so that $\rho(\mathbf{1}) = 1$ and $\rho(A^* A) \geq 0$ for all $A \in \mathcal{U}$.
- Dynamics: strongly continuous group $\tau \equiv \{\tau_t\}_{t \in \mathbb{R}}$ of $*$–automorphisms of $\mathcal{U}$ with generator δ.
- If the state of the system at $t = t_0 \in \mathbb{R}$ is $\rho \in \mathcal{U}^*$, then it evolves as $\rho_t = \rho \circ \tau_t$ for any $t \geq t_0$.
- For any differential family $\{A_t\}_{t \geq t_0} \subset \mathcal{U}$ of observables, one produces some "excitation" by perturbing the dynamics:

  $$\forall\ t \geq t_0 : \quad \partial_t \tau_{t,t_0}(B) = \tau_{t,t_0}(\delta(B) + i[A_t, B]), \quad \tau_{t_0,t_0}(B) := B \in \mathcal{U} .$$

  The state of the system evolves now as $\rho_t = \rho \circ \tau_{t,t_0}$ for any $t \geq t_0$.
- Work performed by the external device at time $t_1 \geq t_0$:

  $$\mathfrak{Q}_\rho(A) := \int_{t_0}^{t_1} \rho \circ \tau_{t,t_0}(\partial_t A_t)\, \mathrm{d}t .$$

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Thermal Equilibrium States

2^{nd} LAW OF THERMODYNAMICS:

- [LY99]: "*one of the most perfect laws in physics*". It has never been faulted by reproducible experiments.
- Kelvin-Planck statement: *Systems at equilibrium are unable to do mechanical work in cyclic processes.*

ALGEBRAIC FORMULATION OF THE 2^{nd} LAW:

- A cyclic process is by definition a differential family $\{A_t\}_{t\geq t_0} \subset \mathcal{U}$ of observables such that $A_{t\geq t_1} = 0$ for some $t_1 \geq t_0$.
- A state $\rho \in \mathcal{U}^*$ is at equilibrium iff the full work $\mathcal{Q}_\rho(A) \geq 0$ for any cyclic process $\{A_t\}_{t\geq t_0} \subset \mathcal{U}$. (Passivity [PW78])
- A state $\varrho \in \mathcal{U}^*$ is at thermal equilibrium iff $\otimes_{j=1}^n \varrho$ is a passive state of $(\mathcal{U}, \tau, \varrho)^n$ for all $n \in \mathbb{N}$. (Complete Passivity [PW78])

Theorem (Pusz–Woronowicz)

ϱ is a thermal equilibrium state iff it is a (τ, β)–KMS state for some $\beta \in [0, \infty]$.

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Interacting Lattice Fermions in Disordered Media

- Host material for conducting fermions: a cubic crystal $\mathfrak{L} := \mathbb{Z}^d$ ($d \in \mathbb{N}$).

- Infinite system of charged fermions: Let $\mathcal{U}$ be the CAR C^*–algebra of the infinite system generated by the identity $\mathbf{1}$ and creation/annihilation operators $\{a_x^*, a_x\}_{x\in\mathfrak{L}}$ satisfying the CAR:

$$a_x a_y + a_y a_x = 0 \ , \qquad a_x a_y^* + a_y^* a_x = \delta_{x,y}\mathbf{1} \ .$$

- Disorder in the crystal modeled by a random external potential coming from a probability space $(\Omega, \mathfrak{A}_\Omega, \mathfrak{a}_\Omega)$ with $\Omega := [-1,1]^{\mathfrak{L}}$.

- Interparticle forces are represented by a two–body potential $v : \mathbb{R}_0^+ \to \mathbb{R}$ from a (Banach) space of short range interactions.

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Electromagnetic Fields

- Electromagnetic potential:

$$\mathbf{A} \equiv \mathbf{A}(t,x) \in \mathbf{C}_0^\infty := \bigcup_{l \in \mathbb{R}^+} C_0^\infty(\mathbb{R} \times [-l,l]^d ; (\mathbb{R}^d)^*) \ .$$

- Electric field in the Weyl gauge: For $\mathbf{A} \in C_0^\infty(\mathbb{R} \times [-l,l]^d ; (\mathbb{R}^d)^*)$ and all $t \in \mathbb{R}$:

$$E_{\mathbf{A}}(t,x) := -\frac{\mathrm{d}\mathbf{A}}{\mathrm{d}t}(t,x) \text{ if } x \in [-l,l]^d \quad \text{and} \quad E_{\mathbf{A}}(t,x) := 0 \text{ else.}$$

- Cyclic electromagnetic process (AC): Since $\mathbf{A} \in \mathbf{C}_0^\infty$, there are $t_0 \leq t_1$ such that

$$\mathbf{A}(t,x) = 0 \quad \text{for all } t \notin [t_0, t_1] \text{ and } x \in \mathbb{R}^d \ .$$

  In particular, one has AC-electric fields:

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Dynamics

- d–dimensional discrete Laplacian $\Delta_{\mathrm{d}} \in \mathcal{B}(\ell^2(\mathfrak{L}))$ (up to a minus sign).

- Electromagnetic discrete Laplacian $\Delta_{\mathrm{d}}^{(\mathbf{A})} \in \mathcal{B}(\ell^2(\mathfrak{L}))$ (up to a minus sign):

$$\langle \mathfrak{e}_x, \Delta_{\mathrm{d}}^{(\mathbf{A})} \mathfrak{e}_y \rangle = \exp\left(i \int_0^1 [\mathbf{A}(t, \alpha y + (1-\alpha)x)]\,(y-x)\mathrm{d}\alpha \right) \langle \mathfrak{e}_x, \Delta_{\mathrm{d}} \mathfrak{e}_y \rangle$$

  for all $x, y \in \mathfrak{L}$, where $\{\mathfrak{e}_x\}_{x\in\mathfrak{L}}$ is the orthonormal basis $\mathfrak{e}_x(y) \equiv \delta_{x,y}$ of $\ell^2(\mathfrak{L})$.

- For $\omega \in \Omega$, there is a unique two–parameter family $\{\tau_{t,s}^{(\omega)}\}_{s,t\in\mathbb{R}}$ of automorphisms of $\mathcal{U}$ formally generated by the commutator $i[H(t), \cdot]$ ("Heisenberg picture") with

$$H(t) := \sum_{x,y\in\mathfrak{L}} \langle \mathfrak{e}_x, \Delta_{\mathrm{d}}^{(\mathbf{A})} \mathfrak{e}_y \rangle a_x^* a_y + \lambda \sum_{x\in\mathfrak{L}} \omega(x) n_x + \sum_{x,y\in\mathfrak{L}} v(|x-y|) n_x n_y,$$

  where $n_x := a_x^* a_x$ is the density operator at lattice site $x \in \mathfrak{L}$.

- For any $\omega \in \Omega$, the automorphism group with $\mathbf{A} \equiv \mathbf{0}$ is denoted by $\tau^{(\omega)}$.

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- For $\omega \in \Omega$, there is a unique two–parameter family $\{\tau_{t,s}^{(\omega)}\}_{s,t\in\mathbb{R}}$ of automorphisms of $\mathcal{U}$ formally generated by the commutator $i[H(t), \cdot]$ ("Heisenberg picture") with

$$H(t) := \sum_{x,y\in\mathfrak{L}} \langle \mathfrak{e}_x, \Delta_{\mathrm{d}}^{(\mathbf{A})} \mathfrak{e}_y \rangle a_x^* a_y + \lambda \sum_{x\in\mathfrak{L}} \omega(x) n_x + \sum_{x,y\in\mathfrak{L}} v(|x-y|) n_x n_y ,$$

  where $n_x := a_x^* a_x$ is the density operator at lattice site $x \in \mathfrak{L}$.

- For any $\omega \in \Omega$, the automorphism group with $\mathbf{A} \equiv \mathbf{0}$ is denoted by $\tau^{(\omega)}$.

Dynamics

- d–dimensional discrete Laplacian $\Delta_{\mathrm{d}} \in \mathcal{B}(\ell^2(\mathfrak{L}))$ (up to a minus sign).

- Electromagnetic discrete Laplacian $\Delta_{\mathrm{d}}^{(\mathbf{A})} \in \mathcal{B}(\ell^2(\mathfrak{L}))$ (up to a minus sign):

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Time–Evolving State

- For all $\omega \in \Omega$, $\rho^{(\omega)}$ is a thermal equilibrium state (2nd law of Thermodynamics).
- In particular, for any cyclic process $\{A_t\}_{t\geq t_0} \subset \mathcal{U}$, the full work $\mathcal{Q}^{(\omega)}(A) \geq 0$.
- By the Pusz-Woronowicz theorem, it means that $\rho^{(\omega)}$ is a $(\tau^{(\omega)}, \beta)$–KMS state for some $\beta \in [0, \infty]$.
- $\beta \in [0, \infty]$ is named *inverse temperature* and results from the 2nd law. It fixes a time scale since ϱ is a (τ_t, β)–KMS state iff ϱ is a $(\tau_{\beta t}, 1)$–KMS state.
- For all $\omega \in \Omega$ and thermal equilibrium state $\rho^{(\omega)}$, define the time–evolving states $\rho_t^{(\omega)}$, $t \in \mathbb{R}$, by:

$$\rho_t^{(\omega)} := \rho^{(\omega)} \circ \tau_{t,t_0}^{(\omega)}.$$

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Genesis of Ohm and Joule's laws

- G.S. Ohm was born in 1789 in Erlangen and is son of a master locksmith.
- Being teacher of mathematics and physics in Cologne, he had been able to elaborate his own experiments on electrical resistivity.
- Inspired by Fourier's theory of heat (1822), he published his famous theory (1827), which was a theoretical deduction of his law from "*first principles*". His theory was at best completely ignored and at worst treated really negatively:

  Ohm's theory, to quote one critic, was "a web of naked fancies", which could never find the semblance of support from even the most superficial observation of facts; "he who looks on the world", proceeds the writer, "with the eye of reverence must turn aside from this book as the result of an incurable delusion, whose sole effort is to detract from the dignity of nature".

- Although at the origin of Ohm's intuition, the relation between heat and electrical conduction has not been established by himself, but J.P. Joule (born in 1818).
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1st Law of Thermodynamics

- Full heat produced by the cyclic electromagnetic process $\mathbf{A} \in \mathbf{C}_0^\infty$:

$$\mathcal{H}^{(\omega)}(\mathbf{A}) := \beta^{-1} S(\rho_{t_1}^{(\omega)}, \rho_{t_0}^{(\omega)}) \in [0, \infty] ,$$

where $S(\rho, \rho')$ is Araki's relative entropy of ρ w.r.t. ρ'.

- Full work of the cyclic electromagnetic process $\mathbf{A} \in \mathbf{C}_0^\infty$:

$$\mathcal{Q}^{(\omega)}(\mathbf{A}) := \int_{t_0}^{t_1} \rho_t^{(\omega)}(\partial_t A_t^{(\mathbf{A})}) \mathrm{d}t \in [0, \infty) .$$

Theorem (Bru-dSP-K – 1st Law)

For any $\mathbf{A} \in \mathbf{C}_0^\infty$ and $\omega \in \Omega$, one has:

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Heat production – Quadratic Response

- For simplicity, consider electromagnetic potentials $\mathbf{A}$ of the form

$$\mathbf{A}_{\eta,l}(t,x) := \eta A(t)\mathbf{1}[x \in [-l/2, l/2]^d]\mathbf{w},$$

where $\eta, l > 0$, $A \in C_0^\infty(\mathbb{R},\mathbb{R})$, and $\mathbf{w}$ is a unit vector in $\mathbb{R}^d$.

- The full heat production or electromagnetic work per unit volume equals

$$\mathcal{Q}_{\eta,l}^{(\omega)} := l^{-d}\mathcal{Q}^{(\omega)}\left(\mathbf{A}_{\eta,l}\right) = l^{-d}\mathcal{H}^{(\omega)}\left(\mathbf{A}_{\eta,l}\right) \in [0,\infty) \ ,$$

Theorem (Bru-dSP – Quadratic response of the heat production)

If $\eta > 0$ is sufficiently small, then there is $Q_l^{(\omega)}$ not depending on η, such that, uniformly w.r.t. to $l > 0$ and $\omega \in \Omega$:

$$\mathcal{Q}_{\eta,l}^{(\omega)} = \eta^2 Q_l^{(\omega)} + \mathcal{O}(\eta^3) \ .$$

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Microscopic AC–Conductivity Measure

- For all smooth electric fields $E = -\partial_t A$ satisfying the AC-condition

$$\int_{\mathbb{R}} E(s)\,\mathrm{d}s = 0 \in \mathbb{R}^d \ ,$$

we have

$$Q_l^{(\omega)} = \frac{1}{2}\int_{\mathbb{R}} \mathrm{d}s \int_{\mathbb{R}} \mathrm{d}t \ \left\langle E(s), \boldsymbol{\Xi}_l^{(\omega)}(t-s)\,E(t)\right\rangle_{\mathbb{R}^d}$$

- By the 2nd law, $Q_l^{(\omega)} \geq 0$ for any $E \in C_0^\infty(\mathbb{R};\mathbb{R}^d)$ and $\boldsymbol{\Xi}_l^{(\omega)} \in C(\mathbb{R};\mathcal{B}(\mathbb{R}^d))$ is conditionally positive definite (or negative definite in the sense of Schoenberg).

- Therefore, there is a Lévy-Khintchine representation of $\boldsymbol{\Xi}_l^{(\omega)}$ with Lévy measure $\mu_l^{(\omega)}$ on $\mathbb{R}\backslash\{0\}$ and

$$Q_l^{(\omega)} = \int_{\mathbb{R}\backslash\{0\}} \mathrm{d}\mu_l^{(\omega)}(\nu)|\hat{E}(\nu)|^2 \ ,$$

where $\hat{E}$ is the Fourier transforms of E with support outside $\nu = 0$.

- $\mu_l^{(\omega)}$ is the (microscopic) AC–conductivity measure we are looking for.

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Conductivity Measure and Joule's Law

By the 1st law, the quantity

$$\mathrm{d}\mu_l^{(\omega)}(\nu)|\hat{E}(\nu)|^2$$

is the heat production due to the component $\hat{E}(\nu)$ of frequency ν of the electric field E, in accordance with Joule's law:

> "...the calorific effects of equal quantities of transmitted electricity are proportional to the resistances opposed to its passage, whatever may be the length, thickness, shape, or kind of metal which closes the circuit: and also that, coeteris paribus, these effects are in the duplicate ratio of the quantities of transmitted electricity; and consequently also in the duplicate ratio of the velocity of transmission."
>
> [Joule, 1840]

We have verified this by using the Legendre–Fenchel transform $Q_l^{(\omega)*}$ of the map

$$E \mapsto Q_l^{(\omega)} = \int_{\mathbb{R}} \mathrm{d}\mu_l^{(\omega)}(\nu)|\hat{E}(\nu)|^2$$

w.r.t. a convenient dual pair.

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Random Time–Evolving State

- We say that $\{\rho^{(\omega)}\}_{\omega\in\Omega}$ is a random thermal equilibrium state if:

  (i) For all $\omega \in \Omega$, $\rho^{(\omega)}$ is a thermal equilibrium state (2nd law) with inverse temperature β.

  (ii) The map $\omega \mapsto \rho^{(\omega)}$ is measurable w.r.t. the (Borel) σ–algebra generated by the weak* topology for states.

- Let $\{\rho^{(\omega)}\}_{\omega\in\Omega}$ be a random equilibrium state and define the (random) time–evolving states $\rho_t^{(\omega)}$, $t \in \mathbb{R}$, by:

$$\rho_t^{(\omega)} := \rho^{(\omega)} \circ \tau_{t,t_0}^{(\omega)}.$$

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Macroscopic AC–Conductivity Measure

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for all smooth electric fields E satisfying the AC-condition almost surely survives the limit $l \to \infty$. There is a limiting non–random AC-conductivity measure μ_∞, as $l \to \infty$, as some Lévy measure.

Theorem (Existence of the macroscopic cond. measure)

Assume that the random external potential $\omega \in \Omega$ is ergodic.

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Final Remarks

- For finite l, the conductivity measure $\mu_l^{(\omega)}$ is finite, has finite first moment and is strictly positive.
- $\mu_l^{(\omega)}$ can be identified with the spectral measure of the Liouvillean of the system w.r.t. to an explicit vector in the GNS representation of the equilibrium state $\rho^{(\omega)}$.
- μ_∞ is the trivial measure if $v = \lambda = 0$ (i.e., no disorder and no interparticle forces, perfect conductor case) or in the limit $\lambda \to \infty$ ($v = 0$, perfect insulator case), but is strictly positive, in general.
- Green–Kubo relations: If the fluctuations of the current w.r.t. $\rho^{(\omega)}$ converge to a finite value as $l \to \infty$, then μ_∞ is the Fourier transform of the time correlation of (bosonic) fields w.r.t. the vacuum of the Fock representation of the corresponding CCR algebra of current fluctuations.
- $\mu_l^{(\omega)}$ and μ_∞ determine the current linear response in accordance with Ohm's law.
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