Some Thoughts about *“Approach to Equilibrium”*

A joint work with Vojkan Jakšić (McGill) and Clément Tauber (Strasbourg)

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Mathematical physics: new developments and perspectives (Jan’s 65th)

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Introduction

Approach to Equilibrium

Uhlenbeck-Ford, Lectures in Statistical Mechanics (1963)

3. The approach to equilibrium; the ideas of Boltzmann. How can one "explain" the irreversible behaviour of macroscopic systems from the strictly reversible mechanical model? This question, which I call the problem of Boltzmann, has dominated the whole initial development of statistical mechanics and it is still being discussed. In its simplest form, one must "explain" in which sense an isolated (that is a conservative) mechanical system consisting of a very large number of molecules approaches thermal equilibrium, in which all "macroscopic" variables have reached steady values. This is sometimes called the *zeroth law of thermodynamics* and it expresses the most typical irreversible behaviour of macroscopic systems familiar from common observation.

Approach to Equilibrium & The Second Law

J. Uffink: Bluff your Way in the Second Law of Thermodynamics.
Stud. Hist. Phil. Mod. Phys. 32 (2001).

It is often said that this behaviour of thermodynamical systems (i.e. the approach to equilibrium) is accompanied by an increase of entropy, and a consequence of the second law. But this idea actually lacks a theoretical foundation: for a non-equilibrium state there is in general no thermodynamic entropy –or temperature– at all. We get no further than where Clausius was in 1864 (see page 28): the second law cannot be seen as a statement about the quantities of the system, but also involves its environment. Planck (1897, § 112) too emphasised that the approach to equilibrium has nothing to do with the second law. This aspect of time-asymmetry is woven much deeper in the theory.

Approach to Equilibrium vs. Return to Equilibrium

Commun. math. Phys. 31, 171—189 (1973)

Return to Equilibrium

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Received October 24, 1972

Abstract. The problem of return to equilibrium is phrased in terms of a C^*-algebra $\mathfrak{A}$, and two one-parameter groups of automorphisms τ, τ^P corresponding to the unperturbed and locally perturbed evolutions. The asymptotic evolution, under τ, of τ^P-invariant, and τ^P-K.M.S., states is considered. This study is a generalization of scattering theory and results concerning the existence of limit states are obtained by techniques similar to those used to prove the existence, and intertwining properties, of wave-operators. Conditions of asymptotic abelianness provide the necessary dispersive properties for the return to equilibrium. It is demonstrated that the τ^P-equilibrium states and their limit states are coupled by automorphisms with a quasi-local property; they are not necessarily normal with respect to one another. An application to the $X-Y$ model is given which extends previously known results and other applications, and examples, are given for the Fermi gas.

I. Introduction

We examine general properties of systems whose dynamics have been locally perturbed and illustrate these properties with examples. Our specific interest is whether systems, that have been perturbed in this manner, return to equilibrium under the unperturbed evolution. In this context we consider the behaviour of states which are invariant, or satisfy the K.M.S. condition, for the perturbed dynamics. We demonstrate that this type of problem is tractable with methods which are a natural generalization of scattering theory.

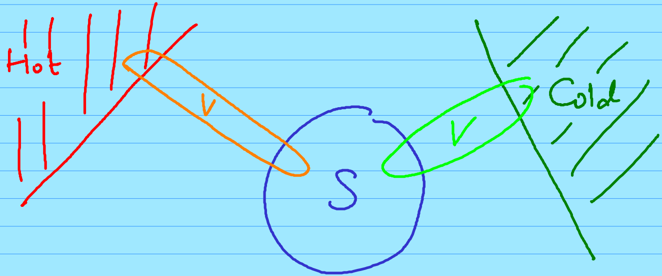
Nonequilibrium Quantum Statistical Mechanics

More recent results (last 25 years) inspired by some deep papers by Ruelle and Gallavotti–Cohen from the mate 90':

- Return to equilibrium for physically relevant models (major contributions by Jan on Pauli-Fierz models).
- Relaxation to non-equilibrium steady states.
- Linear response theory à la Green-Kubo, fluctuation–dissipation.
- Strict positivity of entropy production.
- Repeated measurements and fluctuation relations.
- ...

Nonequilibrium Quantum Statistical Mechanics

Typical configuration: multiple reservoirs, individually in equilibrium, connected to a finite system S



Decoupled dynamics $\tau^t = e^{t\delta}$

Local perturbation $V = V^*$

Coupled dynamics $\tau_V^t = e^{t\delta_V}$, $\delta_V = \delta + i[V, \cdot]$

Most of these results follow the algebraic approach developed in the 70', which provides a rich framework and allows to derive very general, model independent, structural properties. Emblematic example is the entropy balance

$$0 \leq S(\omega \circ \tau_V^t | \omega) = \int_0^t \omega \circ \tau_V^s (\delta_\omega(V)) ds$$

which gives a way to identify entropy production

$$\sigma = \delta_\omega(V)$$

as a quantity related to the underlying modular structure, and deduce its basic properties.

Nonequilibrium Steady States (NESS) are w^*-limit points of the net

$$\overline{\omega}_T = \frac{1}{T}\int_0^T \omega \circ \tau_V^t \, dt$$

and any such NESS ω_+ satisfies

$$\omega_+(\sigma) \geq 0 .$$

However strict positivity of entropy production

$$\omega_+(\sigma) > 0$$

which is related to the singularity of ω_+ w.r.t. ω, can only be achieved in concrete models or under generic conditions.

Approach to equilibrium is more delicate. To our knowledge the only results are either:

- Derivations of a Quantum Boltzmann equation under appropriate closure assumptions (Hugenholtz 1983, Ho-Landau 1997, Erdős-Salmhofer-Yau 2004).

- Concerning quasi-free fermions (which enforces closure) (Lanford-Robinson 1972).

We won't add much to this short list, but..

Framework

Framework

Toolbox: Quantum Spin Systems

- Ruelle: Statistical Mechanics: Rigorous Results
- Bratteli-Robinson: Operator Algebras and Quantum Statistical Mechanics 2
- Israel: Convexity in the Theory of Lattice Gases

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Finite Systems

- $\mathcal{F}$ is the set of finite subsets of the lattice $\mathbb{Z}^d$.
- For $x \in \mathbb{Z}^d$, $\mathcal{H}_x = \mathbb{C}^m$.
- For $\Lambda \in \mathcal{F}$, $\mathcal{H}_\Lambda = \otimes_{x \in \Lambda} \mathcal{H}_x$,
- and $\mathfrak{A}_\Lambda = \mathcal{L}(\mathcal{H}_\Lambda)$ is the C^*-algebra of physical observables.
- States: $\mathfrak{A}_\Lambda \ni A \mapsto \mathrm{tr}_{\mathcal{H}_\Lambda}(\rho A)$.
- von Neumann entropy

$$S(\rho) = -\mathrm{tr}_{\mathcal{H}_\Lambda}(\rho \log \rho) \in [0, m|\Lambda|],$$

and relative entropy

$$S(\rho|\rho_0) = \begin{cases} \mathrm{tr}_{\mathcal{H}_\Lambda}(\rho(\log \rho - \log \rho_0)) \geq 0 & \text{if } \mathrm{Ran}\,\rho \subset \mathrm{Ran}\,\rho_0, \\ +\infty & \text{otherwise.} \end{cases}$$

Framework

Thermodynamic (van Hove) Limit

- Natural isometric injection $\mathfrak{A}_\Lambda \subset \mathfrak{A}_{\Lambda'}$ for $\Lambda \subset \Lambda'$.
- $\mathfrak{A}_{\mathrm{fin}} = \cup_{\Lambda \in \mathcal{F}} \mathfrak{A}_\Lambda \rightsquigarrow$ quasi-local spin algebra $\mathfrak{A} = \overline{\mathfrak{A}_{\mathrm{fin}}}^{\|\ \|}$.
- Natural group action (translations) $\varphi : \mathbb{Z}^d \to \mathrm{Aut}(\mathfrak{A})$.
- Set of states $\mathcal{S}(\mathfrak{A})$, of translation-invariant states $\mathcal{S}_I(\mathfrak{A})$.
- Restriction to finite box $\Lambda = [-l, l]^d \in \mathcal{F}$:

$$\mathcal{S}(\mathfrak{A}) \ni \rho \mapsto \rho_\Lambda \in \mathcal{S}(\mathfrak{A}_\Lambda).$$

- Mean entropy

$$\mathcal{S}_I(\mathfrak{A}) \ni \rho \mapsto s(\rho) = \lim_{\Lambda \uparrow \mathbb{Z}^d} \frac{S(\rho_\Lambda)}{|\Lambda|} \in [0, m],$$

  is an affine weak*-upper semicontinuous function.
- Mean relative entropy

$$s(\rho|\rho_0) = \lim_{\Lambda \uparrow \mathbb{Z}^d} \frac{S(\rho_\Lambda|\rho_{0\Lambda})}{|\Lambda|} \geq 0,$$

  whenever it exists. $s(\rho|\rho_0) = 0 \not\Rightarrow \rho = \rho_0$.

Framework

Interactions

- $\mathcal{B}^r$ the set of **translation invariant** interactions $\Phi = \{\Phi(X)\}_{X \in \mathcal{F}}$

$$\Phi(X) = \Phi(X)^* \in \mathfrak{A}_X, \qquad \Phi(X + x) = \varphi^x(\Phi(X)),$$

  such that for some $r > 0$,

$$\|\Phi\|_r = \sum_{X \ni 0} \|\Phi(X)\| \, \mathrm{e}^{r(|X|-1)} < \infty.$$

- Local Hamiltonian for $\Lambda \in \mathcal{F}$

$$H_\Lambda(\Phi) = \sum_{X \subset \Lambda} \Phi(X).$$

- Mean energy

$$E_\Phi = \sum_{X \ni 0} \frac{\Phi(X)}{|X|}, \qquad \rho(E_\Phi) = \lim_{\Lambda \uparrow \mathbb{Z}^d} \frac{\rho(H_\Lambda(\Phi))}{|\Lambda|}$$

  for $\rho \in \mathcal{S}_I(\mathfrak{A})$.

Framework

Thermodynamics

- Pressure at inverse temperature β

$$P(\beta\Phi) = \lim_{\Lambda \uparrow \mathbb{Z}^d} \frac{1}{|\Lambda|} \log \mathrm{tr}\left(\mathrm{e}^{-\beta H_\Lambda(\Phi)}\right).$$

- Gibbs variational principle [Robinson,Lanford (1967-68)]

$$P(\beta\Phi) = \sup_{\rho \in \mathcal{S}_I(\mathfrak{A})} \left(s(\rho) - \beta\rho(E_\Phi)\right)$$

  Maximizers are *Equilibrium States* for the interaction $\beta\Phi$.

- $\mathcal{S}_{\mathrm{eq}}(\beta\Phi)$ is the set of these equilibrium states. It is a non-empty weak*-compact face of $\mathcal{S}_I(\mathfrak{A})$ and a simplex whose extremal points are extremal translation-invariant states.

Framework

Dynamics & KMS States

- Dynamics $\mathbb{R} \to \mathrm{Aut}(\mathfrak{A})$ is defined as

$$\alpha_\Phi^t(A) = \lim_{\Lambda \uparrow \mathbb{Z}^d} \mathrm{e}^{\mathrm{i}tH_\Lambda(\Phi)} A\, \mathrm{e}^{-\mathrm{i}tH_\Lambda(\Phi)},$$

  and $\mathcal{S}_\Phi(\mathfrak{A})$ demotes the set of α_Φ-invariant states.

- *Thermal equilibrium states* for α_Φ are characterized by the KMS-condition [Haag–Hugenholtz–Winninck 1967]: $\rho \in \mathcal{S}(\mathfrak{A})$ is (α_Φ, β)-KMS if, for all $A, B \in \mathfrak{A}$, the function

$$\mathbb{R} \ni t \mapsto F_{A,B}(t) = \rho(\alpha_\Phi^t(A)B)$$

  has an extension analytic in the strip $\{z \in \mathbb{C} \mid 0 < \mathrm{Im}(z) < \beta\}$, bounded and continuous on its closure, and satisfying the Kubo–Martin–Schwinger boundary condition

$$F_{A,B}(t + \mathrm{i}\beta) = \rho(B\alpha_\Phi^t(A)).$$

  Any (α_Φ, β)-KMS state is α_Φ-invariant.

- $$\rho \in \mathcal{S}_{\mathrm{eq}}(\beta\Phi) \quad \Longleftrightarrow \quad \rho \in \mathcal{S}_I(\mathfrak{A}) \text{ is } (\alpha_\Phi, \beta)\text{-KMS}.$$

Framework

In the following we set $\beta = 1$

Enforcing translation invariance

$\Downarrow$

all local observables are **macro**

Equilibrium Steady States

Equilibrium Steady States

Definition

For $\rho \in \mathcal{S}_l(\mathfrak{A})$, $\Phi \in \mathcal{B}^r$ and $T > 0$ let

$$\overline{\rho}_T = \frac{1}{T} \int_0^T \rho \circ \alpha_\Phi^t \mathrm{d}t,$$

and denote by $\mathcal{S}_+(\rho, \Phi)$ the set of weak*-limit points of the net $(\overline{\rho}_T)_{T>0}$.

Elements of $\mathcal{S}_+(\rho, \Phi)$ are called Equilibrium Steady State (ESS) associated to the initial state ρ and the interaction Φ.

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- Clearly $\mathcal{S}_+(\rho, \Phi)$ is a non-empty subset of $\mathcal{S}_I(\mathfrak{A}) \cap \mathcal{S}_\Phi(\mathfrak{A})$.
- When do we have approach to equilibrium in the sense: $\mathcal{S}_+(\rho, \Phi) \subset \mathcal{S}_{\mathrm{eq}}(\Phi)$?
- When is $\mathcal{S}_+(\rho, \Phi)$ a singleton, *i.e.,* $\overline{\rho}_T \to \rho_+$?
- More generally: What are the properties of ESS following from this definition and not depending on details of ρ and Φ ?

Approach to equilibrium – the Second Law – time's arrow

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A Question of Ruelle

It is unclear to the author whether the evolution of an infinite system should increase its entropy per unit volume. Another possibility is that, when the time tends to ∞, a state has a limit with strictly larger entropy.

David Ruelle (1967)

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Conservation Laws

For any $\rho \in \mathcal{S}_I(\mathfrak{A})$, any $\Phi \in \mathcal{B}^r$ and any $T, t \in \mathbb{R}$, the following hold:

- **Mean Entropy** [Lanford–Robinson 1968].

$$s(\overline{\rho}_T) = s(\rho \circ \alpha_\Phi^t) = s(\rho).$$

- **Mean Energy** [Jakšić–P–Tauber 2022].

$$\overline{\rho}_T(E_\Phi) = \rho \circ \alpha_\Phi^t(E_\Phi) = \rho(E_\Phi).$$

Consequently, (semi-)continuity gives that for any $\rho_+ \in \mathcal{S}_+(\rho, \Phi)$,

$$s(\rho_+) \geq s(\rho), \qquad \rho_+(E_\Phi) = \rho(E_\Phi).$$

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Theorem 1

If approach to equilibrium holds non-trivially, *i.e.*, $\rho \notin \mathcal{S}_\Phi(\mathfrak{A})$ and $\rho_+ \in \mathcal{S}_{\mathrm{eq}}(\Phi)$, then

$$s(\rho_+) > s(\rho).$$

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Proof. Suppose $s(\rho_+) = s(\rho)$, then the variational principle gives

$$P(\Phi) = s(\rho_+) - \rho_+(E_\Phi) = s(\rho) - \rho(E_\Phi)$$

so

$$\rho \in \mathcal{S}_{\mathrm{eq}}(\Phi) \subset \mathcal{S}_\Phi(\mathfrak{A}),$$

a contradiction. □

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a contradiction. □

- Strict increase of the mean entropy $\Rightarrow$ irreversibility.
- This is a conditional result. The only known examples are [Emch-Radin 1970, Lanford-Robinson 1971]. We are seeking unconditional results!

Approach to equilibrium – the Second Law – time's arrow

Weak Gibbs states were introduced in classical dynamical systems by [Yuri 2002]. To our knowledge, they did not appear previously in the quantum context.

Definition

A state $\rho \in \mathcal{S}_I(\mathfrak{A})$ is weak Gibbs for the interaction $\Phi \in \mathcal{B}^r$ whenever, for any finite box $\Lambda = [-l, l]^d \in \mathcal{F}$, there exists a constant C_Λ such that

$$C_\Lambda^{-1} \frac{\mathrm{e}^{-H_\Lambda(\Phi)}}{\mathrm{tr}\left(\mathrm{e}^{-H_\Lambda(\Phi)}\right)} \leq \rho_\Lambda \leq C_\Lambda \frac{\mathrm{e}^{-H_\Lambda(\Phi)}}{\mathrm{tr}\left(\mathrm{e}^{-H_\Lambda(\Phi)}\right)}, \qquad \lim_{\Lambda \uparrow \mathbb{Z}^d} \frac{\log C_\Lambda}{|\Lambda|} = 0.$$

The set of weak Gibbs states for Φ is denoted by $\mathcal{S}_{\mathrm{wg}}(\Phi)$.

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Proposition [Jakšić–P–Tauber 2022], using [Araki 1969] and [Lenci–Rey-Bellet 2005]

- $\mathcal{S}_{\mathrm{wg}}(\Phi) \subset \mathcal{S}_{\mathrm{eq}}(\Phi)$.
- If either $d = 1$ and Φ is finite range, or $d \geq 1$ and $\|\Phi\|_r < r$, then $\mathcal{S}_{\mathrm{wg}}(\Phi) = \mathcal{S}_{\mathrm{eq}}(\Phi)$.

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Conjecture. For any $r > 0$ and $\Phi \in \mathcal{B}^r$, $\mathcal{S}_{\mathrm{wg}}(\Phi) = \mathcal{S}_{\mathrm{eq}}(\Phi)$.

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Remark. For classical spin systems, the equality $\mathcal{S}_{\mathrm{wg}}(\Phi) = \mathcal{S}_{\mathrm{eq}}(\Phi)$ holds for all $\Phi \in \mathcal{B}^0$ [Pfister–Sullivan 2019].

Approach to equilibrium – the Second Law – time's arrow

The following property is a direct consequence of the previous definition

Entropy balance relation for extended translation-invariant spin systems

Suppose that $\Phi \in \mathcal{B}^r$ and $\rho \in \mathcal{S}_{\mathrm{wg}}(\Phi)$. Then, for any $\omega \in \mathcal{S}_I(\mathfrak{A})$ one has

$$0 \leq \lim_{\Lambda \uparrow \mathbb{Z}^d} \frac{S(\omega_\Lambda | \rho_\Lambda)}{|\Lambda|} = s(\omega|\rho) = -s(\omega) + \omega(E_\Phi) + P(\Phi),$$

with equality iff $\omega \in \mathcal{S}_{\mathrm{eq}}(\Phi)$.

and is the central tool in the proof of our main **unconditional** results

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Theorem 2

For $\Psi, \Phi \in \mathcal{B}^r$, suppose that $\mathcal{S}_{\rm eq}(\Psi) = \{\rho\}$ (high temp.) with $\rho \in \mathcal{S}_{\rm wg}(\Psi) \setminus \mathcal{S}_\Phi(\mathfrak{A})$.
Then, any $\rho_+ \in \mathcal{S}_+(\rho, \Phi)$ satisfies

$$\rho_+(E_\Psi) > \rho(E_\Psi).$$

- Strict increase of the mean energy $\Rightarrow$ irreversibility $\rho \notin \mathcal{S}_+(\rho_+, \Psi)$.
- Conjecture: $s(\rho_+) > s(\rho)$.

Approach to equilibrium – the Second Law – time's arrow

Remarks.

- Theorems 1 & 2 display the fundamental irreversibility of approach to equilibrium, contrasting with the reversibility of return to equilibrium.
- Whether $\mathcal{S}_+(\rho, \Phi) \subset \mathcal{S}_{\rm eq}(\Phi)$ is a delicate dynamical problem which can only be answered in the context of concrete models [Emch-Radin 1970, Lanford-Robinson 1971].
- Our results apply to lattice fermions [Araki–Moriya 2003] (with the minimal changes to comply with gauge-invariance).

Outlook

Outlook

- First steps in a research program around approach to equilibrium and time's arrow in classical and quantum statistical mechanics.
- We have related results on adiabatic (*i.e.,* quasi-static) evolution of translation invariant spin systems. More this afternoon in Vojkan's talk.

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Thank you!

All the best for the next 10 years Jan!