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Nonlinear Gibbs, local KMS and dynamical detailed balance conditions

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Abstract

Presently several equivalent characterizations of equilibrium states are known, for example:
– the KMS condition,
– the Boltzmann-Gibbs prescription,
– the detailed balance condition.
Until recently no non-equilibrium analogue of these conditions were known.
From the stochastic limit of quantum theory three natural generalizations of these notions emerged in the past 12 years:
- the local KMS condition
- the nonlinear Boltzmann-Gibbs prescription
- the dynamical detailed balance condition.
The fact that these three conditions are equivalent is quite non trivial.
The present talk will describe the ideas and tools used to prove the above mentioned equivalence.

Short history

The program to apply systematically the stochastic limit (SL) approach to develop a **non equilibrium quantum field Theory** was formulated in:

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Full version in preparation for:
Infinite Dimensional Analysis, Quantum Probability and Related Topics

stationary $\subset$ non equilibrium

Many interesting phenomena are stationary but non equilibrium.
(i) mathematical stationarity: there is a well defined dynamics (reversible or irreversible) which has an invariant state.
(ii)physical stationarity: there is a flow of some quantity with constant physical characteristics.
Examples:
– energy flow: heat conduction
– flow of charges: electrical conductivity
– flow of photons: laser
Flows are related to:
– direction of space
– direction of time.

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General scheme of the stochastic limit technique for the Hamiltonian of the form

$$H^{(\lambda)} = H_0 + \lambda H_I \tag{1}$$

– λ is real parameter,
– H_0 is the free Hamiltonian
– H_I is the interaction Hamiltonian.
Schrödinger equation in interaction picture associated to the Hamiltonian $H^{(\lambda)}$

$$\frac{d}{dt}U_t^{(\lambda)} = -i\lambda H_I(t)U_t^{(\lambda)} \tag{2}$$

$$H_I(t) = e^{itH_0}H_I e^{-itH_0}.$$

idea of the stochastic limit approach:
take time the rescaling

$$t \to t/\lambda^2 \tag{3}$$

in the solution

$$U_t^{(\lambda)} = e^{itH_0} e^{-itH^{(\lambda)}} \tag{4}$$

The rescaling (3) gives the rescaled equation

$$\frac{d}{dt} U^{(\lambda)}_{t/\lambda^2} = -\frac{i}{\lambda} H_I(t/\lambda^2) U^{(\lambda)}_{t/\lambda^2} \tag{5}$$

and the limit $\lambda \to 0$
is equivalent to $\lambda \to 0$ and $t \to \infty$ under the condition that $\lambda^2 t$ tends to a constant.
The limit

$$\lim_{\lambda \to 0} U^{(\lambda)}_{t/\lambda^2} =: U_t$$

captures the dominating contributions
to the dynamics

$$\frac{d}{dt} U_t = -ih_t U_t, \quad h_t = \lim_{\lambda \to 0} \frac{1}{\lambda} H_I(t/\lambda^2) \ , \quad U(0) = 1 \tag{6}$$

the limit of the Heisenberg evolution

$$\lim_{\lambda \to 0} X_t^{(\lambda)} := \lim U^{(\lambda)}_{t/\lambda^2}{}^{\dagger} X U^{(\lambda)}_{t/\lambda^2} = U_t^{\dagger} X U_t \tag{7}$$

where X is an observable
belonging to a certain class: slow observables.

The initial state of the field is a mean zero gauge invariant Gaussian state with correlations:

$$\begin{pmatrix} \langle a_k^+ a_{k'} \rangle & \langle a_k^+ a_{k'}^+ \rangle \\ \langle a_k a_{k'} \rangle & \langle a_k a_{k'}^+ \rangle \end{pmatrix} = \begin{pmatrix} N(k) & 0 \\ 0 & N(k)+1 \end{pmatrix} \delta(k-k')$$

if $N(k)$ depends on k through the energy density $\omega(k)$

$$N(k) = N_0(\omega(k)) \equiv N(\omega_k)$$

then the quotient

$$\frac{\text{Re } (g_i|g_j)^-_\omega}{\text{Re } (g_i|g_j)^+_\omega} = \frac{\langle A(g_i)A^+(S_t g_j)\rangle^\sim}{\langle A^+(g_i)A(S_t g_j)\rangle^\sim} = \frac{N(\omega)+1}{N(\omega)} \quad (8)$$

where $\sim$ means Fourier transform, is independent of the cut–off functions g_i, g_j.

Def.

The quotient (8) is called the (inverse) non equilibrium Gibbs factor.

Defining

$$\tilde{\beta}(k) := \lg \frac{N(k)+1}{N(k)} > 0$$

one has

$$N(k) = \frac{1}{e^{\tilde{\beta}(k)} - 1}$$

$$\frac{N(k)+1}{N(k)} = (e^{\tilde{\beta}(k)} - 1)\left(\frac{1}{e^{\tilde{\beta}(k)} - 1} + 1\right) = e^{\tilde{\beta}(k)}$$

Clearly

$$N(k) = N_0(\omega(k)) \equiv N(\omega_k) \Leftrightarrow \tilde{\beta}(k) = \beta(\omega_k)$$

In the equilibrium it is equal to

and when function $\beta(\ \cdot\ )$ is linear, one finds the usual (inverse) Gibbs factor:

$$e^{\beta\omega(k)}$$

We consider the forward and the backward Heisenberg evolution of an operator X belonging to the slow degrees of freedom of the total system:

$$j_t^{(F)}(X) := U_t^\dagger X U_t \quad \text{for} \qquad ; \; t > 0$$

$$j_t^{(B)}(X) := U_{-t} X U_{-t}^\dagger \quad \text{for} \qquad ; \; t < 0$$

where U_t is the time evolution operator in interaction picture.

After stochastic limit,
taking partial expectation of the field degrees of freedom (denoted $\langle\cdot\rangle$)
of the forward Heisenberg evolution
we obtain the forward master equations for observables

$$\frac{d}{dt}\langle j_t^{(F)}(X)\rangle = i[\Delta, \langle j_t^{(F)}\rangle] - \sum_{\omega\in F}$$

$$\Big(\Gamma_{\omega-}\Big(\frac{1}{2}\{E_\omega^\dagger E_\omega, \langle j_t^{(F)}(X)\rangle\} - E_\omega^\dagger\langle j_t^{(F)}(X)\rangle E_\omega\Big)$$

$$\Big(+\Gamma_{\omega+}\Big(\frac{1}{2}\{E_\omega E_\omega^\dagger, \langle j_t^{(F)}(X)\rangle\} - E_\omega\langle j_t^{(F)}(X)\rangle E_\omega^\dagger\Big)\Big)$$

$$=: \mathcal{L}_F(\langle j_t^{(F)}(X)\rangle) \qquad , \quad \text{for} \quad t \geq 0$$

and taking partial expectation of the field degrees of freedom (denoted $\langle\cdot\rangle$)
of the backward Heisenberg evolution
we obtain the backward master equations for observables

$$\frac{d}{dt}\langle j_t^{(B)}(X)\rangle = i[\Delta, \langle j_t^{(B)}\rangle] + \sum_{\omega\in F}$$

$$\left(\Gamma_{\omega -}\left(\frac{1}{2}\{E_\omega^\dagger E_\omega, \langle j_t^{(B)}(X)\rangle\} - E_\omega^\dagger \langle j_t^{(B)}(X)\rangle E_\omega\right) + \right.$$

$$\left. + \Gamma_{\omega +}\left(\frac{1}{2}\{E_\omega E_\omega^\dagger, \langle j_t^{(B)}(X)\rangle\} - E_\omega \langle j_t^{(B)}(X)\rangle E_\omega^\dagger\right)\right)$$

$$=: -\mathcal{L}_B(\langle j_t^{(B)}(X)\rangle) \qquad , \quad \text{for} \quad t \leq 0$$

the dual master equation (for density matrices) is written as

$$\frac{d}{dt}\rho_S(t) = \mathcal{L}^* \rho_S(t), \quad t \geq 0$$

Similarly, we introduce a master equation associated to $\mathcal{L}_B$ as

$$\frac{d}{dt}\rho_S^{(B)}(t) = -\mathcal{L}_B^* \rho_S^{(B)}(t), \quad t \leq 0$$

Both master equations have the same stationary state ρ_S

The equilibrium state is characterized by the condition:

$$\mathcal{L}(X) - \mathcal{L}_B(X) = 2i[\Delta, X].$$

By direct computation we obtain the deviation from the symmetry condition

$$\mathrm{tr}(\rho_S x \mathcal{L}(y)) = \mathrm{tr}(\rho_S \mathcal{L}_B(x) y)$$

which characterizes equilibrium:

$$\mathrm{tr}\,(\rho_S X \mathcal{L}(Y)) - \mathrm{tr}\,(\rho_S \mathcal{L}_B(X) Y) = \sum_{lm} X_{ll} Y_{mm}$$

$$\Big(\rho_{ll}(\Gamma_{-,\epsilon_l-\epsilon_m} + \Gamma_{+,\epsilon_m-\epsilon_l}) - \rho_{mm}(\Gamma_{-,\epsilon_m-\epsilon_l} + \Gamma_{+,\epsilon_l-\epsilon_m})\Big)$$

$$= \sum_{lm} X_{ll} Y_{mm} \theta(\epsilon_l - \epsilon_m)(J_{1,lm} + J_{2,lm}) - \theta(\epsilon_m - \epsilon_l)(J_{1,ml} + J_{2,m}$$

where

$$X_{ll} := \langle \epsilon_l | X | \epsilon_l \rangle, \quad Y_{mm} := \langle \epsilon_m | Y | \epsilon_m \rangle, \quad \rho_{ll} = \langle \epsilon_l | \rho_S | \epsilon_l \rangle.$$

Choosing

$$X = |\epsilon_a\rangle\langle\epsilon_a| =: P_a, \quad Y = |\epsilon_b\rangle\langle\epsilon_b| =: P_b,$$

one obtains

$$\mathrm{tr}\,(\rho_S P_a \mathcal{L}(P_b)) - \mathrm{tr}\,(\rho_S \mathcal{L}_B(P_a) P_b) =$$

$$= \theta(\epsilon_a - \epsilon_b)(J_{1,ab} + J_{2,ab}) - \theta(\epsilon_b - \epsilon_a)(J_{1,ba} + J_{2,ba})$$

The left hand side describes the balance between two processes: transition from $|\epsilon_a\rangle$ to $|\epsilon_b\rangle$ and its converse in stationary state ρ_S.

Slow degrees of freedom and micro-current

Consider the field number density operator:

$$n_k = a_k^\dagger a_k \qquad k \in \mathbb{R}^d$$

Its Heisenberg evolution after the stochastic limit

$$U_t^\dagger n_k U_t$$

describes the time evolution of the densities of field particles.
Thus its derivative is the number density current.
Its evolution is described by the Langevin equation

$$\frac{d}{dt} U_t^\dagger n_k U_t = \text{white noise Hamiltonian equation}$$

From this equation, taking partial expectation of the field degrees of freedom (denoted $\langle \cdot \rangle$) we find the following dynamical balance equation:

$$\frac{d}{dt} \langle U_t^\dagger n_k U_t \rangle = 2 \sum_{\omega \in F} \delta(\omega(k) - \omega)$$

$$\mathrm{tr}_S \left(\left(\gamma_{-,\omega}(k) E_\omega^\dagger E_\omega - \gamma_{+,\omega}(k) E_\omega E_\omega^\dagger \right) \rho_S(t) \right)$$

where the time evolution of $\rho_S(t)$ obtained by solving the master equation.

Since this equation is in distribution sense, it implies that momentum space is foliated into resonant energy shells and the equation is equivalent to:

$$0 = \sum_{\omega \in F} \delta(\omega(k) - \omega)$$

$$\left(\frac{d}{dt}\langle U_t^\dagger n_k U_t\rangle - 2\mathrm{tr}_S \left(\gamma_{-,\omega}(k) E_\omega^\dagger E_\omega - \gamma_{+,\omega}(k) E_\omega E_\omega^\dagger\right) \rho_S(t)\right)$$

But the energy shells are disjoint and discrete.

This implies the following result.

Theorem. If:

(i) The Liouville spectrum of the system Hamiltonian has no accumulation points.

(ii) The energy density function $k \in \mathbb{R}^d \mapsto \omega(k)$ is "regular enough".

Then the above equation is equivalent to the following dynamical **detailed** balance equation:

$$\forall \omega \in F \qquad ; \qquad \frac{d}{dt}\langle U_t^\dagger \delta(\omega(k) - \omega) n_k U_t \rangle =$$

$$= -2\text{tr}_S \left[\left(\gamma_{-,\omega}(k) E_\omega^\dagger E_\omega - \gamma_{+,\omega}(k) E_\omega E_\omega^\dagger \right) \rho_S(t) \right] \delta(\omega(k) - \omega)$$

(iii) If $\omega(k)$ is positive, then the sum can be restricted to the set F_+ of **positive** Bohr frquencies.

Interpretation of the dynamical detailed balance (DDB) equation:

$$\forall \omega \in F_+ \qquad ; \qquad \frac{d}{dt}\langle U_t^\dagger \delta(\omega(k) - \omega) n_k U_t \rangle =$$

$$= -2\mathrm{tr}_S \left[\left(\gamma_{-,\omega}(k) E_\omega^\dagger E_\omega - \gamma_{+,\omega}(k) E_\omega E_\omega^\dagger \right) \rho_S(t) \right] \delta(\omega(k) - \omega)$$

For each positive Bohr frequency and momentum

$$\omega = \varepsilon_m - \varepsilon_n \in F_+ \qquad ; \qquad k \in \mathbb{R}^d$$

define the average number (ω, k)–micro-current by:

$$\frac{d}{dt}\langle U_t^\dagger \delta(\omega(k) - \omega) n_k U_t \rangle =: J_\omega(t, k)$$

The DDB condition is then:

$$J_\omega(t, k) = 2\mathrm{tr}_S \left(\left(\gamma_{-,\omega}(k) E_\omega^\dagger E_\omega - \gamma_{+,\omega}(k) E_\omega E_\omega^\dagger \right) \rho_S(t) \right)$$

Thus the number density current has a fine structure in terms of (ω, k)–micro-currents:

$$\frac{d}{dt}\langle U_t^\dagger n_k U_t \rangle = 2 \sum_{\omega \in F} \delta(\omega(k) - \omega) J_\omega(t, k)$$

The term *microscopic* here refers to the fact that we define one current for each atomic frequency .

Stationary states under the DDB condition

Corollary. If ρ_S is any stationary state under the forward master equation

$$\rho_S(t) = \rho_S \qquad ; \qquad \forall t$$

then, for each momentum $k \in \mathbb{R}^d$ and positive Bohr frequency $\omega \in F_+$, the (ω, k)–micro-current is constant.
In fact:

$$\frac{d}{dt}\langle U_t^\dagger \delta(\omega(k) - \omega) n_k U_t \rangle =$$

$$= 2\text{tr}_S \left(\left(\gamma_{-,\omega}(k) E_\omega^\dagger E_\omega - \gamma_{+,\omega}(k) E_\omega E_\omega^\dagger \right) \rho_S \right)$$

and the right hand side does not depend on t.

Conclusions.
(i) Under general conditions, for any state ρ_S of the system, the flow of quanta between the modes of the field (environment) and the system is split into a family of independent *microscopic currents*, one for each positive Bohr frequency ω.
(ii) If ρ_S is any stationary state of the system under the forward master equation then any of these microscopic currents is constant.
The sign of this constant determines the direction of the flow:
– from field to system (pumping)
– from system to field (dissipation).
Many flows:
– flow of time
– (micro)–flows of quanta $\forall(\omega, k)$
– (micro)–flows of energy $\forall(\omega, k)$
– ...
Which physical parameters distinguish the different regimes?

$$\frac{d}{dt}\langle U_t^\dagger \delta(\omega(k)-\omega) n_k U_t\rangle =$$

$$= 2\mathrm{tr}_S\left(\left(\gamma_{-,\omega}(k) E_\omega^\dagger E_\omega - \gamma_{+,\omega}(k) E_\omega E_\omega^\dagger\right)\rho_S\right)$$

The micro–susceptibilities (transition rates) are

$$\gamma_{-,\omega}(k) = \gamma_\omega(k)(N(k)+1) \quad , \quad \gamma_{+,\omega}(k) = \gamma_\omega(k)N(k)$$

$$\gamma_\omega(k) = \pi|g_\omega(k)|^2 > 0$$

$$\gamma_{-,\omega}(k) = \gamma_\omega(k)(N(k)+1) > \gamma_{+.\omega}(k) = \gamma_\omega(k)N(k)$$

Generic system Hamiltonians

If the system Hamiltonian is generic
(i.e. its Liouville spectrum is non degenerate),
then for each positive Bohr frequency

$$0 < \omega = \varepsilon_m - \varepsilon_n \in F$$

one has

$$E_\omega = |\epsilon_n\rangle\langle\epsilon_m|$$

Thus

$$E_\omega E_\omega^* = |\epsilon_n\rangle\langle\epsilon_n| \qquad ; \qquad E_\omega^* E_\omega = |\epsilon_m\rangle\langle\epsilon_m|$$

Therefore

$$\frac{d}{dt}\langle U_t^\dagger \delta(\omega(k) - (\epsilon_m - \epsilon_n)) n_k U_t\rangle =$$

$$= 2(\gamma_{-,\epsilon_m - \epsilon_n}(k)\rho_{mm} - \gamma_{+,\epsilon_m - \epsilon_n}\rho_{nn})$$

where

$$\gamma_{-,\omega}(k) = \pi |g_\omega(k)|^2 \ (N(k;\beta,\mu) + 1)$$

$$\gamma_{+,\omega}(k) = \pi |g_\omega(k)|^2 \ N(k;\beta,\mu)$$

Theorem 1 *The following are equivalent:*

(i) ρ *satisfies the local* (H, β)*–KMS condition*

$$\tilde{\rho}\left(xy(t + i\beta(H))\right) = \tilde{\rho}\left(y(t)x\right), \qquad \forall x, y \in \mathcal{B}(\mathcal{H}) \text{ , } \forall t$$
(9)

(ii) $e^{-\beta(H)H}$ *is trace class and*

$$\rho = \rho_{\beta,H} := {Z_\beta}^{-1} e^{-\beta(H)H}, \qquad Z_\beta := \mathrm{tr}\left(e^{-\beta(H)H}\right)$$
(10)

With these notations the local KMS condition can be re–written in the more intuitive form:

$$\varphi\left(xe^{-\beta(H)H}y(t)e^{\beta(H)H}\right) = \varphi\left(y(t)x\right) \text{ ; } \forall x, y \in \mathcal{B}(\mathcal{H}) \text{ , } \forall t \in$$
(11)

Differentiating (11) at $t = 0$ one finds

$$\varphi\left(xe^{-\beta(H)H}\delta(y)e^{\beta(H)H}\right) = \varphi\left(\delta(y)x\right) \qquad (12)$$

where

$$\delta(y) := i[H, y] \qquad ; \qquad y \in \mathcal{B}(\mathcal{H}) \cap \text{Domain}(i[H, \cdot\,])$$

is the infinitesimal generator of the Heisenberg dynamics.

The identity (12) gives the infinitesimal form of the local KMS condition.

Definition 1 *Let $\mathcal{L}$ be a Markov generator, ρ a state on $\mathcal{B}(\mathcal{H})$, and (H, β). The pair $(\rho, \mathcal{L})$ is said to satisfy the infinitesimal form of the irreversible (H, β)–KMS condition*

$$\text{tr}(\rho x e^{-\beta(H)H} \mathcal{L}(y) e^{\beta(H)H}) = \text{tr}(\rho \mathcal{L}(y) x) \qquad (13)$$

for all $x \in \mathcal{B}(\mathcal{H})$ and $y \in$ Domain$(\mathcal{L})$ for which the left hand side of (13) is well defined.