NESS in quantum statistical mechanics

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In this article we describe the construction of canonical Non-Equilibrium Steady States (NESS) for a small quantum system $\mathcal{S}$ coupled to several extended reservoirs $\mathcal{R}_1,\ldots,\mathcal{R}_M$ (see [Nonequilibrium steady states]). We shall work in the framework of C^*-dynamical systems and denote by $\mathcal{O}_0$ the C^*-algebra of $\mathcal{S}$ which we assume to be finite dimensional. Each reservoir $\mathcal{R}_j$ is described by a C^*-algebra $\mathcal{O}_j$. For simplicity we assume that the algebra of the joint system $\mathcal{S}+\mathcal{R}_1+\cdots+\mathcal{R}_M$ is the C^*-tensor product $\mathcal{O}=\mathcal{O}_\mathcal{S}\otimes\mathcal{O}_\mathcal{R}=\otimes_{0\le a\le M}\mathcal{O}_a$. The following is easily adapted to more general cases, e.g., fermionic algebras.

For $0\le a\le M$ let $(\mathcal{O}_a,\tau_a)$ be the C^*-dynamical system describing the isolated subsystem a. The dynamics of the decoupled joint system is $\tau=\otimes_{0\le a\le M}\tau_a$. The dynamics τ_V of the coupled joint system is the local perturbation of τ induced by

$$V=\sum_{1\le j\le M}V_j,\quad V_j=V_j^*\in\mathcal{O}_0\otimes\mathcal{O}_j,$$

where V_j is the interaction between $\mathcal{S}$ and $\mathcal{R}_j$ (see [Quantum dynamical systems]).

Definition 1 *Let ω be a state on $\mathcal{O}$. We say that ω_+ is a NESS of τ_V associated to the reference state ω if there exists a net $t_\alpha\to\infty$ such that*

$$\omega_+(A)=\lim_\alpha\frac{1}{t_\alpha}\int_0^{t_\alpha}\omega\circ\tau_V^t(A)\,\mathrm{d}t,$$

for all $A\in\mathcal{O}$. We denote by $\Sigma_+(\tau_V,\omega)$ the set of these NESS.

A few remarks are in order:

1. By definition the elements of $\Sigma_+(\tau_V,\omega)$ are τ_V-invariant states on $\mathcal{O}$. Moreover, if ω is such a state then $\Sigma_+(\tau_V,\omega)=\{\omega\}$.

2. Strictly speaking, one should exclude the cases where the limit ω_+ turns out to be a KMS state for τ_V. This occurs trivially if ω is such a state, but is also expected when ω is (normal relative to) a KMS state for the decoupled dynamics τ (see [Return to equilibrium]). In this case ω_+ will be ω-normal. In genuine nonequilibrium cases ω_+ is expected to be singular with respect to ω.

3. Entropy production plays a central role in nonequilibrium statistical mechanics. We refer to [Entropy Production] for a discussion of related properties of NESS. Let us just mention here that NESS have a non-negative entropy production rate.

4. Since the set of all states on $\mathcal{O}$ is weak-$*$ compact $\Sigma_+(\tau_V,\omega)$ is not empty.

5. If the perturbation V is time dependent then natural nonequilibrium states (NNES) are defined in a similar way as limit points

$$\omega_+^t(A)=\lim_\alpha\frac{1}{t_\alpha}\int_{-t_\alpha}^t\omega\circ\tau_V^{s\to t}(A)\,\mathrm{d}s.$$

   They satisfy $\omega_+^t\circ\tau_V^{t\to r}=\omega_+^r$ (see [R]).

As stressed in [Nonequilibrium steady states], a NESS should be insensitive to local perturbations of the initial state ω. The following result, proved in [AJPP1], shows that this is indeed the case under a rather weak ergodic hypothesis.

Theorem 2 *Assume that ω is a factor state on $\mathcal{O}$ and that, for any ω-normal state η,*

$$\lim_{t\to\infty} \frac{1}{t} \int_0^t \eta([\tau_V^s(A), B])\, \mathrm{d}s = 0,$$

holds for all A, B in a dense subset of $\mathcal{O}$ (weak asymptotic Abelianness in mean). Then $\Sigma_+(\tau_V, \eta) = \Sigma_+(\tau_V, \omega)$ holds for all ω-normal states η.

In typical applications the reference state ω will be specified by the requirement that its restrictions to the subalgebras $\mathcal{O}_a$ are β_a-KMS states[1] for the corresponding dynamics τ_a. This means that ω is a KMS state at inverse temperature -1 for the dynamics $\sigma_\omega^t = \otimes_a \tau_a^{-\beta_a t}$. In particular, ω is modular and σ_ω is its modular group (see [Tomita-Takesaki theory]). The group σ_ω plays an important and somewhat unexpected role in the mathematical theory of linear response (see [Linear response theory]).

Accordingly, we shall assume in the remaining of this paragraph that ω is modular and denote by $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$ the corresponding GNS representation of $\mathcal{O}$. The enveloping von Neumann algebra $\pi_\omega(\mathcal{O})''$ is in standard form and we denote by J the modular conjugation. If L is the standard Liouvillean of τ then $L_V = L + \pi_\omega(V) + J\pi_\omega(V)J$ is the standard Liouvillean of τ_V. The spectral analysis of L_V yields interesting information on the structure of $\Sigma_+(\tau_V, \omega)$ (see [AJPP1]).

Theorem 3 *Assume that the state ω is modular.*

1. *If $\operatorname{Ker} L_V = \{0\}$ then there is no ω-normal τ_V-invariant state. In particular, any NESS in $\Sigma_+(\tau_V, \omega)$ is purely ω-singular.*
2. *If the assumptions of Theorem 2 hold and if $\operatorname{Ker} L_V \neq \{0\}$ then it is one dimensional and there exists a unique ω-normal τ_V-invariant state ω_V. Moreover, $\Sigma_+(\tau_V, \omega) = \{\omega_V\}$.*

As already mentioned, case 1 in the above theorem is the expected behavior out of equilibrium while case 2 describes a typical equilibrium situation.

To our knowledge, there are two approaches to the construction of NESS which we now describe.

The scattering approach

The first approach was proposed by Ruelle in [R] and rely on the scattering theory of C^*-dynamical systems. We also refer to [FMU] and [JOP] for related papers.

The scattering approach assumes the existence of the strong limit

$$\alpha_V = \mathrm{s} - \lim_{t\to\infty} \tau^{-t} \circ \tau_V^t. \tag{1}$$

If it exists, this limit defines an isometric $*$-endomorphism of $\mathcal{O}$ such that $\alpha_V \circ \tau_V^t = \tau^t \circ \alpha_V$, a so called Møller morphism. α_V is injective but its range $\mathcal{O}_+$, a τ-invariant C^*-subalgebra of $\mathcal{O}$, can be strictly smaller than $\mathcal{O}$. One immediately obtains

Proposition 4 *Assume that the Møller morphism (1) exists and that ω is τ-invariant. It follows that, for all $A \in \mathcal{O}$,*

$$\lim_{t\to\infty} \omega \circ \tau_V^t(A) = \omega_+(A),$$

where $\omega_+ = \omega \circ \alpha_V$. In particular, one has $\Sigma_+(\tau_V, \omega) = \{\omega_+\}$.

[1] chemical potentials can also be prescribed by appropriate definition of τ

If the previous proposition applies then α_V provides an isomorphism between the the coupled dynamical system $(\mathcal{O}, \tau_V, \omega_+)$ and the decoupled one $(\mathcal{O}_+, \tau|_{\mathcal{O}_+}, \omega|_{\mathcal{O}_+})$. Ergodic properties of the latter are therefore inherited by the former. The following proposition is a simple consequence of this fact (see [AJPP1]).

Proposition 5 *Assume that the assumptions of Proposition 4 hold.*

1. *If $\omega|_{\mathcal{O}_+}$ is ergodic for $\tau|_{\mathcal{O}_+}$ then $\Sigma_+(\tau_V, \eta) = \{\omega_+\}$ for any ω-normal state η.*
2. *If $\omega|_{\mathcal{O}_+}$ is mixing for $\tau|_{\mathcal{O}_+}$ then*
$$\lim_{t\to\infty} \eta \circ \tau_V^t(A) = \omega_+(A),$$
holds for all $A \in \mathcal{O}$ and any ω-normal state η.

For a finite system coupled to infinite reservoirs we expect $\mathcal{O}_+ = \mathcal{O}_{\mathcal{R}}$ so that the coupled system out of equilibrium inherit the ergodic properties of the reservoirs.

C^*-scattering is much more difficult than Hilbert-space scattering and the only known technique to deal with it is the basic Cook's method. We refer to [R], [FMU], [AJPP2] and [JOP] for more details and examples.

The Liouvillean approach

This alternative to the scattering approach has been proposed in [JP] where the NESS of a N-level quantum system coupled to ideal Fermi reservoirs is constructed. For this kind of systems it has not yet been possible to obtain the propagation estimates needed to construct the Møller morphism. In fact it is not clear that the scattering approach applies in this case.

In the Liouvillean approach, NESS are related to resonances of a new kind of generator of the dynamics in the GNS representation: The C-Liouvillean. The main advantage of this method is that the required analysis can be performed in a Hilbert space setting. The technical difficulties are related to the fact that the C-Liouvillean is not self-adjoint on the GNS space. We shall only describe the strategy here and refer the reader to [JP] for detailed implementation.

We assume that ω is modular and work directly in the GNS representation $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$, identifying $\mathcal{O}$ with $\pi_\omega(\mathcal{O})$. Recall that σ_ω is the modular group of ω, J the modular conjugation and L, L_V the standard Liouvilleans of τ, τ_V. Denote by Δ_ω the modular operator.

Definition 6 *If $t \mapsto \sigma_\omega^t(V)$ is analytic in the strip $\{z \in \mathbb{C} \,|\, |\mathrm{Im}\, z| < 1/2\}$ and bounded continuous in its closure then the C-Liouvillean of τ_V is the closed operator defined on the domain of L by*
$$K_V = L + V - J\sigma_\omega^{-\mathrm{i}/2}(V)J.$$

Since $J\sigma_\omega^{-\mathrm{i}/2}(V)J \in \pi_\omega(\mathcal{O})'$ one easily checks that $\mathrm{e}^{\mathrm{i}tK_V} A \mathrm{e}^{-\mathrm{i}tK_V} = \tau_V^t(A)$. Moreover, since $L\Omega_\omega = 0$ it follows from modular theory that
$$K_V\Omega_\omega = V\Omega_\omega - J\Delta_\omega^{1/2} V \Delta_\omega^{-1/2} J\Omega_\omega = V\Omega_\omega - J\Delta_\omega^{1/2} V\Omega_\omega = (V - V^*)\Omega_\omega = 0.$$
Hence $\omega \circ \tau_V^t(A) = (\Omega_\omega|\mathrm{e}^{\mathrm{i}tK_V} A\Omega_\omega) = (\mathrm{e}^{-\mathrm{i}tK_V^*}\Omega_\omega|A\Omega_\omega)$ where $K_V^* = L + V - J\sigma_\omega^{\mathrm{i}/2}(V)J$.

Suppose there exists a Gelfand triplet $\mathcal{K} \subset \mathcal{H}_\omega \subset \mathcal{K}'$ and a dense subalgebra $\tilde{\mathcal{O}} \subset \mathcal{O}$ such that $\tilde{\mathcal{O}}\Omega_\omega \subset \mathcal{K}$ and
$$w^*\!-\!\lim_{t\to\infty} \frac{1}{t}\int_0^t \mathrm{e}^{-\mathrm{i}sK_V^*}\Omega_\omega \,\mathrm{d}s = \Psi \in \mathcal{K}',$$
holds in $\mathcal{K}'$. Then the functional $\tilde{\mathcal{O}} \ni A \mapsto (\Psi|A\Omega_\omega)$ extends by continuity to a state ω_+ on $\mathcal{O}$ and we can conclude that $\Sigma_+(\tau_V, \omega) = \{\omega_+\}$. Note that if $\Psi \in \mathcal{H}_\omega$ then ω_+ is ω-normal. Thus, we expect that $\Psi \notin \mathcal{H}_\omega$ in genuine nonequilibrium situations. Under appropriate conditions one can show that Ψ is a zero-resonance vector

of K_V^* i.e., that there exists an extension of K_V^* to $\mathcal{K}'$ of which Ψ is a zero eigenvector. In [JP] and more recently in [MMS] spectral deformation techniques have been used to gain perturbative control on the resonances of K_V^*. This yields a convergent expansion for the NESS ω_+ in powers of the coupling V which, to lowest order, coincide with the weak coupling (van Hove) limit studied in [LS]. It also gives the convergence $\nu \circ \tau_V^t(A) \to \omega_+(A)$ for all ω-normal states ν and all $A \in \mathcal{O}$ with a precise estimates on the exponential rate of convergence for dense sets of such ν and A.

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