C^*-Dynamical Systems
and
Nonequilibrium Quantum Statistical Mechanics

Algebraic Approach to the Thermodynamics
of
Open Quantum Systems

C.-A. Pillet

Centre de Physique Théorique – UMR 6207

Université du Sud – Toulon-Var

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Quantum-Koopmanism

(τ, β)-KMS states $\omega(A\tau^{t+i\beta}(B)) = \omega(\tau^t(B)A)$

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- Creation/annihilation operators

$$a^*(f) f_1 \wedge \cdots \wedge f_n = \sqrt{n+1}\, f_1 \wedge \cdots \wedge f_n \wedge f,$$

$$a(f) f_1 \wedge \cdots \wedge f_n = \frac{1}{\sqrt{n}} \sum_{j=1}^{n} (-1)^{n-j} (f, f_j) f_1 \wedge \cdots \not{f_j} \cdots \wedge f_n.$$

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$$\omega_\beta(a^*(g_1) \cdots a^*(g_n) a(f_m) \cdots a(f_1)) = \delta_{nm} \det\{(f_i, Tg_j)\},$$

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- Local perturbation

$$V = \sum_{k=1}^{K} \prod_{j=1}^{n_k} a^*(g_{kj})a(f_{kj}),$$

  leads to locally interacting Fermi gas.

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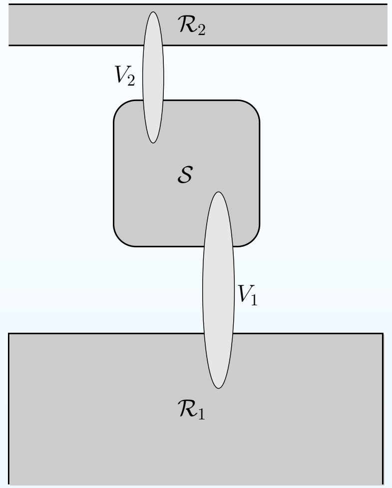

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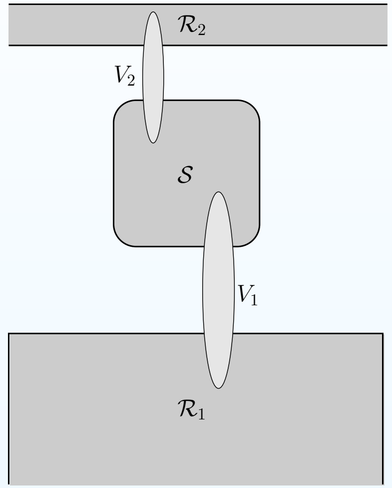

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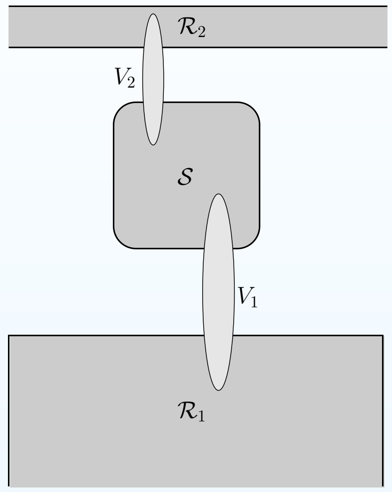

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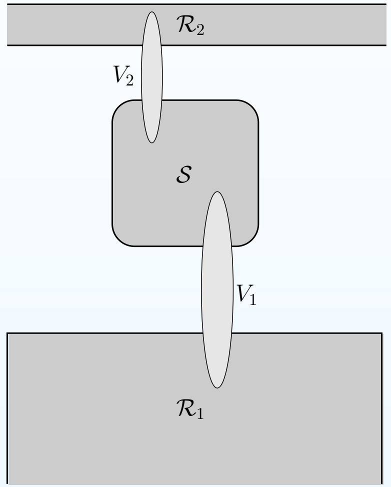

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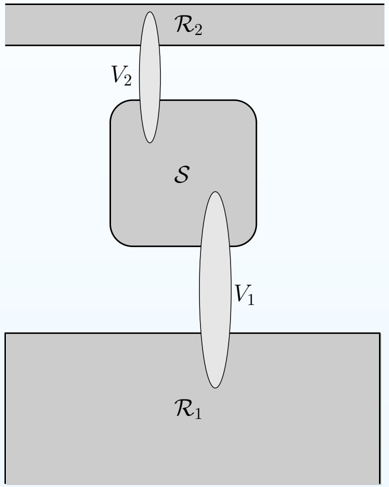

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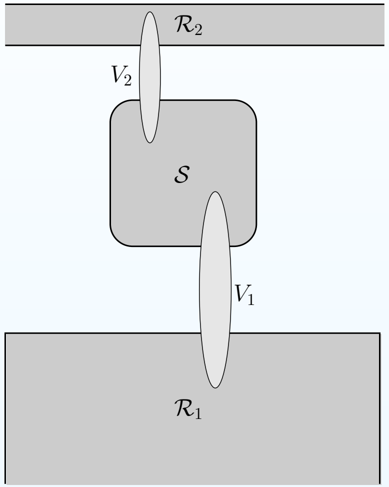
2. Open Quantum Systems



Reservoir $\mathcal{R}_j$: Extended ideal quantum gas $(\mathcal{O}_j, \tau_j^t = \mathrm{e}^{t\delta_j})$.

Small system $\mathcal{S}$: Finite quantum system $(\mathcal{O}_0, \tau_0^t = \mathrm{e}^{t\delta_0})$ (may be absent!).

$(\mathcal{O}, \tau) = \otimes_j (\mathcal{O}_j, \tau_j)$ with multi-KMS reference state $\omega_{\vec{\beta}} = \otimes_j \omega_{\beta_j}$.

Coupling $V = \sum_{j>0} V_j$: Local perturbation $V_j \in \mathcal{O}_0 \otimes \mathcal{O}_j$.

Coupled system $(\mathcal{O}, \tau_V^t = \mathrm{e}^{t(\sum_j \delta_j + i[V, \cdot\,])})$.

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[Ruelle '00]

For all $A \in \mathcal{O}$ and all $\omega_{\vec{\beta}}$–normal state η

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Basic Problem 1. Existence of NESS.

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C^*-scattering theory: [Hepp '70], [Robinson '73], [Botvich-Malyshev '78].

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Theorem. [Aschbacher-Jakšić-Pautrat-P '06] If the C^*-dynamical system $(\mathcal{O}^+, \tau|_{\mathcal{O}^+}, \omega|_{\mathcal{O}^+})$ is mixing then

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

for all $A \in \mathcal{O}$ and all ω-normal states η. Moreover $(\mathcal{O}, \tau_V, \omega^+)$ is mixing.

Remark. The scattering approach does not directly provide information on the rate of convergence in $(*)$.

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Application to open systems. Show that:

1. $(\mathcal{O}_\mathcal{R}, \tau_\mathcal{R}, \omega_\mathcal{R}) \equiv \otimes_{j>0}(\mathcal{O}_j, \tau_j, \omega_{\beta_j})$ is mixing (the easy part).
2. γ^+ exists.
3. $\mathcal{O}^+ = \mathcal{O}_\mathcal{R}$ ($\Rightarrow \omega^+$ independent of $\omega|_{\mathcal{O}_0}$).

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5. CAR $\Rightarrow$ diagrammatic expansion, rooted trees combinatorics.

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Work in GNS representation $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$ of reference state.

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$J = J^* = J^{-1}$: modular conjugation: $J\Delta_\omega J = \Delta_\omega^{-1}$, $J\pi_\omega(\mathcal{O})''J = \pi_\omega(\mathcal{O})'$,

$\sigma_\omega^t(A) \equiv \Delta_\omega^{it} A \Delta_\omega^{-it}$: modular group on $\pi_\omega(\mathcal{O})''$.

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$$\text{if } \exists\Psi \in \mathcal{K}' \text{ s.t. } \mathrm{w}^* - \lim_{t\to\infty} \mathrm{e}^{-iL^* t}\phi = (\Psi, \phi)\Omega_\omega \text{ for all } \phi \in \mathcal{K}, \qquad (*)$$

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Under sufficient regularity assumptions on V spectral deformation techniques allow to control resonances of L and prove $(*)$.

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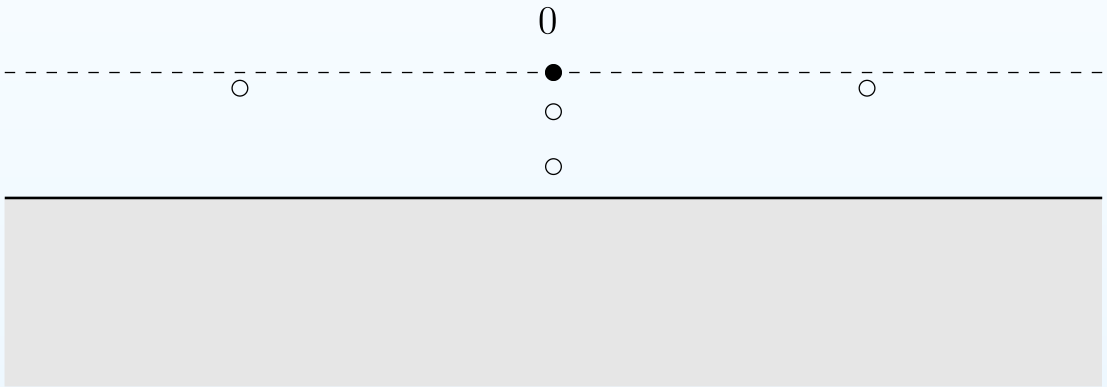

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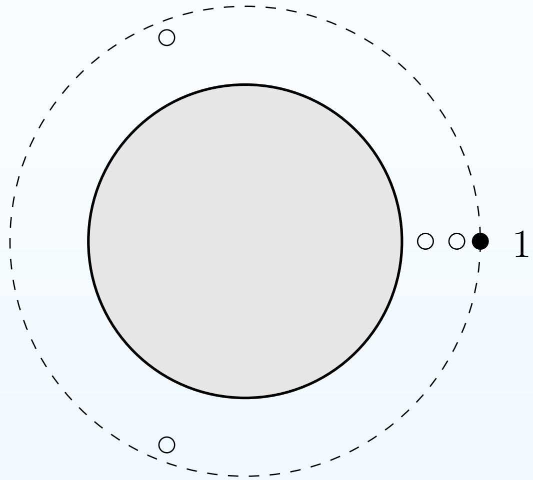

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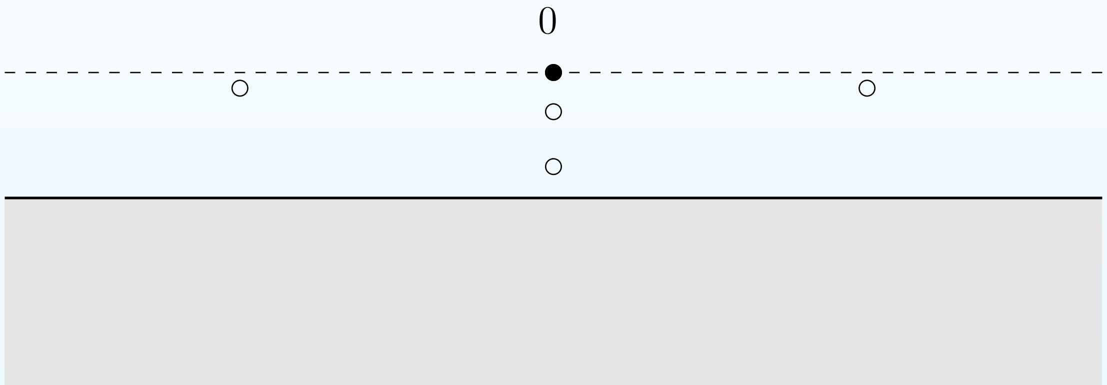

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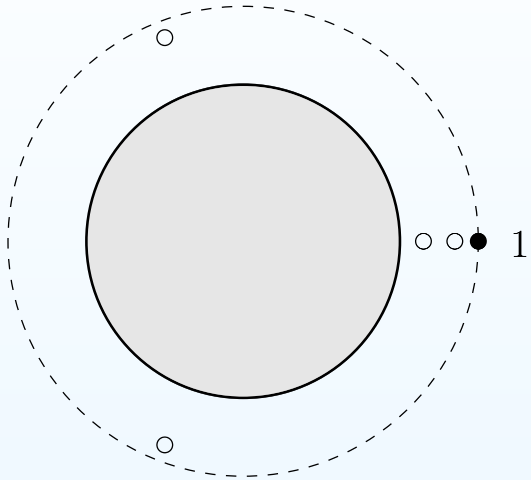

$\mathrm{sp}(e^{-itL^*}|\mathcal{K})$

Imaginary part of resonances control rate of convergence

$$|\eta \circ \tau_V^t(A) - \omega^+(A)| \simeq e^{-\gamma t}$$

3. Entropy Production

$\Phi_j =$ energy flux out of $\mathcal{R}_j = -$rate of change of energy in $\mathcal{R}_j$.

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Total energy is conserved:

$$\sum_{j>0} \Phi_j = \frac{d}{dt}\tau_V^t(H_0 + V)\Big|_{t=0} = \sum_{j>0} \delta_j(H_0 + V) + i[H_0, H_0 + V] + i[V, H_0 + V].$$

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Steady state entropy production rate $= -$ total entropy flux

$$\mathrm{Ep}(\omega_{\vec{\beta}}{}^{+}) \equiv \omega_{\vec{\beta}}{}^{+}(\sigma), \qquad \sigma \equiv -\sum_{j>0} \beta_j \Phi_j.$$

The observable σ plays in this context a similar role as the phase-space contraction rate in dissipative classical dynamical systems.

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Theorem. [Ruelle '01], [Jakšić-P '01] If η is $\omega_{\vec{\beta}}$-normal then

$$\mathrm{Ep}(\omega_{\vec{\beta}}^{\ +}) = -\lim_{t\to\infty} \frac{\mathrm{Ent}(\eta \circ \tau_V^t | \omega_{\vec{\beta}})}{t} \geq 0.$$

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Basic Problem 2. Strict positivity of entropy production

$$\mathrm{Ep}(\omega_{\vec{\beta}}{}^{+}) > 0.$$

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Theorem. [Jakšić-P '02] If $\mathrm{Ep}(\omega_{\vec{\beta}}{}^{+}) > 0$ then $\omega_{\vec{\beta}}{}^{+}$ is not $\omega_{\vec{\beta}}$-normal. Reciproquely, if $\omega_{\vec{\beta}}{}^{+}$ is not $\omega_{\vec{\beta}}$-normal and

$$\limsup_{t\to\infty} \left| \int_0^t \left(\omega_{\vec{\beta}} \circ \tau_V^s(\sigma) - \omega_{\vec{\beta}}{}^{+}(\sigma) \right) ds \right| < \infty,$$

then $\mathrm{Ep}(\omega_{\vec{\beta}}{}^{+}) > 0$.

4. Linear Response

$$\overrightarrow{\beta}_{\rm equ} = (\beta, \beta, \ldots, \beta).$$

$$\omega_{\overrightarrow{\beta}}{}^{+} = \lim_{t\to\infty} \omega_{\overrightarrow{\beta}} \circ \tau_V^t, \quad (|\overrightarrow{\beta} - \overrightarrow{\beta}_{\rm equ}| < \epsilon).$$

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Remark. Order of limits: 1st thermodynamic limit, 2nd long time limit, 3rd weak forcing limit.

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$\mathcal{W} =$ CCR-algebra over $(\mathfrak{C}, \varsigma)$.

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Quasi-free state $\mu_L(W(A)) = \mathrm{e}^{-L(A,A)/2}$
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regular GNS representation $(\mathcal{H}_L, \pi_L, \Omega_L)$ with $\pi_L(W(A)) = \mathrm{e}^{i\phi_L(A)}$.

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Basic Problem 4. Simple Quantum Dynamical CLT:

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holds for all bounded Borel functions $f_1, \ldots, f_n$.

7. Models

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- Quasifree fermions/bosons and XY spin chains ($\rightarrow$ independent particles models): C^*- scattering reduces to Hilbert space scattering leading to Landauer-Büttiker formalism,
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Assumptions. For all j's:

(A1) $\mathfrak{h}_j = L^2(\mathbb{R}_+, ds) \otimes \mathfrak{K}_j$ and $h_j = s$ (spectral representation).

(A2) For some $\delta > 0$ and all a: $e^{-as}\alpha_j(|s|) \in H^2(\{|\mathrm{Im} s| < \delta\}) \otimes \mathfrak{K}_j$ (analyticity).

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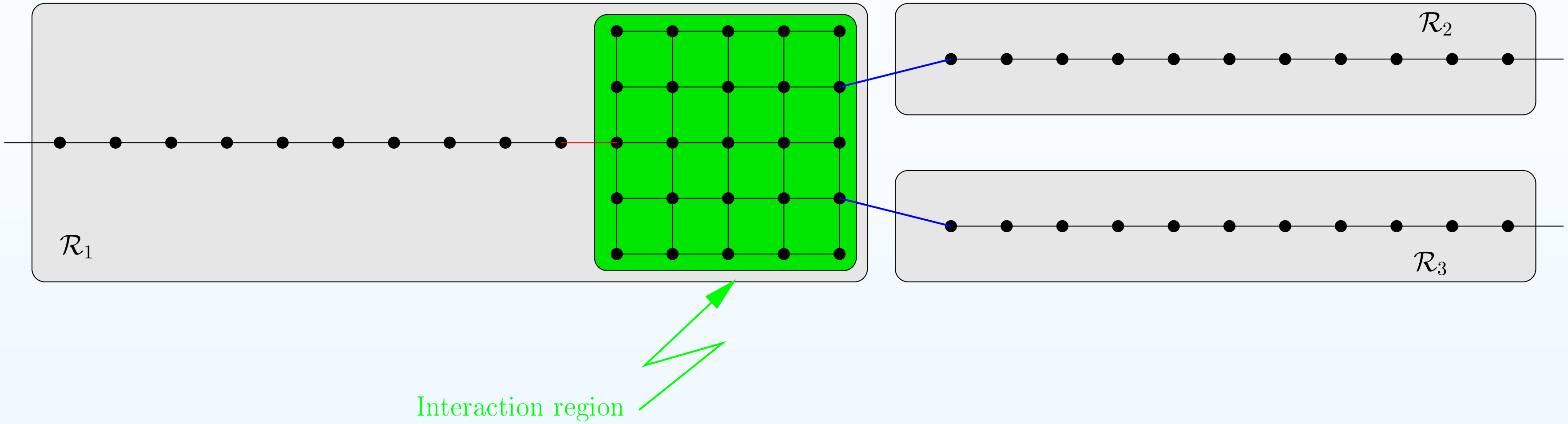
Theorem. [Jakšić-P '02], [Jakšić-Ogata-P, '06] Assume (A1)-(A3) and let $0 < \gamma_1 < \gamma_2$ be given. Then there exists $\Lambda > 0$ such that, for all $0 < |\lambda| < \Lambda$ and $\gamma_1 < \beta_j < \gamma_2$:

1. There exists a NESS $\omega_{\vec{\beta}}{}^{+}$.
2. If the β_j's are not all equal then $\omega_{\vec{\beta}}{}^{+}$ is not $\omega_{\vec{\beta}}$-normal and $\mathrm{Ep}(\omega_{\vec{\beta}}{}^{+}) > 0$.
3. The Green-Einstein-Kubo formulas (1) and (2) hold as well as the Onsager reciprocity relations.

Example 2: Locally Interacting Fermi Gases



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$$\int_{-\infty}^{\infty} |(f, e^{ith} g)| \, dt < \infty,$$

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Example 2: Locally Interacting Fermi Gases

Assumptions. Set $\mathfrak{h} \equiv \oplus_j \mathfrak{h}_j$, $h \equiv \oplus_j h_j$ and $\mathcal{D}_0 \equiv \{u_{jk}, v_{jk}\}$:

(B1) There is a dense subspace $\mathcal{D} \subset \mathfrak{h}$ containing $\mathcal{D}_0$ and such that

$$\int_{-\infty}^{\infty} |(f, e^{ith} g)|\, dt < \infty,$$

for all $f, g \in \mathcal{D}$.

(B2) $h\mathcal{D}_0 \subset \mathcal{D}$.

(B3) There is a complex conjugation on $\mathfrak{h}$ which commute with h and such that u_{jk}, v_{jk} are real (Time reversal invariance).

Theorem. [Jakšić-Ogata-P '06], [Jakšić-Pautrat-P '07] If (B1) holds then there exists $\Lambda > 0$ such that, for $0 < |\lambda| < \Lambda$:

1. There exists a NESS $\omega_{\vec{\beta}}{}^{+}$.
2. If (B2) also holds then the Green-Einstein-Kubo formula (1) holds.
3. If, in addition, (B3) holds then the Green-Einstein-Kubo formula (2) and the Onsager reciprocity relations hold. Moreover QDCLT holds for $\mathfrak{C} = \{\Phi_1, \Phi_2, \ldots\}$.