Landauer-Büttiker formulas in systems of independent fermions

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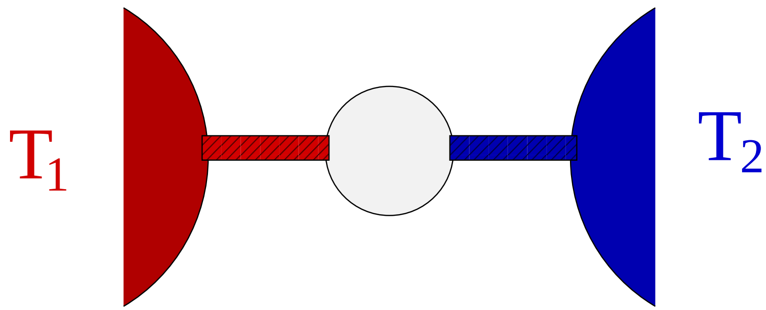
[A, Pillet] *J.Stat.Phys.* **112** (2003) 1153–75
[A, Jakšić, Pautrat, Pillet] *J.Math.Phys.* **48** (2007) 032101 1–28

Contents

What is the general physical question?

• one confined sample $\mathcal{S}$ coupled to several extended reservoirs $\mathcal{R}_j$



Example $j = 1, 2$ with temperatures T_1 and T_2

• initially, reservoirs in thermal equilibrium at different temperatures

other intensive parameters, e.g. chemical potentials

• for large times, coupled system approaches a nonequilibrium steady state carrying nontrivial currents driven by the thermodynamic forces

How do these currents relate to the underlying scattering process?

1. Model

• general interacting system too complicated

$\Rightarrow$ study simplified system of independent fermions

Remark current for interacting fermions in general not expressible by scattering data

1.1 Setting [A, Jakšić, Pautrat, Pillet 07]

observables

• C^*-algebra $\mathcal{A}(\mathfrak{h})$ over one-particle Hilbert space $\mathfrak{h}$ with CAR

$$\{a(f), a^*(g)\} = (f, g) \quad \text{and} \quad \{a^*(f), a^*(g)\} = \{a(f), a(g)\} = 0$$

Remark identify generators with $a^\sharp(f) \in \mathcal{L}(\mathfrak{F}(\mathfrak{h}))$ in Fock representation

• write one-particle Hilbert space as direct sum

$$\mathfrak{h} = \mathfrak{h}_\mathcal{S} \oplus \underbrace{(\oplus_j \mathfrak{h}_j)}_{\mathfrak{h}_\mathcal{R}}$$

Example chain with sample $\mathbb{Z}_\mathcal{S}$ and reservoirs $\mathbb{Z}_1$, $\mathbb{Z}_2$: $\ell^2(\mathbb{Z}_\mathcal{S} \cup \mathbb{Z}_1 \cup \mathbb{Z}_2) = \ell^2(\mathbb{Z}_\mathcal{S}) \oplus \ell^2(\mathbb{Z}_1) \oplus \ell^2(\mathbb{Z}_2)$

states

• normalized $\omega(1) = 1$, positive $\omega(A^*A) \geq 0$ linear functionals ω on $\mathcal{A}(\mathfrak{h})$

Remark set of states is convex subset of Banach space dual of $\mathcal{A}(\mathfrak{h})$, and weak-$*$ compact with neighborhood $\mathcal{U}(\omega; A_1, \ldots, A_n; \varepsilon) = \{\omega' : |\omega'(A_k) - \omega(A_k)| < \varepsilon \text{ for all } k\}$

• two-point function defines density ϱ with $0 \leq \varrho \leq 1$

$$\omega(a^*(g)a(f)) = (f, \varrho\, g)$$

(anti)-linearity, positivity

• a state is quasi-free iff

$$\omega(a^*(g_n)...a^*(g_1)a(f_1)...a(f_m)) = \delta_{nm} \det\{(f_i, \varrho\, g_j)\}$$

Example $\varrho = \varrho(h)$: free Fermi gas with energy density $\varrho(\varepsilon)$

dynamics

- described by uncoupled and coupled Hamiltonians h_0 and h
- Bogoliubov $*$-automorphism groups

$$\tau_0^t(a(f)) = a(\mathrm{e}^{\mathrm{i}th_0} f), \quad \tau^t(a(f)) = a(\mathrm{e}^{\mathrm{i}th} f)$$

Remarks (1) the pair $(\mathcal{A}(\mathfrak{h}), \tau^t)$ is C^*-dynamical system, i.e. dynamics is strongly continuous

(2) free bosons: W^*-dynamical system, i.e. W^*-algebra with σ-weakly continuous dynamics only

Assumptions on the Hamiltonians h_0 and h

(H1) $h_0, h \geq -E_0$

(H2) $h - h_0 \in \mathcal{L}^1$

(H3) $\sigma_{\mathrm{sc}}(h) = \emptyset$

- for the case of partitioning $h_0 = h_{\mathcal{S}} \oplus \underbrace{(\oplus_j h_j)}_{h_{\mathcal{R}}}$

(H4) $\sigma_{\mathrm{ess}}(h_{\mathcal{S}}) = \emptyset$

$\mathcal{L}^1$ trace class operators, more general couplings (H2') in 3.2 below

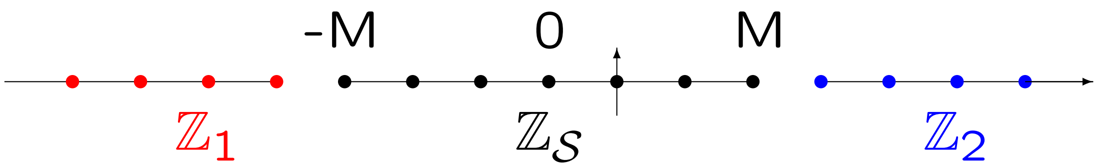
Example **XY chain** [A, Pillet 03]

- coupled Hamiltonian with anisotropy γ and magnetic field λ

$$H = -\frac{1}{4}\sum_{x\in\mathbb{Z}}\Big[(1+\gamma)\sigma_1^{(x)}\sigma_1^{(x+1)} + (1-\gamma)\sigma_2^{(x)}\sigma_2^{(x+1)} + 2\lambda\sigma_3^{(x)}\Big]$$

quasi-local UHF spin algebra over finite subsets of $\mathbb{Z}$

- uncoupled Hamiltonian by removing bonds at sites $-M$ and M



- Araki-Jordan-Wigner transformation

$\Rightarrow$ free fermions with $h = (\cos\xi - \lambda)\otimes\sigma_3 + \gamma\sin\xi\otimes\sigma_2$ and $h_0 = h - v$

Remark self-dual CAR setting: $B(f) = a^*(f_1) + a(\bar{f}_2)$ for $f \in \mathfrak{h}^{\oplus 2}$ with $\mathfrak{h} = \ell^2(\mathbb{Z})$ and $v \in \mathcal{L}^0$, cf. 3.3

$\Rightarrow$ (H1)-(H4) satisfied

1.2 Nonequilibrium steady states (NESS)

• [Ruelle 01] NESS ω_+ w.r.t. ω_0 is weak-$*$ limit point of net

$$\frac{1}{T}\int_0^T \mathrm{d}t\, \omega_0 \circ \tau^t, \quad T > 0$$

ω_0 reference state

• we use Ruelle's scattering approach to NESS

Remark spectral approach [Jakšić, Pillet 02]: NESS as resonances of C-Liouvillian

Proposition Assume (H1)–(H3), and let the reference state ω_0 be
(a) quasi-free with density ϱ_0,
(b) τ_0^t-invariant.

Then, there exists a unique NESS ω_+. Moreover, if $c \in \mathcal{L}^1$,

$$\begin{aligned} \omega_+(\mathrm{d}\Gamma(c)) &= \mathrm{tr}(\varrho_+ c), \\ \varrho_+ &= \Omega\varrho_0\Omega^* + \sum_{\varepsilon\in\sigma_{\mathrm{pp}}(h)} 1_\varepsilon(h)\varrho_0 1_\varepsilon(h). \end{aligned}$$

Proof [Kato-Birman theory] $\Rightarrow$ wave operator

$$\Omega = \mathrm{s-}\lim_{t\to\infty} \mathrm{e}^{\mathrm{i}th}\mathrm{e}^{-\mathrm{i}th_0}1_{\mathrm{ac}}(h_0)$$

exists and is complete

$$\omega_0(\tau^t(a^*(f)a(g))) = \\ (\mathrm{e}^{-\mathrm{i}th_0}\mathrm{e}^{\mathrm{i}th}\,[1_{\mathrm{ac}}(h) + 1_{\mathrm{pp}}(h)]g, \varrho_0\,\mathrm{e}^{-\mathrm{i}th_0}\mathrm{e}^{\mathrm{i}th}\,[1_{\mathrm{ac}}(h) + 1_{\mathrm{pp}}(h)]f)$$

□

Example **XY chain**

- quasi-free reference state with reservoirs in thermal equilibrium (KMS)

$$\varrho_0 = (1 + \mathrm{e}^{-k_0})^{-1}, \quad k_0 = 0 \oplus \beta_1 h_1 \oplus \beta_2 h_2$$

- using partial wave operators and asymptotic projections

$$\varrho_+ = \Omega\varrho_0\Omega^* = (1 + \mathrm{e}^{-k_+})^{-1}, \quad k_+ = (\beta - \delta\,\mathrm{sign}\,V)h$$

$\beta = (\beta_1 + \beta_2)/2$, $\delta = (\beta_1 - \beta_2)/2$, and V asymptotic velocity

1.3 Flux observables

We describe fluxes of conserved extensive thermodynamic quantities entering the sample $\mathcal{S}$ from the reservoirs $\mathcal{R}_j$.

- charge $q^* = q$ with $\mathrm{e}^{\mathrm{i}th_0}\, q\, \mathrm{e}^{-\mathrm{i}th_0} = q$

Example $q = h_j$ energy (q not necessarily bounded) or $q = 1_j$ particle number of reservoir $\mathcal{R}_j$

- extensive charge $Q = \mathrm{d}\Gamma(q)$

- rate of change of extensive charge (formal)

$$\Phi_q = -\frac{\mathrm{d}}{\mathrm{d}t}\bigg|_{t=0} \mathrm{e}^{\mathrm{i}t\mathrm{d}\Gamma(h)} Q \mathrm{e}^{-\mathrm{i}t\mathrm{d}\Gamma(h)} = \mathrm{d}\Gamma(\varphi_q)$$

$$\varphi_q = -\mathrm{i}[h, q]$$

Example **XY chain** $\varphi_q \in \mathcal{L}^0$ with $q = h_1$

$\mathcal{L}^0$ finite rank operators

Problem

in general, $\Phi_q = \mathrm{d}\Gamma(\varphi_q)$ with $\varphi_q = -\mathrm{i}[h, q]$ is *not* observable

$\mathrm{d}\Gamma(\varphi) \in \mathcal{A}(\mathfrak{h}) \Leftrightarrow \varphi \in \mathcal{L}^1$

$\Rightarrow$ regularization

• regularization

charge q is tempered iff

$$q_\Lambda = q\, 1_{(-\infty,\Lambda]}(h_0) \in \mathcal{L} \quad \text{for all } \Lambda \in \mathbb{R}$$

$\mathcal{L}$ bounded operators

$$\varphi_{q_\Lambda} = -\mathrm{i}\,[\underbrace{h - h_0}_{\in\,\mathcal{L}^1}, q_\Lambda] \in \mathcal{L}^1 \quad \Rightarrow \quad \Phi_{q_\Lambda} = \mathrm{d}\Gamma(\varphi_{q_\Lambda}) \text{ is observable}$$

additional regularization for (H2') in 3.2 below

• define NESS expectation of tempered charge flux by

$$\omega_+(\Phi_q) = \lim_{\Lambda\to\infty} \omega_+(\Phi_{q_\Lambda})$$

Lemma Assume q to be a tempered charge. Then,

$$\omega_+(\Phi_{q_\Lambda}) = \mathrm{tr}(\varrho_0 \Omega^* \varphi_{q_\Lambda} \Omega).$$

Proof

$$\omega_+(\Phi_{q_\Lambda}) = \mathrm{tr}(\varrho_+ \varphi_{q_\Lambda}) = \mathrm{tr}(\Omega \varrho_0 \Omega^* \varphi_{q_\Lambda}) + \sum_{\varepsilon \in \sigma_{\mathrm{pp}}(h)} \mathrm{tr}(\varrho_0 1_\varepsilon(h) \varphi_{q_\Lambda} 1_\varepsilon(h))$$

the second term vanishes since the flux φ_{q_Λ} is a commutator

$$1_\varepsilon(h)\varphi_{q_\Lambda} 1_\varepsilon(h) = -\mathrm{i}\, 1_\varepsilon(h)[h - h_0, q_\Lambda] 1_\varepsilon(h) = 0$$

$\square$

2. Landauer-Büttiker formulas

The Landauer-Büttiker theory expresses NESS currents by means of the scattering matrix $S = \Omega_+^* \Omega_-$ of the underlying scattering process on the one-particle space.

wave operators $\Omega_\pm = \text{s}-\lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}th}\mathrm{e}^{-\mathrm{i}th_0}1_{\mathrm{ac}}(h_0)$ and $\Omega \equiv \Omega_+$

We show that, for systems in the independent electrons approximation, the Landauer-Büttiker theory derives from Ruelle's scattering approach to NESS.

2.1 General structure

Theorem [AJPP07] Assume (H1)–(H3), and let
(a) ω_0 be a τ_0-invariant, quasi-free reference state with density ϱ_0,
(b) q be a tempered charge with $\operatorname{ess\,sup}_{\varepsilon\in\sigma_{\mathrm{ac}}(h_0)}\|\varrho_0(\varepsilon)\|\|q(\varepsilon)\| < \infty$.

Then,

$$\omega_+(\Phi_q) = \int_{\sigma_{\mathrm{ac}}(h_0)} \frac{\mathrm{d}\varepsilon}{2\pi}\,\mathrm{tr}(\varrho_0(\varepsilon)[q(\varepsilon) - S^*(\varepsilon)q(\varepsilon)S(\varepsilon)]).$$

Proof by stationary scattering theory for perturbations of trace class type

major ingredients only, can be made rigorous everywhere

- we first extract the kernel $D_\Lambda(\varepsilon)$

$$
\begin{aligned}
\omega_+(\Phi_{q_\Lambda}) &= \mathrm{tr}(\varrho_0\Omega^*\varphi_{q_\Lambda}\Omega)\\
&= \mathrm{i}\,\mathrm{tr}(\varrho_0\Omega^*[q_\Lambda, h-h_0]\Omega)
\end{aligned}
$$

$h-h_0 = x^*y \in \mathcal{L}^1$ with $x, y \in \mathcal{L}^2$ Hilbert-Schmidt operators

$$
= \mathrm{i}\,\mathrm{tr}(\varrho_0\Omega^*[q_\Lambda x^*y - x^*yq_\Lambda]\Omega)
$$

$U:\, \mathfrak{h}_{\mathrm{ac}}(h_0) \to \int_{\sigma_{ac}(h_0)} \mathfrak{h}(\varepsilon)\,\mathrm{d}\varepsilon$, energy shell $\mathfrak{h}(\varepsilon)$

$$
\begin{aligned}
&= \mathrm{i}\,\mathrm{tr}(\varrho_0 U^*U\Omega^*[q_\Lambda x^*y - x^*yq_\Lambda]\Omega U^*U)\\
&= \mathrm{i}\,\mathrm{tr}(U\varrho_0U^*\,[U(xq_\Lambda\Omega)^*(U(y\Omega)^*)^* - U(x\Omega)^*(U(yq_\Lambda\Omega)^*)^*])
\end{aligned}
$$

τ_0^t-invariance $\mathrm{e}^{\mathrm{i}th_0}\varrho_0\mathrm{e}^{-\mathrm{i}th_0} = \varrho_0$

$$
= \mathrm{i}\int_{\sigma_{\mathrm{ac}}(h_0)} \mathrm{d}\varepsilon\ \mathrm{tr}(\varrho_0(\varepsilon)D_\Lambda(\varepsilon)),
$$

and, with $Z(a,\varepsilon)\psi = (Ua^*\psi)(\varepsilon)$ for $a \in \mathcal{L}^2$,

$$
D_\Lambda(\varepsilon) = Z(xq_\Lambda\Omega,\varepsilon)Z^*(y\Omega,\varepsilon) - Z(x\Omega,\varepsilon)Z^*(yq_\Lambda\Omega,\varepsilon)
$$

• we compute $D_\Lambda(\varepsilon)$ in four steps:

(1) relate $Z(a\Omega,\varepsilon)$ to the perturbed resolvent $r(\varepsilon - \mathrm{i}\delta)$ (formal)

strong, weak, weak abelian wave operator ⇒ resolvent

$$\begin{aligned} Z(a\Omega,\varepsilon)\psi &= \lim_{\delta\downarrow 0} \delta\int_0^\infty \mathrm{d}t\, \mathrm{e}^{-\delta t}(U\mathrm{e}^{\mathrm{i}th_0}\mathrm{e}^{-\mathrm{i}th}a^*\psi)(\varepsilon) \\ &= \lim_{\delta\downarrow 0} \mathrm{i}\delta(Ur(\varepsilon-\mathrm{i}\delta)a^*\psi)(\varepsilon) \end{aligned}$$

(2) relate $r(\varepsilon - \mathrm{i}\delta)$ to the bordered free resolvent $yr_0(\varepsilon-\mathrm{i}\delta)x^*$

iterate resolvent identity with $h - h_0 = x^*y$

$$r = r_0 - r_0x^*y(r_0 - rx^*yr_0) = r_0 - r_0x^* \underbrace{(1-yrx^*)}_{(1+yr_0x^*)^{-1} = Q} yr_0$$

(3) compute boundary values of bordered resolvents (limiting absorption principle)

$$\mathrm{i}\delta(Ur(\varepsilon-\mathrm{i}\delta)a^*\psi)(\varepsilon) = (Ua^*\psi)(\varepsilon) - (Ux^*Q(\varepsilon-\mathrm{i}\delta)yr_0(\varepsilon-\mathrm{i}\delta)a^*\psi)(\varepsilon)$$

$\mathcal{L}^2 - \lim_{\delta\to 0} ar_0(\varepsilon \pm \mathrm{i}\delta)b$ with $a, b \in \mathcal{L}^2$ exists for a.e. $\varepsilon \in \mathbb{R}$

$$\delta \downarrow 0 \;\Rightarrow\; Z(a\Omega,\varepsilon) = Z(a,\varepsilon) - Z(x,\varepsilon)Q(\varepsilon - \mathrm{i}0)yr_0(\varepsilon-\mathrm{i}0)a^*$$

(4) relate $D_\Lambda(\varepsilon)$ to the on-shell scattering matrix $S(\varepsilon)$

$$D_\Lambda(\varepsilon) = Z(xq_\Lambda\Omega,\varepsilon)Z^*(y\Omega,\varepsilon) - Z(x\Omega,\varepsilon)Z^*(yq_\Lambda\Omega,\varepsilon)$$

plug in $Z(a\Omega,\varepsilon)$ and use $S(\varepsilon) = 1 - 2\pi\mathrm{i}\, Z(x,\varepsilon)Q(\varepsilon+\mathrm{i}0)Z^*(y,\varepsilon)$

$$= \frac{1}{2\pi\mathrm{i}}\left[q_\Lambda(\varepsilon) - S^*(\varepsilon)q_\Lambda(\varepsilon)S(\varepsilon)\right]$$

hence, the regularized mean flux becomes

$$\omega_+(\Phi_{q_\Lambda}) = \int_{\sigma_{\mathrm{ac}}(h_0)} \frac{\mathrm{d}\varepsilon}{2\pi}\,\mathrm{tr}(\varrho_0(\varepsilon)[q_\Lambda(\varepsilon) - S^*(\varepsilon)q_\Lambda(\varepsilon)S(\varepsilon)])$$

- finally, we remove the regularizing cut-off

$$|\omega_+(\Phi_{q_\Lambda})| \leq 2\int_{\sigma_{\mathrm{ac}}(h_0)} \frac{\mathrm{d}\varepsilon}{2\pi}\,\|\varrho_0(\varepsilon)\|\|q(\varepsilon)\|\|1 - S(\varepsilon)\|_1$$

use $\int_{\sigma_{\mathrm{ac}}(h_0)} \frac{\mathrm{d}\varepsilon}{2\pi}\,\|1 - S(\varepsilon)\|_1 \leq \|h - h_0\|_1$

$$\leq \underbrace{\sup_{\varepsilon\in\sigma_{\mathrm{ac}}(h_0)} \|\varrho_0(\varepsilon)\|\|q(\varepsilon)\|}_{<\infty \text{ by assumption}}\ \|h - h_0\|_1$$

□

2.2 Landauer-Büttiker formula

The Landauer-Büttiker formula is a corollary of the foregoing theorem under the additional assumption (H4) $\sigma_{\rm ess}(h_{\mathcal{S}}) = \emptyset$.

$\mathfrak{h}(\varepsilon) = \oplus_j \mathfrak{h}_j(\varepsilon)$ channels

- total transmission probability

$$T_{jk}(\varepsilon) = \mathrm{tr}(t_{jk}^*(\varepsilon) t_{jk}(\varepsilon)), \quad S_{jk}(\varepsilon) = \delta_{jk} + \underbrace{t_{jk}(\varepsilon)}_{\text{transmission amplitude } \mathcal{R}_k \to \mathcal{R}_j}$$

Theorem [L-B] Assume also (H4), and let
(a) $\varrho_0 = \oplus_j f_j(h_j)$,
(b) $q = \oplus_j g_j(h_j)$.

Then,

$$\omega_+(\Phi_q) = \sum_{j,k} \int_{\sigma_{\rm ac}(h_j)\cap\sigma_{\rm ac}(h_k)} \frac{\mathrm{d}\varepsilon}{2\pi} T_{jk}(\varepsilon) \, [f_j(\varepsilon) - f_k(\varepsilon)] g_j(\varepsilon).$$

$\omega_+(\Phi_q) = 0$ if "same states" $f_j = f_k$

2.3 Entropy production rate

We further specialize to the situation of heat and charge currents between reservoirs $\mathcal{R}_k$ in thermal equilibrium at different temperatures and chemical potentials.

Corollary [from L-B] Let

(a) $f_j(\varepsilon) = (1 + e^{\beta_j(\varepsilon - \mu_j)})^{-1}$ Fermi-Dirac distribution,

(b) $q_j^{\mathrm{c}} = 1_j$, $q_j^{\mathrm{h}} = h_j$.

Then,

$$\omega_+(\Sigma) = \sum_{j,k} \int_{\sigma_{\mathrm{ac}}(h_j) \cap \sigma_{\mathrm{ac}}(h_k)} \frac{\mathrm{d}\varepsilon}{2\pi} \, \xi_k(\varepsilon) \, T_{kj}(\varepsilon) \, [F(\xi_j(\varepsilon)) - F(\xi_k(\varepsilon))],$$

where $\xi_k(\varepsilon) = \beta_k(\varepsilon - \mu_k)$ and $F(x) = (1 + e^x)^{-1}$, and the entropy production rate observable is

$$\Sigma = -\sum_j \beta_j (\Phi_{q_j^{\mathrm{h}}} - \mu_j \Phi_{q_j^{\mathrm{c}}}).$$

- the channel $j \to k$ is open iff

$$|\{\varepsilon \in \sigma_{\rm ac}(h_j) \cap \sigma_{\rm ac}(h_k) \,|\, T_{kj}(\varepsilon) \neq 0\}| > 0$$

Theorem If there exists an open channel such that $\beta_j \neq \beta_k$ or $\mu_j \neq \mu_k$, then

$$\omega_+(\Sigma) > 0.$$

Proof Use unitarity of the S-matrix (Pauli) to derive a nonnegative lower bound on $\omega_+(\Sigma)$. Strict positivity follows from this bound. □

Remark if system is time reversal invariant, proof of lower bound much simpler

Example **XY chain**

$$\omega_+(\Sigma) = \frac{\delta}{2} \int_0^{2\pi} \frac{d\xi}{2\pi} |\mathbf{p} \cdot \mathbf{h}| \frac{\text{sh}\,(\delta|h|)}{\text{ch}^2(\beta|h|/2) + \text{sh}^2(\delta|h|/2)} > 0 \quad \text{if} \quad \beta_1 \neq \beta_2$$

where $h = \mathbf{h} \otimes \sigma$ and $p = -\mathrm{i}[h, x] = \mathbf{p} \otimes \sigma$

3. Remarks

3.1 Kinetic transport coefficients

similar expressions for $L_{kj}^{\mathrm{uv}} = \partial_{X_j^{\mathrm{v}}}\, \omega_+(\Phi_{q_k^{\mathrm{u}}})|_{X=0}$, where $\beta_k = \beta - X_k^{\mathrm{h}}$ and $\beta_k\mu_k = \beta\mu + X_k^{\mathrm{c}}$

3.2 Generalized couplings

(H2') $r^p - r_0^p \in \mathcal{L}^1$ for some $p \in \{-1\} \cup \mathbb{N}$

- additional regularization for $p \in \mathbb{N}$

$f_\eta(x) = x(1+\eta x)^{-(p+1)} \;\Rightarrow\; \varphi_{q_\Lambda}^{\eta} = -i[\underbrace{f_\eta(h) - f_\eta(h_0)}_{\in \mathcal{L}^1}, q_\Lambda] \in \mathcal{L}^1$

- use Birman's invariance principle for $f_\eta(h_0)$ and $f_\eta(h)$

i.e. "$\Omega_\pm(h, h_0) = \Omega_\pm(f_\eta(h), f_\eta(h_0))$"

3.3 Self-dual CAR

- generalized relations $\{B^*(f), B(g)\} = (f, g)$ and $B(Jf) = B^*(f)$
- quasi-free state: pfaffian instead of determinant

Example truly anisotropic XY chain

Thank you for your attention!