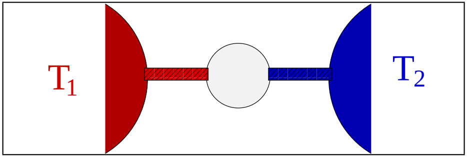
A Rigorous Derivation of the Landauer-Büttiker Formalism



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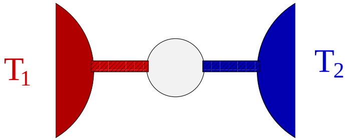
Contents

What are we physically interested in?

Open systems: Fundamental paradigm

- A confined sample is coupled to several extended thermal reservoirs at different temperatures.



- For large times, the suitably coupled system is expected to approach a unique NonEquilibrium Steady State (NESS).
- The NESS carries a nontrivial current driven by the thermodynamic force.
- How does this current relate to the underlying scattering process?

What are we physically interested in?

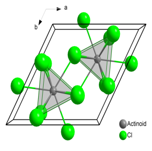
Specific model: XY chain [Lieb *et al.* 61, Araki 84]

- The Heisenberg Hamiltonian density reads

$$H_x = \sum_{n=1,2,3} J_n \sigma_n^{(x)} \sigma_n^{(x+1)} + \lambda \sigma_3^{(x)},$$

and the XY chain is the special case with $J_3 = 0$.

Experiments $SrCuO_2$, Sr_2CuO_3 [Sologubenko *et al.* 01] with $J_3 \neq 0$
$PrCl_3$ [D'Iorio *et al.* 83, Culvahouse *et al.* 69] with $J_1 = J_2$, $J_3 \approx 0$, *i.e.*, $J_3/J_1 \approx 10^{-2}$, and $\lambda = 0$



Formalism of quantum statistical mechanics

Rigorous foundation in the early 1930s:

1. An observable A is a selfadjoint operator on the Hilbert space of the system.
2. The dynamics of the system is determined by a distinguished selfadjoint operator H, called the Hamiltonian, through $A \mapsto A_t = \mathrm{e}^{\mathrm{i}tH} A \mathrm{e}^{-\mathrm{i}tH}$.
3. A pure state is a vector ψ in the Hilbert space, and the expectation value of the measurement of A in the state ψ is $(\psi, A\psi)$.

Algebraic reformulation and generalization (von Neumann, Jordan, Wigner, ...):

Observables

C^* algebra $\mathfrak{A}$

Dynamics

(Strongly) continuous group τ^t of *-automorphisms on $\mathfrak{A}$

States

Normalized positive linear functionals ω on $\mathfrak{A}$

Example $\mathfrak{A} = \mathcal{L}(\mathfrak{h})$, $\tau^t(A) = \mathrm{e}^{\mathrm{i}tH} A \mathrm{e}^{-\mathrm{i}tH}$, and $\omega(A) = \mathrm{tr}(\varrho A)$.

1.1 Quasifree setting

Observables

- The algebra of observables is given as follows:

Canonical AntiCommutation Relations (CAR) algebra

Let $\mathfrak{h}$ be a complex Hilbert space, called the *one-particle Hilbert space*. The *CAR algebra* $\mathfrak{A} \equiv \mathfrak{A}(\mathfrak{h})$ is the (unique) C^* algebra generated by the identity $\mathbb{1}$ and elements $a(f)$, $f \in \mathfrak{h}$, satisfying:

- $a(f)$ is antilinear in f
- $\{a(f), a(g)\} = 0$
- $\{a(f), a^*(g)\} = (f, g)\, \mathbb{1}$

Sample and subreservoir structure

$$\mathfrak{h} = \mathfrak{h}_{\mathcal{S}} \oplus \mathfrak{h}_{\mathcal{R}} \text{ and } \mathfrak{h}_{\mathcal{R}} = \oplus_{j=1}^{M} \mathfrak{h}_j$$

Example: XY NESS [A-Pillet 03] For $x \in \mathbb{Z}$ s.t. $\mathbb{Z}_{\mathcal{S}} = \{|x| \leq \ell\}$, $\mathbb{Z}_1 = \{x < -\ell\}$, $\mathbb{Z}_2 = \{x > \ell\}$, we have $\mathfrak{h} = \ell^2(\mathbb{Z}) \simeq \ell^2(\mathbb{Z}_{\mathcal{S}}) \oplus \ell^2(\mathbb{Z}_1) \oplus \ell^2(\mathbb{Z}_2)$.

Quasifree setting

Dynamics

- The time evolution has the following structure:

Decoupled and coupled dynamics

The decoupled and the coupled time evolutions are given by groups of *Bogoliubov ∗-automorphisms* acting on the generators as

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

Assumptions [A *et al.* 07]

(A1) $h_0, h \geq -E_0$
(A2) $h - h_0 \in \mathcal{L}^1(\mathfrak{h})$
(A3) $\sigma_{\mathrm{sc}}(h) = \emptyset$

Example: XY NESS $h = \mathrm{Re}(u) \in \mathcal{L}(\mathfrak{h})$ and $h - h_0 = v_L + v_R \in \mathcal{L}^0(\mathfrak{h})$ with $v_L = \mathrm{Re}(u^{-(\ell+1)} p_0 u^\ell)$ and $v_R = \mathrm{Re}(u^\ell p_0 u^{-(\ell+1)})$ (for $J_1 = J_2$ and $\lambda = 0$).

Quasifree setting

States

- States are normalized positive linear functionals on $\mathfrak{A}$, denoted by $\mathcal{E}(\mathfrak{A})$.
- The two-point function is characterized as follows:

Density

The *density* of a state $\omega \in \mathcal{E}(\mathfrak{A})$ is the operator $\varrho \in \mathcal{L}(\mathfrak{h})$ satisfying $0 \leq \varrho \leq 1$ and, for all $f, g \in \mathfrak{h}$,

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

- The class of states we are concerned with is:

Quasifree states

A state $\omega \in \mathcal{E}(\mathfrak{A})$ with density $\varrho \in \mathcal{L}(\mathfrak{h})$ is called *quasifree* if

$$\omega(a^*(f_n)...a^*(f_1)a(g_1)...a(g_m)) = \delta_{nm} \det[(g_i, \varrho f_j)]_{i,j=1}^n.$$

Example: XY chain $\varrho = \varrho(h) = (1 + \mathrm{e}^{\beta h})^{-1}$ is the thermal equilibrium state at inverse temperature β (i.e. the so-called KMS state).

Quasifree setting

States

- For the nonequilibrium situation, we use:

NESS [Ruelle 01]

A *NESS* $\omega_+ \in \mathcal{E}(\mathfrak{A})$ associated with the C^*-dynamical system $(\mathfrak{A}, \tau)$ and the initial state $\omega_0 \in \mathcal{E}(\mathfrak{A})$ is a weak-$*$ limit point for $T \to \infty$ of

$$\left\{ \frac{1}{T} \int_0^T \mathrm{d}t \; \omega_0 \circ \tau^t \,\middle|\, T > 0 \right\}.$$

- There are two rigorous approaches to the construction of NESS.
  (1) The time dependent scattering approach [Ruelle 00]
  (2) The spectral approach [Jakšić-Pillet 02]

  We will use the first approach.

1.2 NESS existence and uniqueness

Proposition: NESS density [A *et al.* 07]

Assume (A1)–(A3), and let the initial state $\omega_0 \in \mathcal{E}(\mathfrak{A})$ be
(1) quasifree with density $\varrho_0 \in \mathcal{L}(\mathfrak{h})$,
(2) τ_0^t-invariant.

Then, there exists a unique NESS $\omega_+ \in \mathcal{E}(\mathfrak{A})$ with density $\varrho_+ \in \mathcal{L}(\mathfrak{h})$ given by

$$\varrho_+ = w_+ \varrho_0 w_+^* + \sum_{e \in \mathrm{spec_{pp}}(h)} 1_e(h) \varrho_0 1_e(h).$$

Def: $1_e(h), 1_{\mathrm{ac}}(h) \in \mathcal{L}(\mathfrak{h})$ denote the spectral projections. The wave operator $w_\pm \equiv w_\pm(h, h_0) \in \mathcal{L}(\mathfrak{h})$ is defined by $w_\pm := \mathrm{s} - \lim_{t \to \pm\infty} \mathrm{e}^{ith} \mathrm{e}^{-ith_0} 1_{\mathrm{ac}}(h_0)$.

Example: XY NESS [A-Pillet 03] $\varrho_0 = (1 + \mathrm{e}^{k_0})^{-1}$, where $k_0 = 0 \oplus \beta_1 h_1 \oplus \beta_2 h_2$, and, with $\beta = (\beta_1 + \beta_2)/2$, $\delta = (\beta_1 - \beta_2)/2$, and the asymptotic velocity v, we have

$$\varrho_+ = w_+ \varrho_0 w_+^* = (1 + \mathrm{e}^{k_+})^{-1} \quad \text{with} \quad k_+ = (\beta - \delta\, \mathrm{sign}\, v) h.$$

1.3 NESS currents

Current observables

- Charge currents are defined as follows:

Charge

$q \in \mathcal{L}(\mathfrak{h})$ is called a *charge* if $q = q^*$ and $\mathrm{e}^{\mathrm{i}th_0} q \mathrm{e}^{-\mathrm{i}th_0} = q$ for all $t \in \mathbb{R}$.

Charge current

The *charge current* $\varphi_q \in \mathcal{L}^1(\mathfrak{h})$ w.r.t. charge q is defined by

$$\varphi_q = \mathrm{i}[q, h - h_0].$$

The *extensive charge current* is $\Phi_q = \mathrm{d}\Gamma(\varphi_q) \in \mathfrak{A}$.

Example: XY NESS $q = h_j \in \mathcal{L}(\mathfrak{h})$ is the energy of subreservoir $j = 1, 2$, and $\varphi_q \in \mathcal{L}^0(\mathfrak{h})$.

2.1 General structure

Landauer-Büttiker formalism

The Landauer-Büttiker transport formalism for systems of independent electrons expresses the steady currents flowing through the small sample coupled to extended reservoirs in thermal equilibrium in terms of the one-electron scattering matrix $S = w_+^* w_-$.

Theorem: General Landauer-Büttiker formalism [A *et al.* 07]

Assume (A1)–(A3), and let

(1) $\omega_0 \in \mathcal{E}(\mathfrak{A})$ be a τ_0^t-invariant, quasifree initial state with density $\varrho_0 \in \mathcal{L}(\mathfrak{h})$,

(2) $q \in \mathcal{L}(\mathfrak{h})$ a charge,

(3) $|||\varrho_0(e)|||\,|||q(e)|||_{L^\infty(\sigma_{\mathrm{ac}}(h_0))} < \infty$.

Then, the NESS current can be expressed as

$$\omega_+(\Phi_q) = \frac{1}{2\pi} \int_{\sigma_{\mathrm{ac}}(h_0)} \mathrm{d}e \quad \mathrm{tr}(\varrho_0(e)[q(e) - S^*(e) q(e) S(e)]).$$

General structure

Proof.

1. With $\omega(\mathrm{d}\Gamma(c)) = \mathrm{tr}(\varrho c)$ for $c \in \mathcal{L}^1(\mathfrak{h})$, the factorization $h - h_0 = x^* y$ for some $x, y \in \mathcal{L}^2(\mathfrak{h})$, and the direct integral representation $U : \mathfrak{h}_{\mathrm{ac}}(h_0) \to \int_{\sigma_{\mathrm{ac}}(h_0)}^{\oplus} \mathrm{d}e\ \mathfrak{h}(e)$, we have, with $w \equiv w_+$,

$$\begin{aligned}
\omega_+(\Phi_q) &= \mathrm{tr}(\varrho_0 w^* \varphi_q w) + \sum_{e \in \mathrm{spec}_{\mathrm{pp}}(h)} \mathrm{tr}(\varrho_0 \underbrace{1_e(h)\varphi_q 1_e(h)}_{=0}) \\
&= \mathrm{i}\,\mathrm{tr}(\varrho_0 w^* [q, h - h_0] w) \\
&= \mathrm{i}\,\mathrm{tr}(\varrho_0 w^* (q x^* y - x^* y q) w) \\
&= \mathrm{i}\,\mathrm{tr}(\varrho_0 U^* U w^* (q x^* y - x^* y q) w U^* U) \\
&= \mathrm{i}\,\mathrm{tr}(U \varrho_0 U^* \, [U(xqw)^* (U(yw)^*)^* - U(xw)^* (U(yqw)^*)^*]) \\
&= \mathrm{i} \int_{\sigma_{\mathrm{ac}}(h_0)} \mathrm{d}e \ \ \mathrm{tr}(\varrho_0(e) D(e)).
\end{aligned}$$

For $a \in \mathcal{L}^2(\mathfrak{h}_{ac}(h_0), \mathfrak{h})$, the map $Z(a, e) \in \mathcal{L}^2(\mathfrak{h}, \mathfrak{h}(e))$ is defined by $Z(a, e)\psi = (Ua^*\psi)(e)$, and we can write the kernel as

$$D(e) = Z(xqw, e) Z^*(yw, e) - Z(xw, e) Z^*(yqw, e).$$

General structure

Stationary scattering theory expresses the dynamical wave operator in terms of the resolvents of the Hamiltonians. Using this scheme, we compute $D(e)$ in four steps.

2. [Relate $Z(aw, e)$ to $r_{e-\mathrm{i}\delta}(h)$] Formally, we have

$$\begin{aligned} Z(aw,e)\psi &= \lim_{\delta\to 0+} \delta \int_0^\infty \mathrm{d}t\, \mathrm{e}^{-\delta t} (U \mathrm{e}^{\mathrm{i}th_0} \mathrm{e}^{-\mathrm{i}th} a^* \psi)(e) \\ &= \lim_{\delta\to 0+} \mathrm{i}\,\delta (U r_{e-\mathrm{i}\delta}(h) a^* \psi)(e). \end{aligned}$$

3. [Relate $r_{e-\mathrm{i}\delta}(h)$ to $y r_{e-\mathrm{i}\delta}(h_0) x^*$] Iterating the resolvent identity, we get

$$r_{e-\mathrm{i}\delta}(h) = r_{e-\mathrm{i}\delta}(h_0) - r_{e-\mathrm{i}\delta}(h_0) x^* Q(e-\mathrm{i}\delta) y r_{e-\mathrm{i}\delta}(h_0),$$

where we define $Q(e-\mathrm{i}\delta) = (1 + y r_{e-\mathrm{i}\delta}(h_0) x^*)^{-1}$.

General structure

4. [Compute boundary values] Plugging the foregoing into $Z(aw, e)$, we have $\mathrm{i}\,\delta(Ur_{e-\mathrm{i}\delta}(h)a^*\psi)(e) = (Ua^*\psi)(e) - (Ux^*Q(e-\mathrm{i}\delta)yr_{e-\mathrm{i}\delta}(h_0)a^*\psi)(e)$.
   With the sufficiently regular factorization of $h - h_0$, the limit $\delta \to 0^+$ yields
   $$Z(aw, e) = Z(a, e) - Z(x, e)Q(e - \mathrm{i}0)yr_{e-\mathrm{i}0}(h_0)a^*,$$
   where we used that, for $a, b \in \mathcal{L}^2(\mathfrak{h})$, the limit $\lim_{\delta\to 0^+} ar_{e\pm\mathrm{i}\delta}(h_0)b$ exists in $\mathcal{L}^2(\mathfrak{h})$ for a.e. $e \in \mathbb{R}$ (abstract limiting absorption principle).
5. [Relate $D(e)$ to $S(e)$] Plugging the foregoing into $D(e)$ and using that $S(e) = 1 - 2\pi\mathrm{i}Z(x, e)Q(e + \mathrm{i}0)Z^*(y, e)$, we find
   $$D(e) = \frac{1}{2\pi\mathrm{i}}\,(q(e) - S^*(e)q(e)S(e)).$$
6. Finally, the assertion is well-defined since
   $$|\omega_+(\Phi_q)| \le \frac{1}{\pi}\int_{\sigma_{\mathrm{ac}}(h_0)} \mathrm{d}e\ \ \|\varrho_0(e)\|\|q(e)\|\|S(e) - 1\|_1 < \infty,$$
   where we use $\int_{\sigma_{\mathrm{ac}}(h_0)} \mathrm{d}e\ \|S(e) - 1\|_1 \le 2\pi\|h - h_0\|_1$ and (3).

□

2.2 Landauer-Büttiker formula

Landauer-Büttiker formula

We make the following additional assumptions:

(A4) $h_0 = h_\mathcal{S} \oplus h_\mathcal{R}$ and $h_\mathcal{R} = \oplus_{j=1}^M h_j$ (*partitioning*)

(A5) $\sigma_{\rm ess}(h_\mathcal{S}) = \emptyset$

Corollary: Landauer-Büttiker formula [A *et al.* 07]

Assume (A1)–(A5), and let

(1) $\varrho_\mathcal{R} = \oplus_{j=1}^M f_j(h_j)$,

(2) $q_\mathcal{R} = \oplus_{j=1}^M g_j(h_j)$,

(3) $\max_{j,k}\{|f_j g_k|_{L^\infty(\sigma_{\rm ac}(h_j)\cap\sigma_{\rm ac}(h_k))} < \infty\}$.

Then, the NESS current can be expressed as

$$\omega_+(\Phi_q) = \frac{1}{2\pi}\sum_{j,k=1}^M \int_{\sigma_{\rm ac}(h_j)\cap\sigma_{\rm ac}(h_k)} {\rm d}e \quad T_{jk}(e)\,[f_j(e) - f_k(e)]\,g_j(e).$$

Def: $T_{jk} = {\rm tr}(t_{jk}^* t_{jk})$ with $t_{jk} = S_{jk} - \delta_{jk}$ denotes the transmission probability.

3. Remarks

Unbounded charges

Heat currents often stem from charges $q_j = h_j \notin \mathcal{L}(\mathfrak{h})$. The corresponding extensive charge current is i.g. not observable. Regularizing charges q s.t.

$$q 1_{(-\infty,\Lambda]}(h_0) \in \mathcal{L}(\mathfrak{h})$$

for all $\Lambda \in \mathbb{R}$, leads to the LB-formalism in the limit $\Lambda \to \infty$.

More general couplings

The assumption (A2) can be generalized to

$$r_\zeta(h)^p - r_\zeta(h_0)^p \in \mathcal{L}^1(\mathfrak{h}),$$

where $\zeta = -(E_0 + 1)$ and $p \in \{-1\} \cup \mathbb{N}$. This time, the extensive charges require a regularization of the Hamiltonians. Using Birman's invariance principle, the LB-formalism can again be recovered.

Remarks

Entropy production

Using the foregoing remarks, the NESS expectation of the entropy production observable generated by the charges $q = h_j$ and $q = 1_j$,

$$\sigma = -\sum_{j=1}^{M} \beta_j (\Phi_{h_j} - \mu_j \Phi_{1_j}),$$

can be expressed with the help of the LB-formalism. Moreover, it allows to derive the strict positivity of the entropy production, i.e. $\omega_+(\sigma) > 0$.

Example: XY NESS [A-Pillet 03] $\omega_+(\sigma) > 0$ by time dependent scattering theory.

Linear response theory

The LB-formalism leads to expressions for the kinetic transport coefficients,

$$L_{kj}^{\mathrm{hc}} = \partial_{X_j^{\mathrm{c}}} \omega_+(\Phi_{q_k^{\mathrm{h}}})|_{X=0},$$

where $\beta_k = \beta - X_k^{\mathrm{h}}$, $\beta_k \mu_k = \beta\mu + X_k^{\mathrm{c}}$, and $X = (X_1^{\mathrm{h}}, ..., X_M^{\mathrm{c}})$. Moreover, they satisfy the Onsager reciprocity relations.

Summary

Results

1. **(Content)** A generalized LB-formalism is rigorously derived in the context of open quantum system, i.e., for systems of independent electrons, the NESS currents flowing through a sample coupled to several reservoirs are expressed in terms of the underlying scattering process.
2. **(Mathematics)** The mathematical framework being C^* algebras (CAR), the derivation is carried out using functional analysis in the form of stationary scattering theory on the one-electron Hilbert space.
3. **(Assumptions)** The assumptions on the sample-reservoir coupling are of general nature.
4. **(Applications)** Our general framework allows, e.g., for the derivation of:
   - Strict positivity of the entropy production
   - Linear response theory