Transport in quasi-free Fermionic systems

Joint work with

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CAR algebras & free dynamics

One particle Hilbert space $\mathfrak{h}$

One particle Hamiltonian h and charge $q (= I)$

CAR algebras & free dynamics

One particle Hilbert space $\mathfrak{h}$

$\downarrow$

$a^*(f)/a(f)$ on Fermionic Fock space $\Gamma_-(\mathfrak{h})$

$H = d\Gamma(h)$ and $Q = d\Gamma(q)$

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Groups of $*$-automorphisms $\begin{cases} \tau^t(a(f)) = e^{itH}a(f)e^{-itH} = a(e^{ith}f) \\ \vartheta^s(a(f)) = e^{isQ}a(f)e^{-isQ} = a(e^{is}f) \end{cases}$

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Charge sectors $\mathrm{CAR}_n(\mathfrak{h}) = \{A \in \mathrm{CAR}(\mathfrak{h}) | \vartheta^s(A) = e^{ins} A\}$

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Gauge-invariant subalgebra $\mathrm{CAR}_0(\mathfrak{h})$ generated by monomials

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Gauge invariant state on $\mathrm{CAR}(\mathfrak{h})$: $\omega \circ \vartheta^s = \omega$

$$\updownarrow$$

State on $\mathrm{CAR}_0(\mathfrak{h})$

Gauge-invariant states

ω completely determined by $F_n(f_1, \ldots, f_n; g_1, \ldots, g_n) = \omega(a^*(g_1) \cdots a^*(g_n) a(f_n) \cdots a(f_1))$

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ω satisfies Wick's theorem

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for any finite dimensional $\mathfrak{K} \subset \mathfrak{h}$, ω maximizes von Neumann entropy $S(\omega_{|\,\mathrm{CAR}(\mathfrak{K})})$
at fixed density ϱ

KMS states

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$(\tau^t \circ \vartheta^{-\mu t}, \beta)$-KMS state on $\mathrm{CAR}(\mathfrak{h})$ for some $\mu \in \mathbb{R}$

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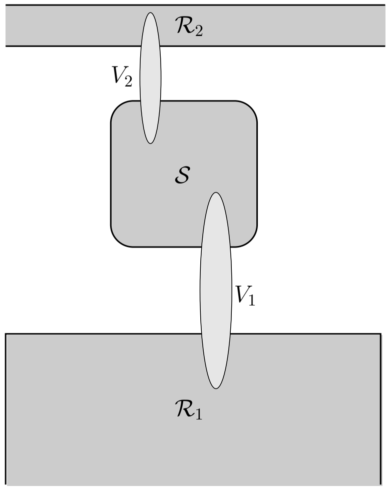
Grand canonical ensemble at inverse temperature β and chemical potential μ

The Electronic Black Box



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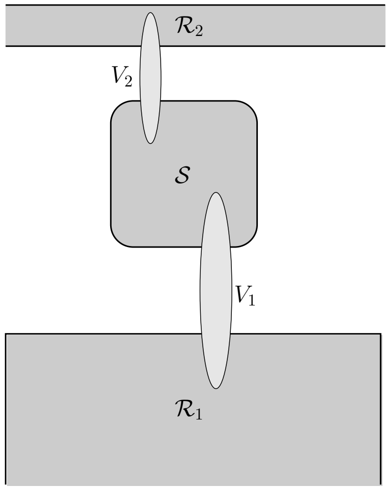

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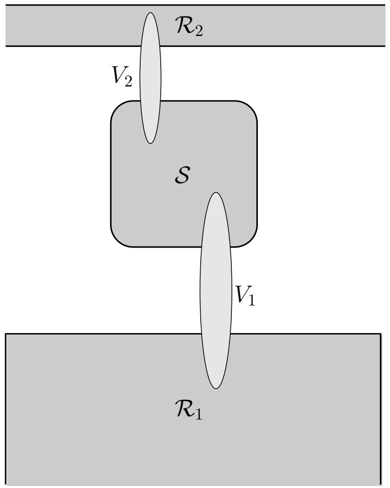

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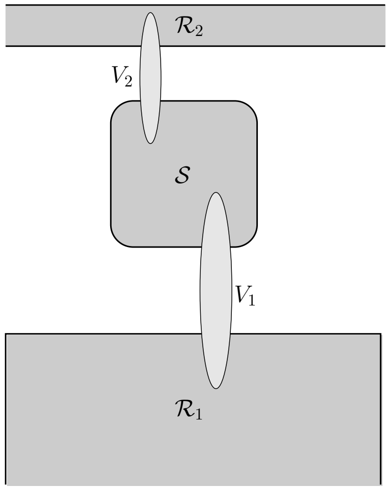

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Coupled one particle Hamiltonian $h = h_0 + V_1 + \cdots$

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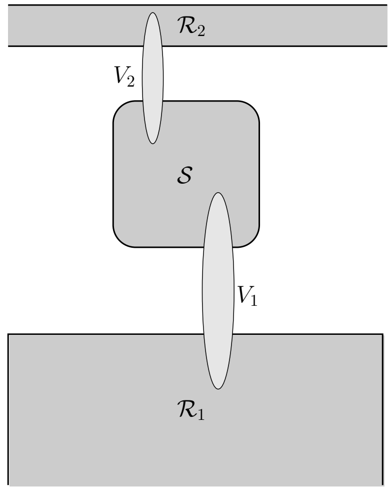

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Example 1: Finite rank coupling (e.g. Tight Binding Models)

$V_j = |f_j\rangle\langle g_j| + |g_j\rangle\langle f_j|$ with $f_j \in \mathfrak{h}_{\mathcal{S}}$ and $g_j \in \mathfrak{h}_{\mathcal{R}_j}$

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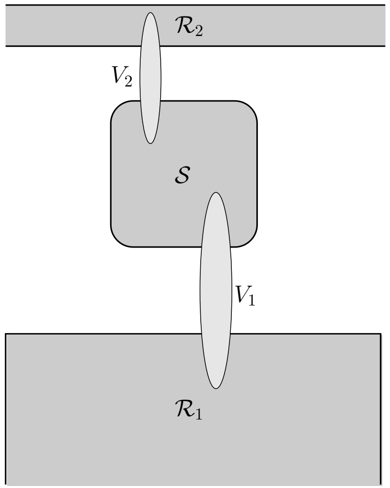

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Example 2: Decoupling Boundary Conditions (e.g. Continuous Models)

$$\mathfrak{h} = L^2(\Lambda),\ \Lambda = \Lambda_{\mathcal{S}} \cup \Lambda_{\mathcal{R}_j} \cup \cdots$$

$$h = -\Delta,\ h_0 = -\Delta_{\Lambda_{\mathcal{S}}} \oplus -\Delta_{\Lambda_{\mathcal{R}_j}} \oplus \cdots$$

Ruelle scattering approach to NESS

Initial state ω_0

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$\mathrm{s} - \lim_{t\to\infty} \tau_0^{-t} \circ \tau^t = \gamma_-$ exists

and ω_0 is τ_0-invariant.

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Unique NESS $\omega_+ = \omega_0 \circ \gamma_-$

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C^*-scattering on $\mathrm{CAR}(\mathfrak{h}_{\mathrm{ac}}(h))$ reduces to Hilbert scattering

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- For trace class c on $\mathfrak{h}$ one has $\omega_+(d\Gamma(c)) = \mathrm{tr}(\varrho_+ c)$ with

$$\varrho_+ = \Omega_- \varrho_0 \Omega_-^* + \sum_{\varepsilon \in \mathrm{sp}_{\mathrm{pp}}(h)} P_\varepsilon \varrho_0 P_\varepsilon$$

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Example 1: The heat flux out of reservoir $\mathcal{R}_k$ is given by

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Example 2: The charge flux out of reservoir $\mathcal{R}_k$ is given by

$$\Phi_k^c = d\Gamma(-i[h, 1_k])$$

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Fluxes need regularization!

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Definition: A tempered conserved charge is a self-adjoint operator q on $\mathfrak{h}$ commuting with h_0 and such that

$$q^{(\Lambda)} = q 1_{]-\infty,\Lambda]}(h_0)$$

is bounded for all $\Lambda \in \mathbb{R}$.

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For $\eta > 0$ set $f_\eta(\varepsilon) = \varepsilon(1 + \eta\varepsilon)^{-(p+1)}$

Definition: Let q be a tempered conserved charge. The regularized flux is

$$\Phi^\eta_{q^{(\Lambda)}} = d\Gamma(\varphi^\eta_{q^{(\Lambda)}}), \qquad \varphi^\eta_{q^{(\Lambda)}} = -i[f_\eta(h), q^{(\Lambda)}].$$

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For $\eta > 0$ set $f_\eta(\varepsilon) = \varepsilon(1 + \eta\varepsilon)^{-(p+1)}$

$$\varphi^{\eta}_{q^{(\Lambda)}} = -i[f_\eta(h), q^{(\Lambda)}]$$

Observe: Under Hypothesis (H2) the regularized flux $\varphi^{\eta}_{q^{(\Lambda)}}$ is trace class

$$\varphi^{\eta}_{q^{(\Lambda)}} = -i[f_\eta(h) - f_\eta(h_0), q^{(\Lambda)}]$$

hence $\Phi^{\eta}_{q^{(\Lambda)}} \in \mathrm{CAR}_0(\mathfrak{h})$.

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Definition: If q is a tempered conserved charge and ω a state with density ϱ we define

$$\omega(\Phi_q) = \lim_{\Lambda\to\infty} \lim_{\eta\to 0} \omega(\Phi^{\eta}_{q^{(\Lambda)}}) = \lim_{\Lambda\to\infty} \lim_{\eta\to 0} \mathrm{tr}(\varrho \varphi^{\eta}_{q^{(\Lambda)}})$$

whenever these limits exist.

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Proposition: If q is a tempered conserved charge and ω a state with density $\varrho = \varrho(h)$ such that $\varrho(h) - \varrho(h_0)$ is trace class

$$\omega(\Phi_q) = 0.$$

In particular, under Hypothesis (H1)-(H3) steady currents vanish at equilibrium.

No transport from point spectrum

Recall $\omega_+(d\Gamma(c)) = \mathrm{tr}(\varrho_+ c)$ with

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Proposition. If ω is a state with density ϱ such that $(\varrho - \varrho_0)1_{\mathrm{ac}}(h)$ is compact (ω needs not be quasi-free), then

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T \omega \circ \tau^t(\Phi^\eta_{q^{(\Lambda)}})\, dt = \omega_+(\Phi^\eta_{q^{(\Lambda)}}).$$

A general steady current formula

Direct integral decomposition $U : \mathfrak{h}_{\rm ac}(h_0) \longrightarrow \int_{{\rm sp}_{\rm ac}(h_0)}^{\oplus} \mathfrak{h}(\varepsilon) d\varepsilon$

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Theorem II. Under Hypothesis (H1)-(H3), if q is a tempered conserved charge such that

$$\operatorname*{ess-sup}_{\varepsilon \in \mathrm{sp_{ac}}(h_0)} (1 + E_0 + \varepsilon)^{p+1} \|\varrho_0(\varepsilon)\| \, \|q(\varepsilon)\| < \infty,$$

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Theorem IV. Under Hypothesis (H1)-(H4) one has

$$L_{kj}^{\mathrm{uv}} = -\int_{\mathrm{sp_{ac}}(h_0)} \varepsilon^{n_{\mathrm{u}}+n_{\mathrm{v}}} f_{\mathrm{eq}}(\varepsilon)(1 - f_{\mathrm{eq}}(\varepsilon)) D_{kj}(\varepsilon) \frac{d\varepsilon}{2\pi}.$$

Here $n_{\mathrm{c}} = 0$, $n_{\mathrm{h}} = 1$, $f_{\mathrm{eq}}(\varepsilon) = (1 + e^{\beta(\varepsilon-\mu)})^{-1}$ and

$$D_{kj}(\varepsilon) = T_{kj}(\varepsilon) - \delta_{kj} \sum_l T_{kl}(\varepsilon).$$

Onsager relations

If the system is Time Reversal Invariant

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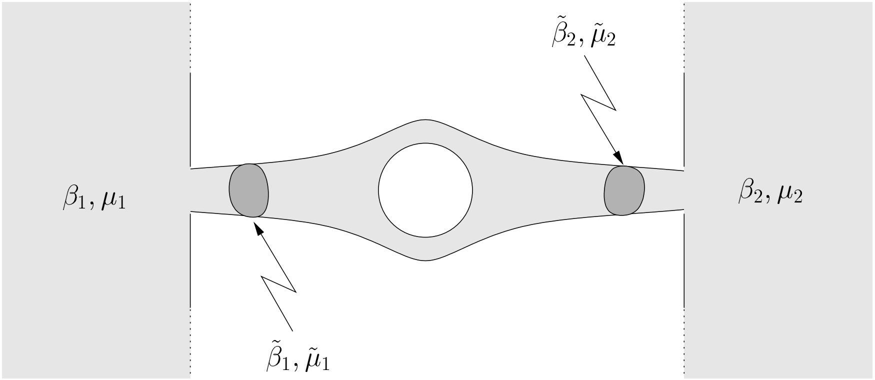
Local thermodynamic parameters



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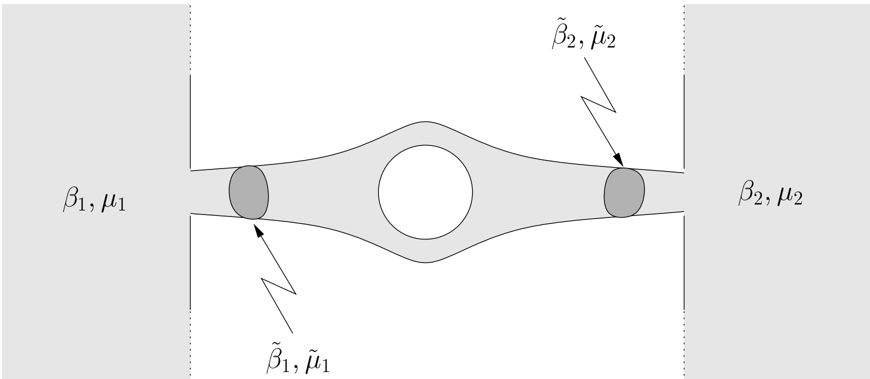

↓

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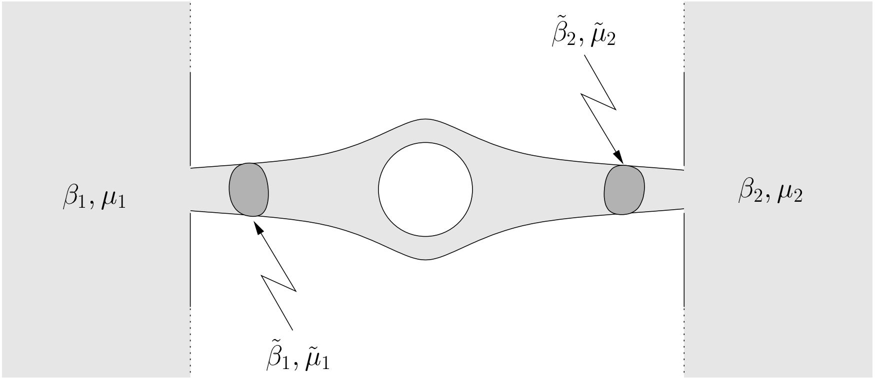

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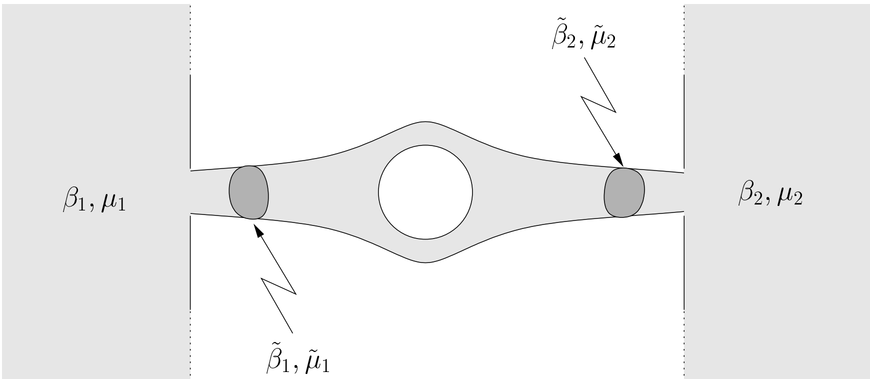

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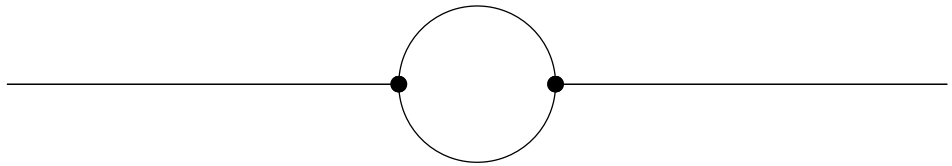
Warning: $\tilde L_{jk}^{\mathrm{uv}}$ do not satisfy Onsager relations!

Local thermodynamic parameters

Example. Two 1-D wires at zero temperature coupled to $\mathcal{S}$.



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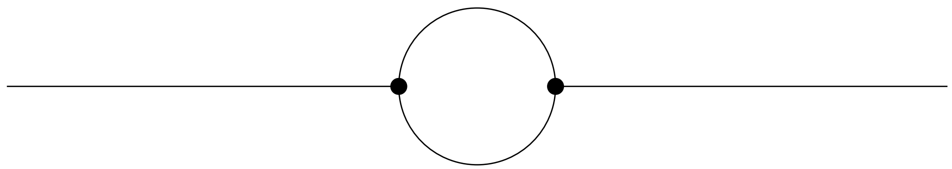

Theorem IV yields the electric resistance

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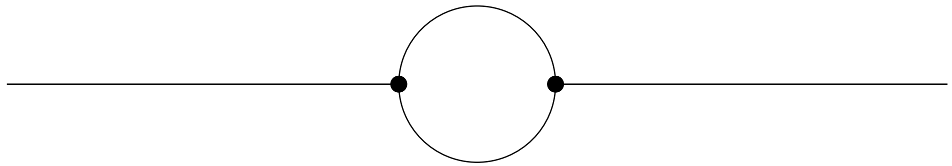

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where $T(\mu)$ is the transmission probability through the sample. Computing the average density in the wires to determine the local temperature gives

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Proof of Theorem I

Gauge invariance and uniform continuity of $A \mapsto \omega_0 \circ \tau^t(A)$

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Hilbert-Schmidt operators are h_0 and h-smooth

$\downarrow$

$Q(\varepsilon \pm i0) = (1 + y r_0(\varepsilon \pm i0) x^*)^{-1} = 1 - y r(\varepsilon \pm i0) x^*$ exists for a.a. $\varepsilon \in \mathbb{R}$

Proof of Theorem II

Special case $p = -1$ *i.e.* $h = h_0 + v$ with trace class v

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$v = x^* y = y^* x$ with Hilbert-Schmidt x and y

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$\mathfrak{K} \ni u \mapsto Z(a, \varepsilon) u = (U a^* u)(\varepsilon) \in \mathfrak{h}(\varepsilon)$

defines, for a.a. $\varepsilon \in \mathbb{R}$, a Hilbert-Schmidt $Z(a, \varepsilon) : \mathfrak{K} \longrightarrow \mathfrak{h}(\varepsilon)$ such that

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$$Q(z)=(1+yr_0(z)x^*)^{-1}, \qquad Q(\bar{z})^*=(1+xr_0(z)y^*)^{-1}$$

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$$Z(a,\varepsilon)^*Z(b,\varepsilon)=\frac{1}{2\pi i}a(r_0(\varepsilon+i0)-r_0(\varepsilon-i0))b^*$$

Proof of Theorem II

Stationary formula for the Møller operators

$$(U\Omega_-^* a^* u)(\varepsilon) = \lim_{\delta \downarrow 0} \delta \int_0^\infty e^{-\delta t} (U e^{-ith_0} e^{ith} a^* u)(\varepsilon)\, dt = \lim_{\delta \downarrow 0} \delta \int_0^\infty (U e^{it(h-\varepsilon+i\delta)} a^* u)(\varepsilon)$$

$$= \lim_{\delta \downarrow 0} i\delta (U r(\varepsilon - i\delta) a^* u)(\varepsilon) = (U a^* u)(\varepsilon) - (U x^* Q(\varepsilon - i0) y r_0(\varepsilon - i0) a^* u)(\varepsilon)$$

Proof of Theorem II

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$$Z(a\Omega_-, \varepsilon) = Z(a, \varepsilon) - Z(x, \varepsilon) Q(\varepsilon - i0) y r_0(\varepsilon - i0) a^*$$

$$Z(a\Omega_-, \varepsilon)^* = Z(a, \varepsilon)^* - a r_0(\varepsilon + i0) x^* Q(\varepsilon + i0) Z(x, \varepsilon)^*$$

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Stationary formula for the scattering matrix

$$S(\varepsilon) = I - 2\pi i Z(x,\varepsilon) Q(\varepsilon + i0) Z(y,\varepsilon)^* = I - 2\pi i Z(y,\varepsilon) Q(\varepsilon - i0) Z(x,\varepsilon)^*$$

Proof of Theorem II

$$\omega_+(\Phi_{q^{(\Lambda)}}) = \mathrm{tr}((U\varrho_0 U^*)U\Omega_-^* \varphi_{q^{(\Lambda)}}\Omega_- U^*)$$

$$\varphi_{q^{(\Lambda)}} = -i[h - h_0, q^{(\Lambda)}] = i[q^{(\Lambda)}, v] = i((xq^{(\Lambda)})^* y - x^*(yq^{(\Lambda)}))$$

Proof of Theorem II

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$$D(\varepsilon) = i(Z(xq^{(\Lambda)}\Omega_-, \varepsilon)Z(y\Omega_-, \varepsilon)^* - Z(x\Omega_-, \varepsilon)Z(yq^{(\Lambda)}\Omega_-, \varepsilon)^*)$$

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$$\begin{aligned}
Z(x\Omega_-,\varepsilon) &= Z(x,\varepsilon)(I - Q(\varepsilon - i0)yr_0(\varepsilon - i0)x^*) = Z(x,\varepsilon)Q(\varepsilon - i0)\\
Z(xq^{(\Lambda)}\Omega_-,\varepsilon) &= q^{(\Lambda)}(\varepsilon)Z(x,\varepsilon) - Z(x,\varepsilon)Q(\varepsilon - i0)yr_0(\varepsilon - i0)q^{(\Lambda)}x^*\\
Z(y\Omega_-,\varepsilon)^* &= (I - yr_0(\varepsilon + i0)x^*Q(\varepsilon + i0))Z(y,\varepsilon)^* = Q(\varepsilon + i0)Z(y,\varepsilon)^*\\
Z(yq^{(\Lambda)}\Omega_-,\varepsilon)^* &= Z(y,\varepsilon)^*q^{(\Lambda)}(\varepsilon) - yq^{(\Lambda)}r_0(\varepsilon + i0)x^*Q(\varepsilon + i0)Z(y,\varepsilon)^*
\end{aligned}$$

Proof of Theorem II

$$
\begin{aligned}
D(\varepsilon) &= i(q^{(\Lambda)}(\varepsilon)Z(x,\varepsilon)Q(\varepsilon+i0)Z(y,\varepsilon)^* - Z(x,\varepsilon)Q(\varepsilon-i0)Z(y,\varepsilon)^* q^{(\Lambda)}(\varepsilon) \\
&+ Z(x,\varepsilon)Q(\varepsilon-i0)[yq^{(\Lambda)}(r_0(\varepsilon+i0)-r_0(\varepsilon-i0))x^*]Q(\varepsilon+i0)Z(y,\varepsilon)^*)
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$$\downarrow$$

$$D(\varepsilon) = \frac{1}{2\pi}(q^{(\Lambda)}(\varepsilon) - S(\varepsilon)^* q^{(\Lambda)}(\varepsilon) S(\varepsilon))$$

Proof of Theorem II

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General case $p > 0$: use the invariance principle

$\ell_0 = f_\eta(h_0), \quad \ell = f_\eta(h) \quad \Rightarrow \quad \ell - \ell_0$ trace class

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$$\downarrow$$

$$
W_\pm = \mathrm{s}-\lim_{t\to\pm\infty} e^{it\ell} e^{-it\ell_0} 1_{\mathrm{ac}}(\ell_0)
$$

$$
\Omega_\pm = W_\pm 1_{E_+}(h_0) + W_\mp 1_{E_-}(h_0)
$$

where $E_\pm = \{\varepsilon | \pm f_\eta'(\varepsilon) > 0\}$