On transport in quantum devices

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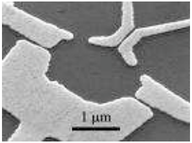
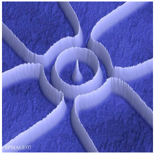
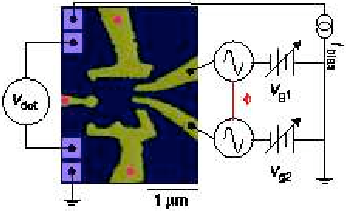
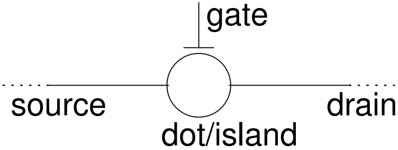
La théorie quantique des petites aux grandes échelles

Some pictures









Outline

Quantum pumps: The scattering approach

Quantization of charge transport

Quantum pumps: The topological approach

A comparison

Counting statistics

The determinant for independent particles

Application to tunnel junction

Collaborators: Y. Avron, S. Bachmann, A. Elgart, I. Klich, L. Sadun, G. Ortelli

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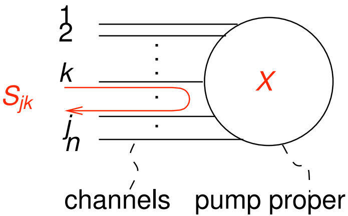
Quantum pumps

Charge quantum mechanically transferred between leads due to parametric operations, e.g. changing gate voltages.
Idealized:



- independent electrons ($e = +1$)
- each channel filled up to Fermi energy μ with incoming electrons
- $S = S(X) = (S_{jk})$ scattering $n \times n$ matrix at energy μ given the pump configuration X (w.r.t. to reference configuration X_0)
- At fixed X: no net current

Charge transport

(Büttiker, Thomas, Prêtre) Under a slow change $X \to X + dX$, and hence $S \to S + dS$, a net charge

$$đ Q_j = \frac{\mathrm{i}}{2\pi}((dS)S^*)_{jj}$$

leaves the pump through channel j

Remarks

- $$đ Q_j = \frac{\mathrm{i}}{2\pi}((dS)S^*)_{jj}$$

is a thermodynamic formula: exchanged charge $đ Q_j$ expressed through static quantities $S(X)$ (& their variation) accessible from the outside, (cf. work $đ W = -pdV$);
$\int_A^B đ Q_j$ depends on path, but not on its time parameterization.
- $\oint đ Q_j \neq 0$: it is a pump!

• Kirchhoff's law does not hold:

$$\sum_{j=1}^{n} đQ_j = \frac{\mathrm{i}}{2\pi}\operatorname{tr}((dS)S^*) = \frac{\mathrm{i}}{2\pi} d\log\det S$$

$$= -d\xi \neq 0$$

where "$\xi(\mu) = \operatorname{Tr}(P(\mu, X) - P(\mu, X_0))$" is the Krein spectral shift and $P(\mu, X) = \theta(\mu - H(X))$ is the spectral projection for the Hamiltonian $H(X)$.
$=$ is Friedel sum rule/Birman-Krein formula

$$\det S = \mathrm{e}^{2\pi \mathrm{i}\xi(\mu)}$$

• But

$$\oint \sum_{j=1}^{n} đQ_j = 0$$

A semiclassical/adiabatic picture

$E \in [0, \infty)$: 1-particle energy spectrum in a channel
$\rho(E)$: occupation of incoming states, e.g.
$\rho(E) = \theta(\mu - E)$ (at temperature $\beta^{-1} = 0$)
or $\rho(E) = (1 + e^{\beta(E-\mu)})^{-1}$
$S(E, t) = S(E, X(t))$: static scattering matrix $S(E, X)$ at energy E along slowly varying $X = X(t)$.
out state: channel j, energy E, time of passage t at fiducial point under X_0
$\mathcal{T}(E, t) = -i \frac{\partial S}{\partial E} S^*$: *Eisenbud-Wigner time delay:*
$t - \mathcal{T}_{jj}$ time of passage of in state corresponding to same out state under $X(t)$.
$\mathcal{E}(E, t) = i \frac{\partial S}{\partial t} S^*$: *Martin-Sassoli energy shift:*
$E - \mathcal{E}_{jj}$ energy of in state under $X(t)$.

Incoming charge during $[0, T]$ in lead j

$$\frac{1}{2\pi}\int_0^T dt \int_0^\infty dE\rho(E)$$

($2\pi =$ size of phase space cell of a quantum state)
Outgoing charge

$$\frac{1}{2\pi}\int_0^T dt' \int_0^\infty dE'\rho(E)$$

where
$(E', t') \mapsto (E, t) = (E' - \mathcal{E}_{jj}(E', t'), t' - \mathcal{T}_{jj}(E', t'))$
maps outgoing to incoming data
Net charge (linearize in $\mathcal{E}$)

$$Q_j = -\frac{1}{2\pi}\int_0^T dt \int_0^\infty dE\rho'(E)\mathcal{E}_{jj}(E, t)$$

For $\rho(E) = \theta(\mu - E)$ this equals $Q_j = \int_0^T dt\dot{Q}_j(t)$ with

$$\dot{Q}_j(t) = \frac{1}{2\pi}\mathcal{E}_{jj}(\mu, t) = \frac{\mathrm{i}}{2\pi}(\frac{\partial S}{\partial t}S^*)_{jj}$$

(cf. BPT)

What's behind: Adiabatic evolution in absence of gap

- Adiabatic evolution

$$H = H_s, \qquad s = \varepsilon t$$

$$\mathrm{i}\frac{d}{ds} U_\varepsilon(s, s_0) = \varepsilon^{-1} H_s U_\varepsilon(s, s_0), \qquad U_\varepsilon(s_0, s_0) = 1$$

  in the limit $\varepsilon \to 0$. Assume dH_s/ds compact operator (device).

- Initial state (1-particle density matrix) at s_0: spectral projection

$$P_{s_0} = \theta(\mu - H_{s_0})$$

  with μ Fermi energy.

- State at s

$$P_\varepsilon(s) = U_\varepsilon(s, s_0) P_{s_0} U_\varepsilon(s, s_0)^* \qquad (\neq P_s)$$

- Current operator at distance a from the device: $I_j(a)$

Theorem. For $s > s_0$,

$$\lim_{a\to\infty}\lim_{\varepsilon\downarrow 0}\varepsilon^{-1}\mathrm{tr}(P_\varepsilon(s)I_j(a)) = \frac{\mathrm{i}}{2\pi}\Big(\frac{dS}{ds}(s,\mu)S(s,\mu)^*\Big)_{jj}$$

Remarks.

- Order of limits: Ammeter is many wavelengths away from the pump, but reached within $\ll \varepsilon^{-1}$ (adiabatic time).
- Generalization to positive temperature.
- Most adiabatic theorems discuss

$$U_\varepsilon(s,s_0)PU_\varepsilon(s,s_0)^*$$

  where P is the spectral projection of H_{s_0} onto (i) an isolated part of its spectrum or (ii) an embedded eigenvalue. Here (iii) $P = \theta(\mu - H_{s_0})$ corresponds to a gapless part of continuous spectrum.

An idea from the proof

- Scattering is about comparing two dynamics:

$$\text{scattering matrix} = U_I(+\infty, -\infty)$$

  $U_I(t', t)$: propagator in the interaction picture.
- Answer in terms of static scattering matrix: generators $(H_{s'}, H_s) \rightsquigarrow S(s', s)$.
  At $s' = s$: may replace $(dS/ds)S^* \rightsquigarrow dS/ds$
- Starting point is non-autonomous dynamics $H_{\varepsilon t}$, hence dynamic scattering matrix: generators $(H_{s+\varepsilon t}, H_s) \rightsquigarrow \mathcal{S}(s)$.
  Then
  $\rho(H_s)$ incoming 1-pdm (e.g. $\rho(H_s) = \theta(\mu - H_s)$)
  $\mathcal{S}(s)\rho(H_s)\mathcal{S}^*(s)$ outgoing 1-pdm

An idea from the proof: $S(s', s)$ vs. $\mathcal{S}(s)$

- Linearize $H_{s+\varepsilon t} = H_s + \varepsilon \dot{H}_s t + \ldots$. Scattering operator (dynamic) in Born approximation

$$\begin{aligned}\mathcal{S}(s) &= 1 - \mathrm{i}\varepsilon \int_{-\infty}^{\infty} dt\, \mathrm{e}^{\mathrm{i}H_s t}(\dot{H}_s t)\mathrm{e}^{-\mathrm{i}H_s t} + \ldots \\ &\equiv 1 + \varepsilon \mathcal{S}^{(1)}(s) + \ldots\end{aligned}$$

  whence

$$\mathcal{S}\rho(H_s)\mathcal{S}^* = \rho(H_s) + \varepsilon[\mathcal{S}^{(1)}(s), \rho(H_s)] + \ldots$$

- Linearize for $s' \to s$

$$H_{s'} = H_s + (s' - s)\dot{H}_s + \ldots$$

  Scattering operator (static) in Born approximation

$$\begin{aligned}S(s', s) &= 1 - \mathrm{i}(s' - s) \int_{-\infty}^{\infty} dt\, \mathrm{e}^{\mathrm{i}H_s t}\dot{H}_s \mathrm{e}^{-\mathrm{i}H_s t} + \ldots \\ &\equiv 1 + (s' - s)\partial_{s'} S(s', s)|_{s'=s} + \ldots\end{aligned}$$

An idea from the proof (cont.)

$$\mathcal{S}^{(1)}(s) = -\mathrm{i}\int_{-\infty}^{\infty} dt\, \mathrm{e}^{\mathrm{i}H_s t}\dot{H}_s t \mathrm{e}^{-\mathrm{i}H_s t}$$

$$\partial_{s'} S(s',s)|_{s'=s} = -\mathrm{i}\int_{-\infty}^{\infty} dt\, \mathrm{e}^{\mathrm{i}H_s t}\dot{H}_s \mathrm{e}^{-\mathrm{i}H_s t}$$

Claim:

$$[\mathcal{S}^{(1)}(s), \rho(H_s)] = -\mathrm{i}\partial_{s'} S(s',s)\big|_{s'=s}\rho'(H_s)$$

Remark: relates dynamic $\to$ static, $\rho \to \rho'$.
Proof immediate for $\rho(\lambda) = \mathrm{e}^{-\mathrm{i}\lambda\tau}$, $-\mathrm{i}\rho'(\lambda) = -\tau \mathrm{e}^{-\mathrm{i}\lambda\tau}$:

$$\begin{aligned}\mathcal{S}^{(1)}(s)\mathrm{e}^{-\mathrm{i}H_s\tau} &= \mathrm{e}^{-\mathrm{i}H_s\tau}(-\mathrm{i})\int_{-\infty}^{\infty} dt\, \mathrm{e}^{\mathrm{i}H_s t}\dot{H}_s \cdot (t-\tau)\mathrm{e}^{-\mathrm{i}H_s t} \\ &= \mathrm{e}^{-\mathrm{i}H_s\tau}\big(\mathcal{S}^{(1)}(s) - \tau\partial_{s'} S(s',s)|_{s'=s}\big)\end{aligned}$$

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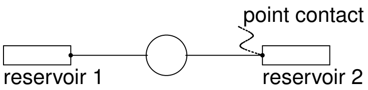
Further transport properties

- Noise

$$\langle\langle n_j^2 \rangle\rangle = \frac{1}{(2\pi)^2} \int_{-\infty}^{\infty} \int_0^T \frac{1 - |(S(t)S^*(t'))_{jj}|^2}{(t-t')^2} dt\, dt'$$

- Energy dissipated to reservoirs



$$\underbrace{\langle E_j \rangle}_{\text{energy delivered to reservoir } j} - \underbrace{\mu \langle n_j \rangle}_{\text{can be reclaimed from reservoir}} = \frac{1}{4\pi} \int_0^T (\mathcal{E}^2)_{jj} dt$$

Remark (dissipation inequality): For any source

$$\langle \dot{E} \rangle - \mu \langle \dot{n} \rangle \geq \pi \langle \dot{n} \rangle^2$$

- related to $P = RI^2$ with $R \geq \pi = (1/2)(h/e^2)$ (point contact resistance; $e = \hbar = 1$)
- for pumps: $(\mathcal{E}^2)_{jj} \geq (\mathcal{E}_{jj})^2$

Theorem: Optimal pump processes

Hypotheses: • cyclic process: $X(0) = X(T)$ • fix a lead, j

The following are equivalent:

- Dissipation inequality is saturated (minimal dissipation)
- No noise: $\langle\langle n_j^2 \rangle\rangle = 0$
- The charge transported in a cycle is quantized:

$$n_j = \langle n_j \rangle \in \mathbb{Z}$$

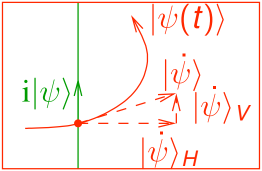
Note: holds for arbitrary number number of leads n (instead of 2)

The content is geometric

The Hopf map

Unit sphere $S^{2n-1} \subset \mathbb{C}^n$ preserved by circle action $|\psi\rangle \mapsto e^{i\theta}|\psi\rangle$

$$S^{2n-1}/\sim = P\mathbb{C}^{n-1}$$



S^{2n-1} (fibre bundle)

connection 1-form
$\langle i\psi|\dot{\psi}\rangle = -i\langle\psi|\dot{\psi}\rangle$

Hopf map π $\downarrow$

$P\mathbb{C}^{n-1}$ (base space)

Geometric interpretation of optimality

Recall: $\mathcal{E} = \mathrm{i}\dot{S}S^* = -\mathrm{i}S\dot{S}^*$

Let $\langle\psi(t)| = j$-th row of $S(t)$ (incoming state feeding channel j)

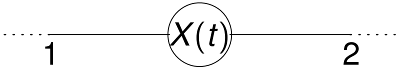
$$\langle\psi(t)|\psi(t)\rangle = 1$$
$$\mathrm{i}(\dot{S}S^*)_{jj} = \mathcal{E}_{jj} = -\mathrm{i}\langle\psi|\dot{\psi}\rangle$$

Charge transport $\langle n_j\rangle = (2\pi)^{-1}\oint \mathcal{E}_{jj}dt$ is holonomy (Berry phase).

If process proceeds along fiber, $|\psi(t)\rangle = \mathrm{e}^{\mathrm{i}\theta(t)}|\psi(0)\rangle$, then

- $\mathcal{E}_{jj} = \dot{\theta}$ and $(2\pi)^{-1}\oint \dot{\theta}dt$ is the winding number
- $|(S(t)S^*(t'))_{jj}|^2 = |\langle\psi(t)|\psi(t')\rangle|^2 = 1$: no noise
- $(\mathcal{E}^2)_{jj} = \langle\dot{\psi}|\dot{\psi}\rangle = \langle\dot{\psi}|\psi\rangle\langle\psi|\dot{\psi}\rangle = (\mathcal{E}_{jj})^2$: minimal dissipation

Quantized transport



Cyclic process: $X(0) = X(T)$

Theorem. The charge transported in a cycle is quantized

$$n_j = \langle n_j \rangle \in \mathbb{Z} \qquad (j = 1, 2)$$

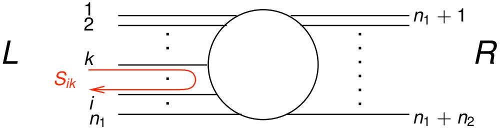
iff scattering matrix $S(t)$ is of the form

$$S(t) = \begin{pmatrix} e^{i\varphi_1(t)} & 0 \\ 0 & e^{i\varphi_2(t)} \end{pmatrix} S_0$$

Then n_j is the winding number of $\varphi_j(t)$, $(j = 1, 2)$

Quantized transport (cont.)

Generalization to many channels:



In a cycle, the charge delivered to the Left (resp. Right) channels as a whole is quantized iff

$$S(t) = \begin{pmatrix} U_1(t) & 0 \\ 0 & U_2(t) \end{pmatrix} S_0$$

with $U_j(t)$ unitary $n_j \times n_j$-matrices ($j = 1, 2$). The charge is the winding number of $\det U_j(t)$.

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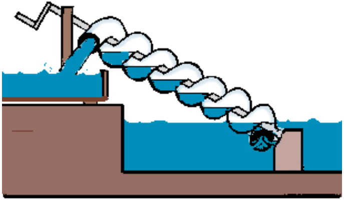
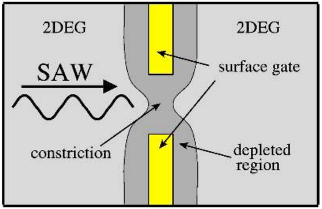
Some examples





The setup of the topological approach

Infinitely extended 1-dimensional system

$$H(s) = -\frac{d^2}{dx^2} + V(s,x) \qquad \text{on } L^2(\mathbb{R}_x)$$

depending on parameter s, real. Potential V doubly periodic

$$V(s, x + L) = V(s, x), \qquad V(s + 2\pi, x) = V(s, x)$$

Change s slowly with time t.

Hypothesis. The Fermi energy lies in a spectral gap for all s.

Theorem (Thouless 1983). The charge transported (as determined by Kubo's formula) during a period and across a reference point is an integer, C.

(What's behind: Adiabatic evolution in presence of gap)

The integer as a Chern number

$\psi_{nks}(x)$: n-th Bloch solution of quasi-momentum $k \in [0, 2\pi/L]$ (Brillouin zone), normalized over $x \in [0, L]$ (unique up to phase).

$$C = \sum_n C_n \equiv \sum_n \frac{\mathrm{i}}{2\pi} \int_{\mathbb{T}} \Big(\langle \frac{\partial \psi_{nks}}{\partial s} | \frac{\partial \psi_{nks}}{\partial k} \rangle - \langle \frac{\partial \psi_{nks}}{\partial k} | \frac{\partial \psi_{nks}}{\partial s} \rangle \Big) ds\, dk$$

- sum extends over filled bands n
- integral over torus $\mathbb{T} = [0, 2\pi] \times [0, 2\pi/L]$
- as a rule, phase can be chosen such that $|\psi_{nks}\rangle$ is smooth only locally $\mathbb{T}$
- integrand (curvature) is smooth globally
- C_n is Chern number, obstruction to global section $|\psi_{nks}\rangle$

Generalizations

1) n channels:

$$H(s) = -\frac{d^2}{dx^2} + V(s,x) \qquad \text{on } L^2(\mathbb{R}_x, \mathbb{C}^n)$$

with $V(s,x) = V^*(s,x) \in M_n(\mathbb{C})$.

2) Time, but not space periodicity is essential. Sufficient: Fermi energy lies in a spectral gap for all s. What about C?
Let $z \notin \sigma(H(s))$ and $\psi(x)$, $\chi(x) \in M_n(\mathbb{C})$ with

$$\begin{aligned} (H(s) - z)\psi(x) &= 0, \qquad \psi(x) \to 0 \ (x \to +\infty) \\ \chi(x)(H(s) - z) &= 0, \qquad \chi(x) \to 0 \ (x \to -\infty) \end{aligned}$$

with $\psi(x)$, $\chi(x)$ regular for some $x \in \mathbb{R}$. Wronskian

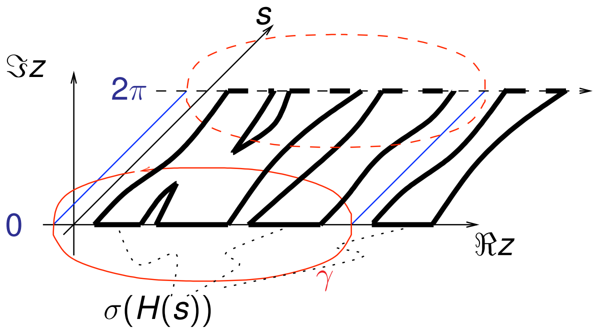
$$W(\chi, \psi; x) = \chi(x)\psi'(x) - \chi'(x)\psi(x) \in M_n(\mathbb{C})$$

is independent of x for solutions ψ, χ. Normalize:
$W(\chi, \psi; x) = 1$.

Theorem. The transported charge is

$$C = \frac{\mathrm{i}}{2\pi} \int_{\mathbb{T}} \mathrm{tr}\Big(W(\frac{\partial \chi}{\partial s}, \frac{\partial \psi}{\partial z}; x) - W(\frac{\partial \chi}{\partial z}, \frac{\partial \psi}{\partial s}; x) \Big) ds\, dz$$

(any x). This is the Chern number of the bundle of solutions ψ on $(s, z) \in \mathbb{T} = [0, 2\pi] \times \gamma$.



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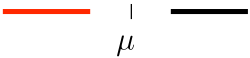
Are Thouless' and Büttiker's approaches incompatible?

- Topological approach: Fermi energy μ in gap: no states there



  Charge transport attributed to energies way below μ

- Scattering approach: Depends on scattering at Fermi energy

  Charge transport attributed to states at energy μ

Truncate potential V to interval $[0, L]$

$$H(s) = -\frac{d^2}{dx^2} + V(s,x)\chi_{[0,L]}(x) \qquad \text{on } L^2(\mathbb{R}_x, \mathbb{C}^n)$$

Gap closes.

A comparison (cont.)

Scattering matrix

$$S_L(s) = \begin{pmatrix} R_L & T'_L \\ T_L & R'_L \end{pmatrix}$$

exists at Fermi energy.

Theorem

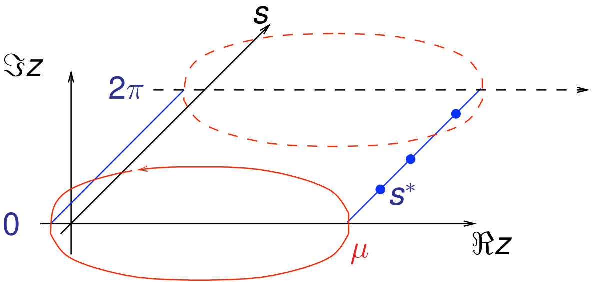
- As $L \to \infty$,

  $$S_L(s) \to \begin{pmatrix} R(s) & 0 \\ 0 & R'(s) \end{pmatrix}$$

  exponentially fast, with R, R' unitary. Hence: conditions for quantized transport attained in the limit.
- Charge transport in both descriptions agree: Winding number of det R is Chern number C.

Sketch of proof

- Solution $\psi_{z,s}(x)$ for $(z, s) \in \mathbb{T}$
  - $\psi_{z,s}(x)$ or $\psi'_{z,s}(x)$ regular at any $x \in \mathbb{R}$
  - $\psi_{z,s}(x = 0)$ regular except for $(z = \mu, s)$ at discrete values s^* of s.
  - Except for these critical points, there is a global section $\psi_{z,s}$ (e.g. $\psi_{z,s}(0) = 1$)



Sketch of proof (cont.)

- Near a given critical point ($z = \mu, s = s^*$) let $\psi_{z,s}$ be a local section, analytic in z (e.g. $\psi'_{z,s}(0) = 1$)

$$L(z,s) := \psi'^{*}_{\bar{z},s}(0)\psi_{z,s}(0)$$

  is analytic with $L(z,s) = L(\bar{z},s)^*$
- Generically, $L(z,s)$ has a simple eigenvalue $\lambda(z,s)$ vanishing to first order at (μ, s^*); $\lambda(z,s) \in \mathbb{R}$ for $z \in \mathbb{R}$
-

$$C = -\sum_{s^*} \text{winding number of } \lambda(z,s) \text{ around } (\mu, s^*)$$

$$= \sum_{s^*} \operatorname{sgn}\left(\frac{\partial\lambda}{\partial z}\frac{\partial\lambda}{\partial s}\right)\Big|_{(z=\mu,s=s^*)} = -\sum_{s^*} \operatorname{sgn}\left(\frac{\partial\lambda}{\partial s}\right)\Big|_{(z=\mu,s=s^*)}$$

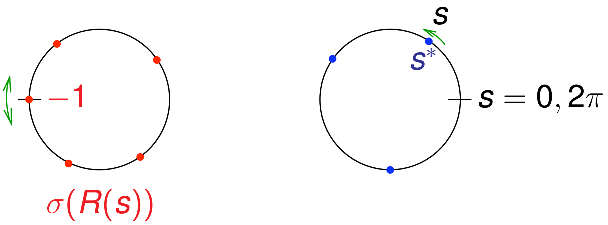
- $\partial\lambda/\partial z < 0$ for $z \in \mathbb{R}$ (Sturm oscillation)

Sketch of proof (cont.)

- Matching condition at $x = 0$ yields ($L \to \infty$)

$$R(s) = (\mathrm{i}\sqrt{\mu}\psi_{\mu,s}(0) - \psi'_{\mu,s}(0))(\mathrm{i}\sqrt{\mu}\psi_{\mu,s}(0) + \psi'_{\mu,s}(0))^{-1}$$

$R(s)$ has eigenvalue -1 iff $\psi_{\mu,s}(0)$ is singular



- Eigenvalue crossing is counterclockwise iff $\partial\lambda/\partial s|_{(z=\mu, s=s^*)} < 0$
- Together:

$$\begin{aligned} C &= \#\text{ eigenvalue crossings of } R \text{ at } z = -1 \\ &= \text{winding number of } \det R \end{aligned}$$

□

Summary

- Scattering approach: gapless systems, finite scatterer; transport based on scattering matrix and attributed to states, both at Fermi energy; quantized in special cases only
- Topological approach: gapped systems, infinite device; transport attributed to states way below Fermi energy; quantized
- A comparison has been obtained.

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Noises

R resistance

1. Equilibrium noise: • no voltage applied; • temperature β^{-1}

Q: charge flowed during time T

$$\langle Q \rangle = 0$$

$$\underbrace{\frac{\langle Q^2 \rangle}{T}}_{\text{fluctuation}} = \underbrace{\frac{2}{\beta R}}_{\text{dissipation}} \qquad \text{(Johnson, Nyquist 1928)}$$

2. Non-equilibrium noise: • voltage V; • zero temperature

$$\frac{\langle Q \rangle}{T} = \frac{V}{R} \qquad \text{(Ohm)}$$

$$\langle\langle Q^2 \rangle\rangle := \langle Q^2 \rangle - \langle Q \rangle^2 \qquad \text{(shot noise \ldots)}$$

Classical shot noise

$$\langle\langle Q^2 \rangle\rangle = e\langle Q \rangle \qquad \text{(Schottky 1918)}$$

(e electron charge)

Interpretation. Poisson distribution (parameter λ)

$$n: \text{ number of electrons}$$

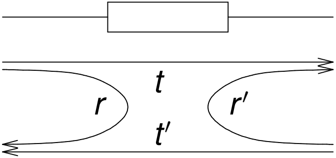
$$p_n = \mathrm{e}^{-\lambda}\frac{\lambda^n}{n!}$$

$$\langle n \rangle = \lambda, \qquad \langle\langle n^2 \rangle\rangle = \lambda$$

Charge: $Q = en$

$$\langle\langle Q^2 \rangle\rangle = e^2\lambda = e\langle Q \rangle$$

Quantum shot noise



$p = |t|^2$ transmission probability
$q = 1 - |t|^2$ reflection probability

$$\langle\langle Q^2 \rangle\rangle = e\langle Q \rangle (1 - |t|^2) \qquad \text{(Khlus 1987, Lesovik 1989)}$$

Interpretation. Binomial distribution with N attempts

$$p_n = \binom{N}{n} p^n q^{N-n}$$

$$\langle n \rangle = Np, \qquad \langle\langle n^2 \rangle\rangle = Np(1-p)$$

Besides: For bias V the semi-classical count is $N = VT/(2\pi)$.

The generating function of counting statistics

p_n	probability of transfer of n electrons
$\chi(\lambda) = \sum_{n \in \mathbb{Z}} p_n e^{i\lambda n} = \langle e^{i\lambda \Delta Q} \rangle$	moment generating function: $\langle n^k \rangle = (-i d/d\lambda)^k \chi(\lambda)\|_{\lambda=0}$
$\log \chi(\lambda)$	cumulant generating function

- For binomial statistics:

$$\log \chi(\lambda, t) = \frac{Vt}{2\pi} \log((1 - T) + e^{i\lambda} T)$$

- For a random variable with outcomes α_n:

$$\chi(\lambda) = \sum_{n \in \mathbb{Z}} p_n e^{i\lambda \alpha_n}$$

Quantum mechanics and measurement

Hilbert space with vectors $|\psi\rangle$ (pure states) and operators, representing

• mixed state: $\rho \geq 0$, $\mathrm{tr}\rho = 1$; pure if indecomposable, i.e. $\rho = |\psi\rangle\langle\psi|$ is rank 1 projection.

• observable $A^* = A = \sum_i \alpha_i P_i$ (spectral decomposition)

• evolution U unitary; $\rho \mapsto U\rho U^*$

Measurement of A:

$$\rho \mapsto \sum_i P_i \rho P_i \qquad \text{(“collapse of the state”)}$$

with $\mathrm{tr}(P_i\rho P_i) = \mathrm{tr}(\rho P_i)$ probability of outcome α_i.

Two measurements of A, with evolution U in between.

$$\rho \mapsto \sum_{i,j} P_j U P_i \rho P_i U^* P_j$$

with $\mathrm{tr}(U^* P_j U P_i \rho P_i)$ probability of history (α_i, α_j)

Quantum mechanics and measurement (cont.)

Moment generating function for difference of outcomes

$$\chi(\lambda) = \sum_{i,j} \mathrm{tr}(U^* P_j U P_i \rho P_i) \mathrm{e}^{\mathrm{i}\lambda(\alpha_j - \alpha_i)} = \sum_i \mathrm{tr}(U^* \mathrm{e}^{\mathrm{i}\lambda A} U P_i \rho P_i) \mathrm{e}^{-\mathrm{i}\lambda \alpha_i}$$

If $[A, \rho] = 0$, then: $P_i \rho P_i = P_i \rho$ (no collapse at 1st measurement) and

$$\chi(\lambda) = \mathrm{tr}(U^* \mathrm{e}^{\mathrm{i}\lambda A} U \mathrm{e}^{-\mathrm{i}\lambda A} \rho)$$

Charge and current

Consider the operators (on the appropriate Hilbert space of the system)

$Q(t)$	charge on the Right lead
$I(t) = \mathrm{i}[H, Q(t)]$	current through the junction

$$Q(t) - Q(0) = \int_0^t dt' \, I(t')$$

ΔQ in quantum mechanics

$$Q(t) - Q(0) = \int_0^t dt' I(t')$$

Single (?) measurement (Levitov, Lesovik 1992)

$$\Delta Q = Q(t) - Q(0)$$

$$\chi(\lambda, t) = \langle \mathrm{e}^{\mathrm{i}\lambda(Q(t)-Q(0))} \rangle$$

$$\langle\langle (\Delta Q)^k \rangle\rangle = \int_0^t d^k t \langle\langle I(t_1) \ldots I(t_k) \rangle\rangle$$

($d^k t = dt_1 \ldots dt_k$)
But: $Q(t)$, $Q(0)$ are based at different times; have integer spectrum, while $Q(t) - Q(0)$ does not. (This protocol not pursued.)

ΔQ in quantum mechanics (cont.)

$$Q(t) - Q(0) = \int_0^t dt' I(t')$$

Two measurements (Levitov, Lesovik 1993)

- Measure charge $Q(0)$ in R at time $t = 0$ and so prepare initial state $\langle \cdot \rangle$
- Wait till t
- Measure charge $Q(t)$ in R
- Transferred ΔQ is difference of the two measurements.
- ΔQ is an integer!

ΔQ in quantum mechanics (cont.)

Generating function:

$$\chi(\lambda, t) = \langle e^{iHt} e^{i\lambda Q} e^{-iHt} e^{-i\lambda Q} \rangle \equiv \langle e^{i\lambda Q(t)} e^{-i\lambda Q} \rangle$$

Proof. $\chi(\lambda, t) = \langle e^{i\lambda Q(t)} \rangle e^{-i\lambda q}$ with q: eigenvalue of $Q = Q(0)$ in $\langle \cdot \rangle$ □

Relation to current: If $[Q, I] = 0$

$$\langle\langle (\Delta Q)^k \rangle\rangle = \int_0^t d^k t \langle\langle T(I(t_1) \ldots I(t_k)) \rangle\rangle$$

Proof. $\chi(\lambda, t) = \langle e^{iHt} e^{-iH(\lambda)t} \rangle$ with

$$\begin{aligned} H(\lambda) &= e^{i\lambda Q} H e^{-i\lambda Q} \\ &= H - i\lambda [H, Q] = H - \lambda I \end{aligned}$$

Dyson expansion for $e^{iHt} e^{-iH(\lambda)t}$ □

Outline

Quantum pumps: The scattering approach

Quantization of charge transport

Quantum pumps: The topological approach

A comparison

Counting statistics

The determinant for independent particles

Application to tunnel junction

Second quantization: from one to many particles

1-particle: Hilbert space $\mathcal{H}$, operator A

many particles (fermions): Hilbert space

$$\mathcal{F}(\mathcal{H}) = \bigoplus_{n=0}^{\infty} \bigwedge^{n} \mathcal{H} \qquad \text{(Fock space)}$$

Operator, acting on $\bigwedge^n \mathcal{H}$

$$\Gamma(A) = A \otimes \ldots \otimes A \qquad \text{(for independent evolutions)}$$

$$d\Gamma(A) = \sum_{i=1}^{n} 1 \otimes \ldots \otimes A \otimes \ldots \otimes 1 \qquad \text{(for additive observables)}$$

For a trace class operator A

$$\mathrm{Tr}_{\mathcal{F}(\mathcal{H})}\, \Gamma(A) = \det_{\mathcal{H}}(1 + A)$$

(Fredholm determinant)

Second quantization (cont.)

$0 \leq N \leq 1$ 1-particle density matrix; $N|\psi\rangle = \nu|\psi\rangle$ means "the 1-particle state $|\psi\rangle$ is occupied with probability ν in the many-particle state ρ"

Quasi-free state: Uncorrelated many-particle state determined by 1-particle density matrix N

$$\rho = \frac{\Gamma(M)}{Z} \qquad (Z = \operatorname{Tr} \Gamma(M))$$

with $N = M(1+M)^{-1}$, resp. $M = N(1-N)^{-1}$.
In fact, on $\mathcal{F}[|\nu\rangle] = \oplus_{n=0}^{1} \wedge^n [|\nu\rangle]$,

$$\frac{1_0 + \frac{\nu}{\nu'} 1_1}{1 + \frac{\nu}{\nu'}} = \nu' 1_0 + \nu 1_1 \qquad (\nu' = 1 - \nu)$$

Example:

$$M = \mathrm{e}^{-\beta H}, \qquad N = (1 + \mathrm{e}^{\beta H})^{-1}.$$

Remark: $[N, A] = 0$ implies $[\rho, d\Gamma(A)] = 0$.

Main formula (Levitov, Lesovik)

Hypothesis: $[Q, N] = 0$; means "state does not collapse under 1st measurement".

Then

$$\chi(\lambda) = \det(1 - N + \mathrm{e}^{\mathrm{i}\lambda U^* Q U} N \mathrm{e}^{-\mathrm{i}\lambda Q})$$

Derivation:

$$\begin{aligned}
\chi(\lambda) &= \mathrm{Tr}\big(\Gamma(U)^* \mathrm{e}^{\mathrm{i}\lambda d\Gamma(Q)} \Gamma(U) \mathrm{e}^{\mathrm{i}\lambda d\Gamma(Q)} \rho\big) \\
&= \frac{\mathrm{Tr}\,\Gamma(U^* \mathrm{e}^{\mathrm{i}\lambda Q} U \mathrm{e}^{-\mathrm{i}\lambda Q} M)}{\mathrm{Tr}\,\Gamma(M)} = \frac{\det(1 + U^* \mathrm{e}^{\mathrm{i}\lambda Q} U \mathrm{e}^{-\mathrm{i}\lambda Q} M)}{\det(1 + M)} \\
&= \det(1 - N + U^* \mathrm{e}^{\mathrm{i}\lambda Q} U \mathrm{e}^{-\mathrm{i}\lambda Q} N)
\end{aligned}$$

A consequence

$$\langle n\rangle = -\mathrm{i}\chi'(0) = \mathrm{tr}(\underbrace{U^* Q U - Q}_{\Delta Q\text{: transmitted charge}})N$$

$$\begin{aligned}\langle\langle n^2\rangle\rangle &= -(\log\chi)''(0)\\ &= \mathrm{tr}(N(\Delta Q)(1-N)\Delta Q)\\ &= \underbrace{\mathrm{tr}(N(1-N)(\Delta Q)^2)}_{\text{thermal noise } \propto \beta^{-1}} + \underbrace{\frac{1}{2}\mathrm{tr}(\mathrm{i}[\Delta Q, N])^2}_{\text{shot noise}}\end{aligned}$$

thermal noise: fluctuation in the source of particles
shot noise: fluctuation in the transmission of particles
(cf. Büttiker)

Questions

Is the determinant Fredholm?

$$\chi(\lambda) = \det(1 - N + e^{i\lambda U^* Q U} N e^{-i\lambda Q})$$

Is $Z < \infty$?

Yes, if both • leads and • energy range are finite.

But: Bounds on these quantities are physically irrelevant, because

- transport is across the dot (compact in space)
- transport occurs near the Fermi energy (compact in energy)

Hence: Such bounds ought not to be necessary mathematically.

A quick fix

$$\chi(\lambda) = \det(1 - N + e^{i\lambda U^* Q U} N e^{-i\lambda Q}) = \det(N' + e^{i\lambda Q_U} N e^{-i\lambda Q})$$

with $N' := 1 - N$ occupation of hole states;
$Q_U := U^* Q U$ (Heisenberg) evolution of Q.

Multiply determinant by

$$\text{"} \det(e^{-i\lambda N_U Q_U}) \cdot \det(e^{i\lambda N Q}) = e^{i\lambda \mathrm{tr}(QN - Q_U N_U)} = 1 \text{"}$$

Result: regularized determinant

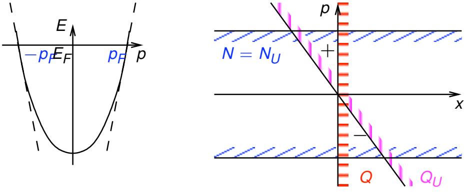
$$\chi(\lambda) = \det(e^{-i\lambda N_U Q_U} N' e^{i\lambda N Q} + e^{i\lambda N'_U Q_U} N e^{-i\lambda N' Q})$$

- Particle-hole symmetry: $(N, \lambda) \leftrightarrow (N', -\lambda)$
- Determinant is Fredholm under reasonable assumptions
- Analogy with $\det_2(1 + A) = \det(1 + A)e^{-\mathrm{tr} A}$ (A Hilbert-Schmidt).

An illustrative example

$\log \chi(\lambda) \rightsquigarrow \log \chi(\lambda) + \mathrm{i}\lambda \mathrm{tr}(QN - Q_U N_U)$: Only 1st cumulant affected.

Example: free particles in a lead.



dispersion relation

phase space

Before regularization: $\langle n \rangle = \mathrm{tr}(Q_U - Q)N$

- trace vanishes by compensation between $+$ and $-$
- trace class norm ($\propto$ area of $\pm$) diverges as $p_F \to \infty$

After regularization:

$$\langle n \rangle = \mathrm{tr}(Q_U - Q)N + \mathrm{tr}(QN - Q_U N_U) = \mathrm{tr} Q_U (N - N_U)$$

- vanishes as operator.

A more fundamental approach

for systems with infinitely many degrees of freedom

Algebraic approach to quantum theory

- observables A: elements of C^*-algebra $\mathcal{A}$
- (mixed) states ω: positive, normalized linear functionals on $\mathcal{A}$

$$\omega(A) : \text{expectation of } A \text{ in } \omega$$

The GNS construction: Given a state ω there are

- a Hilbert space $\mathcal{H}_\omega$
- a representation π_ω of $\mathcal{A}$
- a cyclic vector $\Omega_\omega \in \mathcal{H}_\omega$

such that

$$\omega(A) = (\Omega_\omega, \pi_\omega(A)\Omega_\omega)$$

Note: also mixed states are realized as vectors; then

$$\underbrace{\overline{\pi_\omega(\mathcal{A})}}_{\substack{\text{von Neumann algebra} \\ \text{(observables)}}} \subsetneq \underbrace{\mathcal{B}(\mathcal{H}_\omega)}_{\text{bounded operators}}$$

CAR-Algebra

(Recall: $\mathcal{H}$ 1-particle Hilbert space with operators U, Q, N)

- Algebra $\mathcal{A}(\mathcal{H})$ generated by $a^*(f)$, $a(f)$, $(f \in \mathcal{H})$ with canonical anticommutation relations

$$\{a(f), a^*(g)\} = \langle f|g\rangle, \qquad \{a(f), a(g)\} = 0$$

- States: $0 \leq N \leq 1$ defines a quasi-free state ω by

$$\omega(a^*(f)a(g)) = \langle g|N|f\rangle \qquad \text{(\& Wick's lemma)}$$

Note: the states in the example

$N = 0$	vacuum
$N = \theta(-H)$	Fermi sea
$N = (1 + \mathrm{e}^{\beta H})^{-1}$	Fermi-Dirac distribution

cannot be realized in each other's GNS space.

E.g. for $N = 0$: $\mathcal{H}_\omega \cong \mathcal{F}(\mathcal{H})$

A theorem

(Recall: $\mathcal{H}$ 1-particle Hilbert space with operators U, Q, N)
Under suitable and reasonable assumptions
1. The algebra automorphisms $a^*(f) \mapsto a^*(Uf)$ and $a^*(f) \mapsto a(\mathrm{e}^{\mathrm{i}\lambda Q} f)$ are unitarily implementable: There exists (non-unique) $\widehat{U}$ and $\mathrm{e}^{\mathrm{i}\lambda \widehat{Q}}$ on $\mathcal{H}_\omega$ such that

$$\widehat{U}\pi_\omega(a^*(f)) = \pi_\omega(a^*(Uf))\widehat{U} \qquad \text{etc.}$$

2. $\widehat{Q} \in \overline{\pi_\omega(\mathcal{A})}$ (observable meaning: renormalized charge)
3. The moment generating function

$$\chi(\lambda) := (\Omega_\omega, \widehat{U}^* \mathrm{e}^{\mathrm{i}\lambda\widehat{Q}} \widehat{U} \mathrm{e}^{-\mathrm{i}\lambda\widehat{Q}} \Omega_\omega)$$

(not affected by the above non-uniqueness) is given by the regularized determinant seen before.

Methods: Shale-Stinespring, Araki, Jaksic-Pillet

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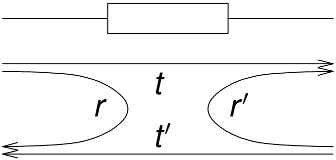
The essential description



$p = |t|^2$ transmission probability
$q = 1 - |t|^2$ reflection probability

Energy independent scattering matrix

$$S = \begin{pmatrix} \mathfrak{r} & \mathfrak{t}' \\ \mathfrak{t} & \mathfrak{r}' \end{pmatrix}$$

for fermions with linear dispersion relation (left, right movers) and Fermi energies μ_L, μ_R.

A discrepancy about the third cumulant

- For single-step measurement of ΔQ:

$$\langle\langle(\Delta Q)^3\rangle\rangle = \int_0^t d^3t \langle\langle I(t_1)\dots I(t_3)\rangle\rangle = -2T^2(1-T)\cdot(Vt/2\pi)$$

- For two-step measurement: $\langle\langle(\Delta Q)^3\rangle\rangle$ equals
  - (Lesovik, Chtchelkatchev 2003)

$$\int_0^t d^3t \langle\langle \mathcal{T}(I(t_1)\dots I(t_3))\rangle\rangle = -2T^2(1-T)\cdot(Vt/2\pi)$$

  - Based on determinant (Lesovik, Levitov): Binomial result

$$T(1-T)(1-2T)\cdot(Vt/2\pi)$$

Same with the above regularization; same by (Salo, Hekking, Pekola 2006) by different means.

Experimental data (Reznikov et al. 2005)

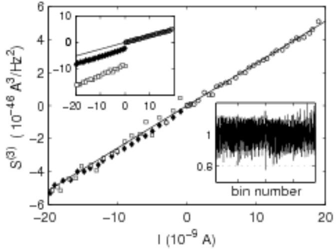


FIG. 3: Measured third cumulant $S^{(3)}$ of the transmitted charge, obtained separately for different current directions. (Markers are the same as in Fig. 2, the straight line is $S^{(3)} = e^2 I$.) Upper inset: $S^{(3)}$ vs. I without amplifier nonlinearity correction; Lower inset: normalized histogram of the linearly swept signal, used to calibrate the A/D converter (see text).

$$I = T \cdot V/2\pi$$

Result is for T small. Sign of slope is consistent with binomial alternative.

Discussion of hypotheses

Recall: the computation by means of $T(I(t_1)\dots I(t_k))$ relies on $[Q, I] = 0$. Typical Hamiltonian for particles with linear dispersion:

$$H = p\sigma_z + V(x) \qquad \text{on } L^2(\mathbb{R};\mathbb{C}^2)$$

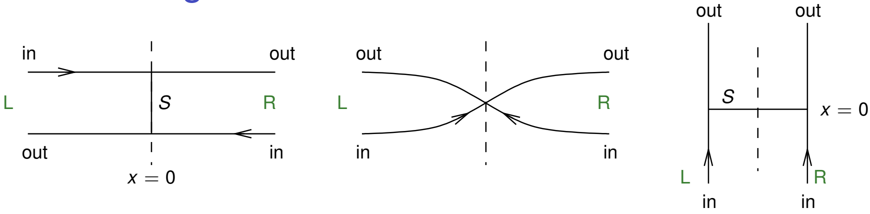
$(V = V^*)$. Then

$$\mathrm{i}[H, x] = \sigma_z$$
$$Q = \theta(x)1, \qquad I = \mathrm{i}[H, Q] = \sigma_z\delta(x)$$

Hence $[Q, I] = 0$.

But the Hamiltonian underlying the essential description is not typical!

Reconstructing the Hamiltonian



$$S = \begin{pmatrix} \mathfrak{r} & \mathfrak{t}' \\ \mathfrak{t} & \mathfrak{r}' \end{pmatrix}$$

H defined on $L^2(\mathbb{R}; \mathbb{C}^2)$ through either

- ("shift and scatter")

  $$(\mathrm{e}^{-\mathrm{i}Ht}\psi)(x) = (1 + (S-1)\theta(0 < x < t))\psi(x-t) \qquad (t > 0)$$

- (Falkensteiner, Grosse 1987) $H = p$ with boundary condition $\psi(0+) = S\psi(0-)$
- (Albeverio, Kurasov 1997)

$$H = p + 2\mathrm{i}\frac{S-1}{S+1}\delta(x) \qquad (\delta = (\delta_+ + \delta_-)/2)$$

Discussion of hypotheses (cont.)

With

$$Q = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \qquad I = \mathrm{i}[H, Q]$$

one has

$$[Q(t), I(t)] = ([Q, S^* QS]\theta(-x) + [SQS^*, Q]\theta(x))\delta(x + t) \neq 0$$

The hypothesis is not satisfied!

Back to the starting point

$$\chi(\lambda, t) = \langle \mathrm{e}^{\mathrm{i}Ht}\mathrm{e}^{\mathrm{i}\lambda Q}\mathrm{e}^{-\mathrm{i}Ht}\mathrm{e}^{-\mathrm{i}\lambda Q}\rangle = \langle \mathrm{e}^{\mathrm{i}\lambda Q(t)}\mathrm{e}^{-\mathrm{i}\lambda Q}\rangle = \langle T\mathrm{e}^{\mathrm{i}\lambda(Q(t)-Q)}\rangle$$

Thus

$$\begin{aligned}
\langle(\Delta Q)^k\rangle &= \langle T(Q(t)-Q)^k\rangle \\
&= T((Q(t_1)-Q)\ldots(Q(t_k)-Q))\big|_{t_1=\ldots=t_k=t} \\
&= \int_0^t dt_1\,\frac{\partial}{\partial t_1}\langle T((Q(t_1)-Q)\ldots(Q(t_k)-Q))\rangle\big|_{t_2=\ldots=t_k=t} \\
&= \int_0^t d^k t\,\frac{\partial}{\partial t_k}\ldots\frac{\partial}{\partial t_1}\langle T((Q(t_1)-Q)\ldots(Q(t_k)-Q))\rangle \\
&= \int_0^t d^k t\,\frac{\partial}{\partial t_k}\ldots\frac{\partial}{\partial t_1}\langle T(Q(t_1)\ldots Q(t_k))\rangle
\end{aligned}$$

Another time ordering

- Hence

$$\langle\langle(\Delta Q)^k\rangle\rangle = \int_0^t d^k t \,\langle\langle T^*(I(t_1)\dots I(t_k))\rangle\rangle$$

  with T^*: Matthews' time ordering: time-derivative outside of the T-ordering (no assumption on $[Q, I]$).

-

$$\begin{aligned} T^*(I(t_1)\dots I(t_k)) = & T(I(t_1)\dots I(t_k)) \\ & + \text{contact terms supported at } t_i = t_j \end{aligned}$$

The discrepancy solved

In the context of the model Hamiltonian the expansion in contact terms of the third cumulant is

$$\langle\langle(\Delta Q)^3\rangle\rangle =$$
$$\int_0^t d^3t\,\langle\langle T\widehat{I}_1\widehat{I}_2\widehat{I}_3\rangle\rangle + 3\int_0^t d^2t\,\langle\langle T\widehat{I}_1[\widehat{Q}_2,\widehat{I}_2]\rangle\rangle + \int_0^t dt_1\,\langle[\widehat{Q}_1,[\widehat{Q}_1,\widehat{I}_1]]\rangle$$

(with $\widehat{\ }$ reminding of second quantization).
It takes the form

$$\begin{aligned}\langle\langle(\Delta Q)^3\rangle\rangle &= (-2T^2(1-T) + 0 + T(1-T))\cdot(Vt/2\pi)\\ &= T(1-T)(1-2T)\cdot(Vt/2\pi)\end{aligned}$$

Binomial result!

Computation of a contact term

- Initial state: fermionic, quasi-free with single-particle density matrix

$$\rho = \begin{pmatrix} \theta(\mu_L - p) & 0 \\ 0 & \theta(\mu_R - p) \end{pmatrix} \qquad (V = \mu_L - \mu_R)$$

  Since $\rho = \rho^2$, the many-particle state $\langle \cdot \rangle$ is pure.
  Since $[Q, \rho] = 0$, the $\langle \cdot \rangle$ is an eigenstate of $\widehat{Q}$.

- Second quantization based the GNS space of $\langle \cdot \rangle$:

$$A \mapsto \widehat{A}$$

  for $[A, \rho] \in$ Hilbert-Schmidt (Shale-Stinespring). One has $\langle \widehat{A} \rangle = 0$ (vacuum substraction)

Computation of a contact term (cont.)

- In the Fock representation ($\rho = 0$): $\widehat{A} = d\Gamma(A)$

$$[\widehat{A}, \widehat{B}] = [d\Gamma(A), d\Gamma(B)] = d\Gamma([A, B]) = \widehat{[A, B]}$$

- In general, corrections by Schwinger terms

$$[\widehat{A}, \widehat{B}] = \widehat{[A, B]} + s(A, B)1$$

$$\begin{aligned} s(A, B) &= \mathrm{tr}([\rho, A]\rho'[B, \rho]) - \mathrm{tr}([\rho, B]\rho'[A, \rho]) \\ &= \mathrm{tr}(\rho A \rho' B \rho) - \mathrm{tr}(\rho' A \rho B \rho') \end{aligned} \qquad (\rho' = 1 - \rho)$$

In particular:

$$\langle [\widehat{A}, \widehat{B}] \rangle = s(A, B)$$

- $\widehat{A}(t) = \widehat{A(t)} + \mathrm{i} \int_0^t dt' \, s(H, A(t'))1$

Computation of a contact term (cont.)

In our case

$$\int_0^t dt_1 \, \langle [\widehat{Q}(t_1), [\widehat{Q}(t_1), \widehat{I}(t_1)]] \rangle = \int_0^t dt_1 \, \langle [\widehat{Q(t_1)}, [\widehat{Q(t_1)}, \widehat{I(t_1)}]] \rangle$$
$$= \int_0^t dt_1 \, s(Q(t_1), [Q(t_1), I(t_1)])$$
$$= T(1-T) \cdot (Vt/2\pi)$$

as announced

Summary

- The correct time ordering for the cumulants of charge ordering is T^*

$$\langle\langle(\Delta Q)^k\rangle\rangle = \int_0^t d^k t \, \langle\langle T^*(I(t_1)\ldots I(t_k))\rangle\rangle$$

- In many cases the $*$ can be omitted. It can not in the simplest case of energy-independent, instantaneous scattering. The difference to the T ordering consists in contact (Schwinger) terms.