Transport in quantum devices and its geometry

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Some pictures of quantum pumps

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

Quantum pumps: The scattering approach

Quantum pumps: The topological approach

A comparison

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Quantum pumps: The scattering approach

Quantum pumps: The topological approach

A comparison
Quantum pumps: The setup

- independent electrons \((e = +1)\)
- no voltage applied; each channel filled up to Fermi energy \(\mu\) with incoming electrons (zero temperature).
- \(S = S(E, X) = (S_{jk})\) scattering \(n \times n\) matrix at electron energy \(E\), given the pump configuration \(X\) (w.r.t. to reference configuration \(X_0\))
- At fixed \(X\): no net current on average.
Charge transport

(Büttiker, Thomas, Prêtre 1994) For slowly varying $X$ transport can be described in terms of static data $S(\mu, X)$: Upon $X \rightarrow X + dX$, and hence $S \rightarrow S + dS$, a net charge

$$\delta n_j = \frac{i}{2\pi}((dS)S^*)_{jj}$$

leaves the pump through channel $j$. 
Charge transport

(Büttiker, Thomas, Prêtre 1994) For slowly varying $X$ transport can be described in terms of static data $S(\mu, X)$: Upon $X \rightarrow X + dX$, and hence $S \rightarrow S + dS$, a net charge

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Remarks

▶ Emitted charge $d n_j$ expressed through static quantities $S(X)$ (& their variation).
▶ $\int_A^B d n_j$ depends on path $X$ from $A$ to $B$, but not on its time parameterization.
▶ $\langle n_j \rangle = \int_A^B d n_j$ is expectation value.
▶ $\oint d n_j \neq 0$: it is a pump!
Charge transport (cont.)

\[ \dot{n}_j = \frac{i}{2\pi} ((dS)S^*)_{jj} \]

More remarks

- Kirchhoff’s law does not hold:

\[ \sum_{j=1}^{n} \dot{n}_j = \frac{i}{2\pi} \text{tr}((dS)S^*) = \frac{i}{2\pi} d \log \det S \]

\[ = - d\xi \neq 0 \]

where “\(\xi(\mu) = \text{Tr}(P(\mu, X) - P(\mu, X_0))\)” 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 \(\det S = e^{2\pi i \xi(\mu)}\)

- But

\[ \oint \sum_{j=1}^{n} \dot{n}_j = 0 \]
Heuristic derivation

\[ S(E, t) = S(E, X(t)) : \text{static scattering matrix } S(E, X) \text{ at energy } E \text{ along slowly varying } X = X(t). \]

\[ T(E, t) = -i \frac{\partial S}{\partial E} S^* : \text{Eisenbud-Wigner time delay:} \]

- \( t \): time of passage at fiducial point of state \( \psi \) (energy \( E \), channel \( j \)) under \( X_0 \)
- \( t - T_{jj} \): time of passage of in state under \( X \) matching out state \( \psi \).

\[ E(E, t) = i \frac{\partial S}{\partial t} S^* : \text{Martin-Sassoli energy shift:} \]

- \( E \): energy of state \( \psi \) (time of passage \( t \), channel \( j \)) under \( X_0 \)
- \( E - E_{jj} \): energy of in state under \( X(t) \) matching out state \( \psi \).

Claim restated: Charge delivered between \( t = 0 \) and \( t = T \)

\[ \langle n_j \rangle = \frac{1}{2\pi} \int_0^T E_{jj}(\mu, t) dt \]
Heuristic derivation (cont.)

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

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

- $2\pi = \text{size of phase space cell of a quantum state}$
- $\rho(E) = \theta(\mu - E)$ occupation of incoming states at zero temperature.

Outgoing charge

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

where

\((E', t') \mapsto (E, t) = (E' - E_{jj}(E', t'), t' - T_{jj}(E', t'))\)

maps outgoing to incoming data

Net charge (linearize in $\mathcal{E}$)

\[
n_j = -\frac{1}{2\pi} \int_0^T dt \int_0^{\infty} dE' \rho'(E) E_{jj}(E, t) = \frac{1}{2\pi} \int_0^T E_{jj}(\mu, t) dt
\]
Quantized transport

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

**Theorem.** The charge transported in a cycle is quantized

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

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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A comparison
Some examples
Quantum pumps: The setup

Infinitely extended 1-dimensional system

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

depending on parameter \( s \), real. Potential \( V \) doubly periodic

\[
V(s, x + L) = V(s, x), \quad V(s + 2\pi, x) = V(s, x)
\]

Change \( s \) slowly with time \( t \).
Quantum pumps: The setup

Ininitely extended 1-dimensional system

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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, \( C \).
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).

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

- 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:

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

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

1) \( n \) channels:

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

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

\[
(H(s) - z)\psi(x) = 0, \quad \psi(x) \to 0 \ (x \to +\infty)
\]

\[
\chi(x)(H(s) - z) = 0, \quad \chi(x) \to 0 \ (x \to -\infty)
\]

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 \( \psi, \chi \). Normalize:

\[
W(\chi, \psi; x) = 1.
\]
Theorem. The transported charge is

\[ C = \frac{i}{2\pi} \int_{\mathbb{T}} \text{tr} \left( W \left( \frac{\partial \chi}{\partial s}, \frac{\partial \psi}{\partial z}; x \right) - W \left( \frac{\partial \chi}{\partial z}, \frac{\partial \psi}{\partial s}; x \right) \right) ds \, dz \]

(any \( x \)). This is the Chern number of the bundle of solutions \( \psi \) on \((s, z) \in \mathbb{T} = [0, 2\pi] \times \gamma\).
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Are Thouless’ and Böttiker’s approaches incompatible?

➤ Topological approach: Fermi energy $\mu$ in gap: no states there

Charge transport attributed to energies way below $\mu$

➤ Scattering approach: Depends on scattering at Fermi energy

Charge transport attributed to states at energy $\mu$
A comparison
Are Thouless’ and Büttiker’s approaches incompatible?

- Topological approach: Fermi energy $\mu$ in gap: no states there

\[
\begin{array}{c}
\mu \\
\end{array}
\]

Charge transport attributed to energies way below $\mu$

- Scattering approach: Depends on scattering at Fermi energy

\[
\begin{array}{c}
\mu \\
\end{array}
\]

Charge transport attributed to states at energy $\mu$

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

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

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.
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 $s$. 

\[ \begin{align*}
\text{Im } z & \quad \text{Re } z \\
0 & \quad 2\pi
\end{align*} \]
Sketch of proof (cont.)

- Near a given discrete 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 \((\mu, s^*)\); \(\lambda(z, s) \in \mathbb{R}\) for \(z \in \mathbb{R}\)

\[
C = - \sum_{s^*} \text{winding number of } \lambda(z, s) \text{ around } (\mu, s^*)
= \sum_{s^*} \text{sgn} \left( \frac{\partial \lambda}{\partial z} \frac{\partial \lambda}{\partial s} \right) \bigg|_{(z=\mu, s=s^*)} = - \sum_{s^*} \text{sgn} \left( \frac{\partial \lambda}{\partial s} \right) \bigg|_{(z=\mu, s=s^*)}
\]

- \(\partial \lambda / \partial z < 0\) for \(z \in \mathbb{R}\) (Sturm oscillation)
Sketch of proof (cont.)

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

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

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

- Eigenvalue crossing is counterclockwise iff

$$\frac{\partial \lambda}{\partial s}|_{(z=\mu, s=s^*)} < 0$$

- Together:

$$C = \# \text{ eigenvalue crossings of } R \text{ at } z = -1$$

= winding number of det $R$
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; generally dissipative
- **Topological approach:** gapped systems, infinite device; transport attributed to states way below Fermi energy; quantized and dissipationless
- A comparison has been obtained.