Transport in quantum devices and its geometry

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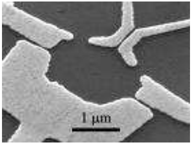
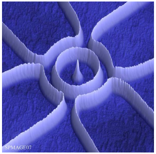
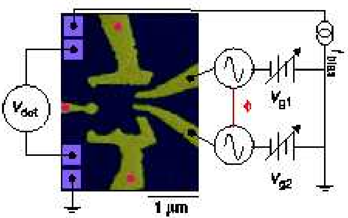
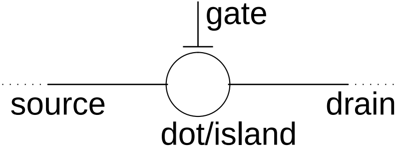
Workshop on Quantum Control
Institut Henri Poincaré

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

Collaborators: Y. Avron, A. Elgart, L. Sadun; G. Ortelli, G. Bräunlich

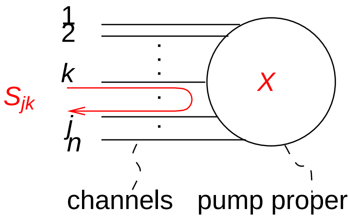
Outline

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 μ 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 $X \to X + dX$, and hence $S \to S + dS$, a net charge

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

leaves the pump through channel j.

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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.)

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

More remarks

- Kirchhoff's law does not hold:

$$\sum_{j=1}^{n} đn_j = \frac{\mathrm{i}}{2\pi}\mathrm{tr}((dS)S^*) = \frac{\mathrm{i}}{2\pi} d \log \det S$$
$$= -d\xi \neq 0$$

  where "$\xi(\mu) = \mathrm{Tr}(P(\mu, X) - P(\mu, X_0))$" 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

$$\oint \sum_{j=1}^{n} đn_j = 0$$

Heuristic derivation

$S(E,t) = S(E,X(t))$: static scattering matrix $S(E,X)$ at energy E along slowly varying $X = X(t)$.

$\mathcal{T}(E,t) = -\mathrm{i}\frac{\partial S}{\partial E} S^*$: *Eisenbud-Wigner time delay:*

t	time of passage at fiducial point of state ψ (energy E, channel j) under X_0
$t - \mathcal{T}_{jj}$	time of passage of in state under X matching out state ψ.

$\mathcal{E}(E,t) = \mathrm{i}\frac{\partial S}{\partial t} S^*$: *Martin-Sassoli energy shift:*

E	energy of state ψ (time of passage t, channel j) under X_0
$E - \mathcal{E}_{jj}$	energy of in state under $X(t)$ matching out state ψ.

Claim restated: Charge delivered between $t = 0$ and $t = T$

$$\langle n_j \rangle = \frac{1}{2\pi} \int_0^T \mathcal{E}_{jj}(\mu, t) dt$$

Heuristic derivation (cont.)

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

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

- $2\pi =$ 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

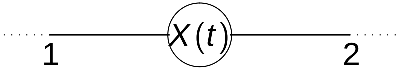
$(E', t') \mapsto (E, t) = (E' - \mathcal{E}_{jj}(E', t'), t' - \mathcal{T}_{jj}(E', t'))$

maps outgoing to incoming data

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

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

Quantized transport



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

Theorem. The charge transported in a cycle is quantized

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

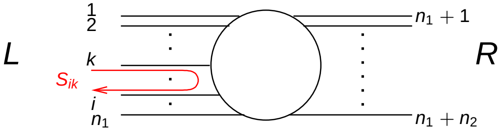
iff scattering matrix $S(t)$ is of the form

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

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

Quantized transport (cont.)

Generalization to many channels:



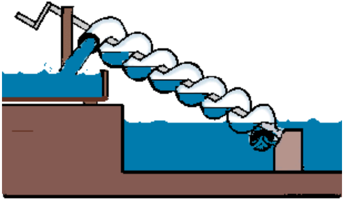
In a cycle, the charge delivered to the Left (resp. Right) channels as a whole is quantized iff

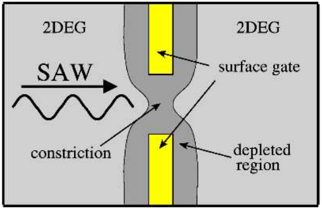
$$S(t) = \begin{pmatrix} U_1(t) & 0 \\ 0 & U_2(t) \end{pmatrix} S_0$$

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

Outline

Some examples





Quantum pumps: The setup

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.

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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).

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

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

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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

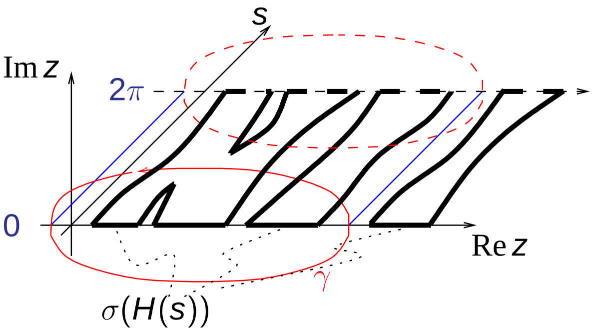
$$W(\chi, \psi; x) = \chi(x)\psi'(x) - \chi'(x)\psi(x) \in M_n(\mathbb{C})$$

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 $(s,z)\in\mathbb{T}=[0,2\pi]\times\gamma$.



Outline

A comparison

Are Thouless' and Büttiker's approaches incompatible?

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

μ

Charge transport attributed to energies way below μ

- Scattering approach: Depends on scattering at Fermi energy

μ

Charge transport attributed to states at energy μ

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

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

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.

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Theorem

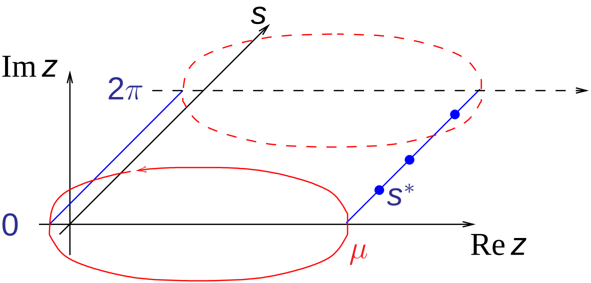
- As $L \to \infty$,

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

  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.



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. $\psi'_{z,s}(0) = 1$)

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

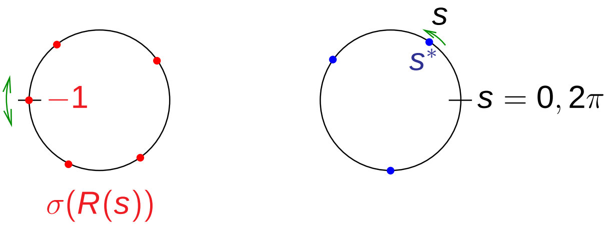
  is analytic with $L(z,s) = L(\bar{z},s)^*$
- Generically, $L(z,s)$ has a simple eigenvalue $\lambda(z,s)$ vanishing to first order at (μ, s^*); $\lambda(z,s) \in \mathbb{R}$ for $z \in \mathbb{R}$
- $$C = -\sum_{s^*} \text{winding number of } \lambda(z,s) \text{ around } (\mu, s^*)$$
  $$= \sum_{s^*} \operatorname{sgn}\Big(\frac{\partial\lambda}{\partial z}\frac{\partial\lambda}{\partial s}\Big)\Big|_{(z=\mu, s=s^*)} = -\sum_{s^*} \operatorname{sgn}\Big(\frac{\partial\lambda}{\partial s}\Big)\Big|_{(z=\mu, s=s^*)}$$
- $\partial\lambda/\partial z < 0$ 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:

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

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.