The Kubo formula and Quantum pumping

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$GIF, $ISF

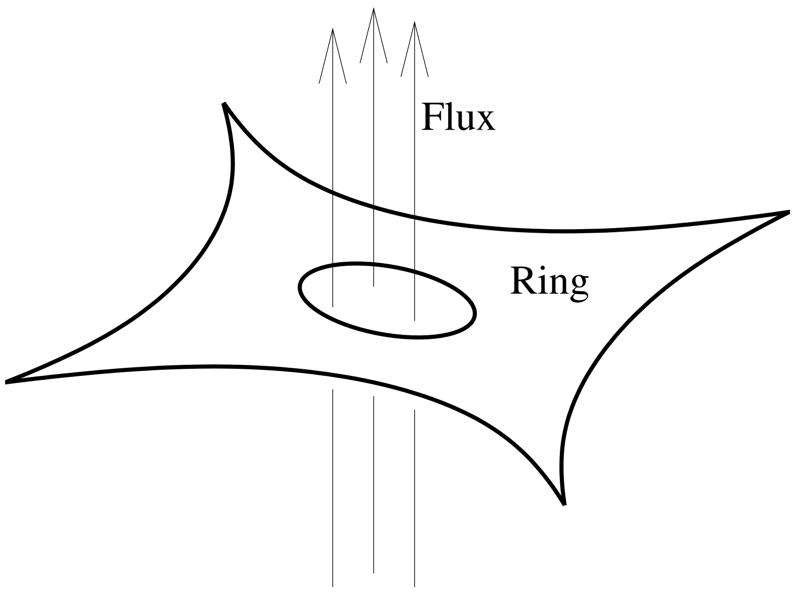
Driven Systems

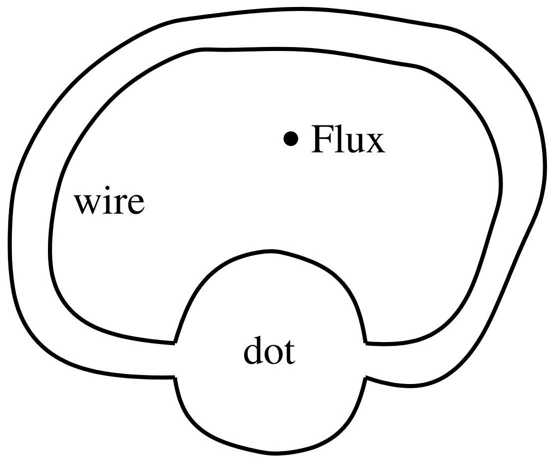
Non interacting "spinless" electrons.

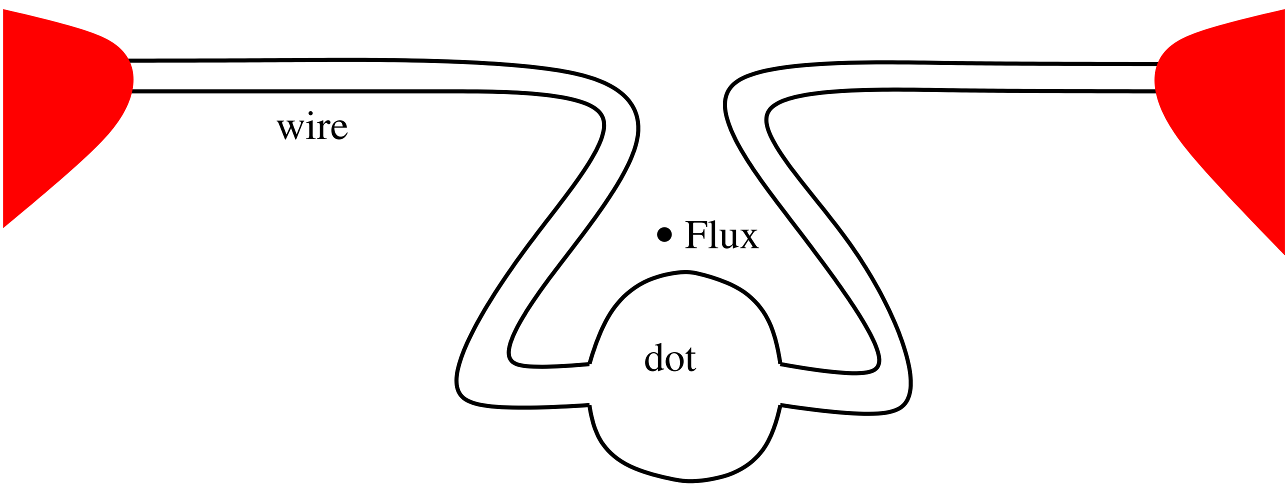
Held by a potential (e.g. AB ring geometry).

$x_1, \ x_2 \ = \$ shape parameters

$x_3 \ = \ \Phi \ = \ (\hbar/e)\phi \ = \$ magnetic flux







"Ohm law"

For one parameter driving by EMF

$$
\begin{aligned}
I &= \boldsymbol{G}^{33} \times (-\dot{x}_3) \\
dQ &= -\boldsymbol{G}^{33}\ dx_3
\end{aligned}
$$

For driving by changing another parameter

$$
\begin{aligned}
I &= -\boldsymbol{G}^{31}\ \dot{x}_1 \\
dQ &= -\boldsymbol{G}^{31}\ dx_1
\end{aligned}
$$

For two parameter driving

$$
\begin{aligned}
I &= -\boldsymbol{G}^{31}\dot{x}_1\ - \boldsymbol{G}^{32}\dot{x}_2 \\
dQ &= -\boldsymbol{G}^{31}\ dx_1\ - \boldsymbol{G}^{32}\ dx_2 \\
Q &= -\oint \boldsymbol{G} \cdot dx
\end{aligned}
$$

and in general

$$
\langle F^k \rangle = -\sum_j \boldsymbol{G}^{kj}\ \dot{x}_j
$$

Linear response theory

$$\mathcal{H} \quad = \quad \mathcal{H}(\boldsymbol{r}, \boldsymbol{p};\ x_1(t), x_2(t), x_3(t))$$

$$F^k \quad = \quad -\frac{\partial \mathcal{H}}{\partial x_k}$$

$$\langle \boldsymbol{F} \rangle_t \ = \int \boldsymbol{\alpha}(t-t')\ \delta \boldsymbol{x}(t')\ dt'$$

$$\begin{tikzcd}
\alpha^{kj}(t-t') \arrow[d] & & \\
\chi^{kj}(\omega) \arrow[d] \arrow[rr] & & (1/\omega) \times \ \mathrm{Im}[\chi^{kj}(\omega)] \arrow[d] \\
\mathrm{Re}[\chi^{kj}(\omega)] & & \boldsymbol{G}^{kj} \arrow[dl] \arrow[dr] & \\
& \boldsymbol{\eta}^{kj} & & \boldsymbol{B}^{kj}
\end{tikzcd}$$

(dissipative) (non-dissipative)

$$\langle F^k \rangle \quad = \quad -\sum_j \boldsymbol{G}^{kj}\ \dot{x}_j$$

What is the problem?

From Kubo formula we get
a formal expression for $\boldsymbol{G}^{kj}$.

Can we trust this expression? Conditions?
Quantum chaos!

How to use this expression?
The bare Kubo formula gives no dissipation!

To define an energy scale Γ
Beyond first order perturbation theory!

Γ in case of isolated system is due to
non-adiabaticity.

Γ affects both the dissipative and the
non-dissipative (geometric) part of the response.

Some references

Adiabatic transport

Thouless (PRL 1983) - Periodic arrays

Avron, Sadun, Raveh, Zur (1988) - Networks with fluxes

Berry, Robbins (JPA 1993) - Geometric magnetism

Linear response theory and Mesoscopics

Imry, Shiren (PRB 1986) - Using Kubo for a closed ring

Wilkinson, Austin (JPA 1995) - Challenging the validity

DC (PRL 1999) - The "quantum chaos" identification of regimes

DC and Kottos (PRL 2000) - The (A, Ω) regimes diagram

DC (PRB+Rapid 2003) - the Kubo approach to pumping

DC, Kottos, Schanz - pumping on networks (in preparation)

Sela, DC, Yakubo - pumping on a ring (in preparation)

Open systems, S matrix formalism

The Landauer / Landauer-Buttiker formula (1970,1986)

Fisher, Lee, Baranger, Stone (1981,1989)

The Buttiker Pretre Thomas [BPT] formula (1994)

Brouwer (1998)

Avron, Elgart, Graf, Sadun

Buttiker, Texier, Moskalets

Marcus - experiments

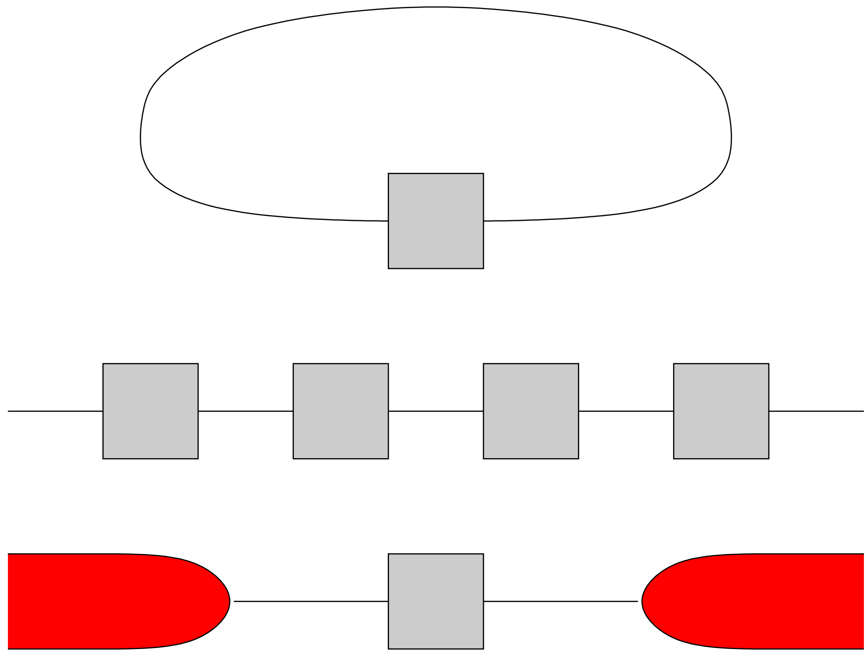
Shutenko, Aleiner, Altshuler (PRB 2000) - quantization?

Entin-Wohlman, Aharony, Levinson (2002) - two delta functions

Driven Systems - classification

$$\mathcal{H} \;=\; \mathcal{H}(\boldsymbol{r},\boldsymbol{p};\; x_1(t), x_2(t), x_3(t))$$

- closed isolated systems
- periodic arrays
- open systems (with reservoirs)
- one of the above interacting with a bath



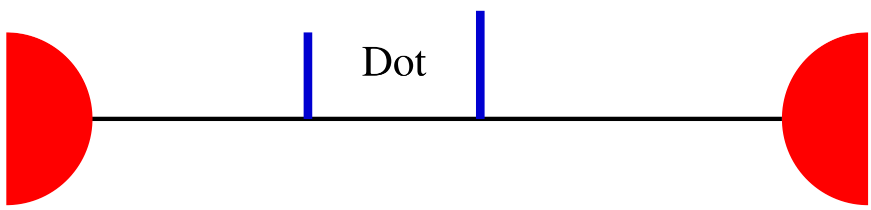
Questions: **Transport? Dissipation?**

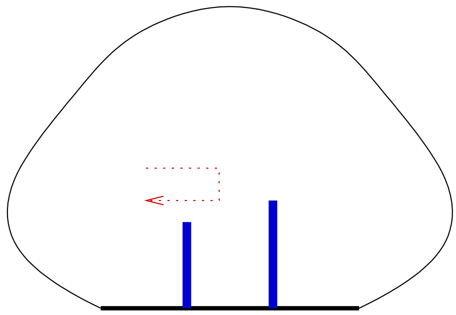
Simple model systems

How can we drive current?

- by changing the height of the potential

- by translating the potential

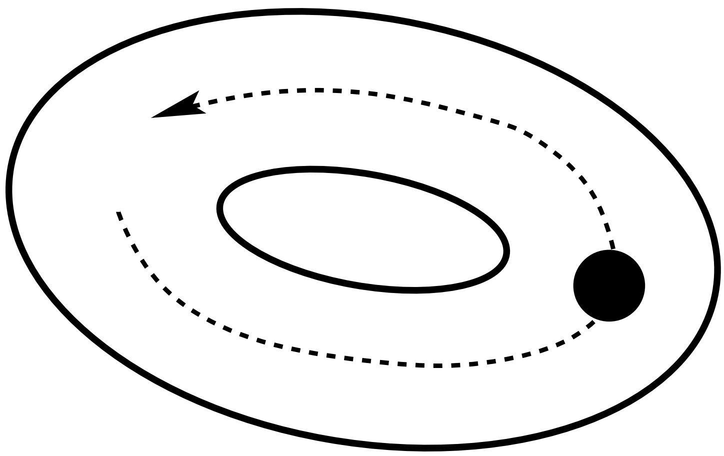




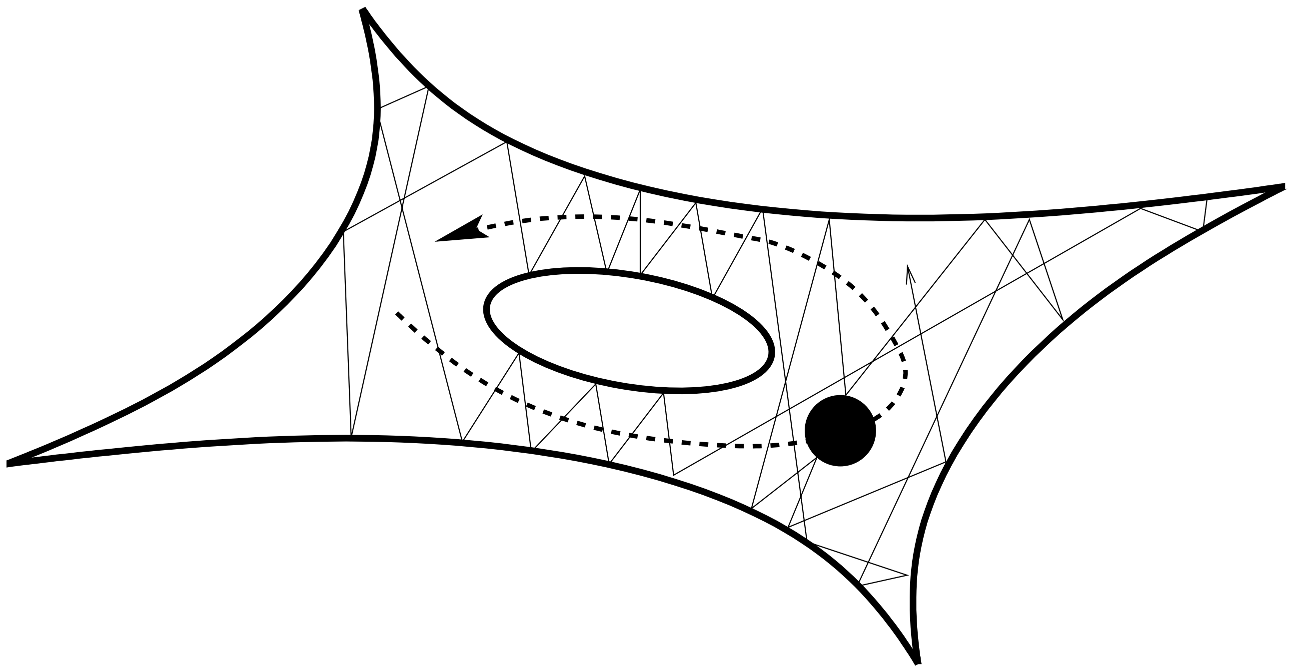
Specific question:

What is the current which is created by translating a scatterer?

The moving scatterer model

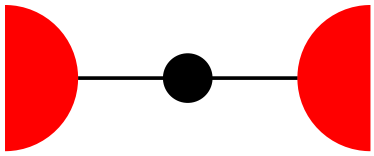


- There is a stationary solution.
- There is no dissipation.
- Pumping: $dQ \propto 1 \times \; dX$

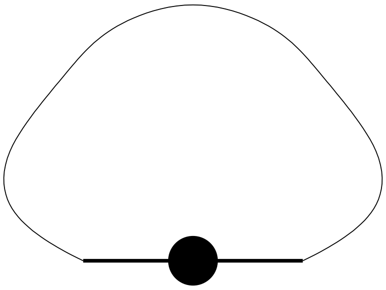


- There is no stationary solution.
- There is dissipation.
- Pumping: $dQ \propto (1-g) \times \; dX$

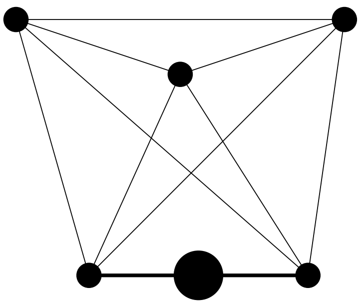
Simple model systems - networks



$$dQ = (1-g_0) \times \frac{e}{\pi} k_{\mathrm{F}} \times dX$$



$$dQ = 1 \times \frac{e}{\pi} k_{\mathrm{F}} \times dX$$



$$dQ = \left[\frac{g_T}{1-g_T}\right] \left[\frac{1-g_0}{g_0}\right] \times \frac{e}{\pi} k_{\mathrm{F}} \times dX$$

Adiabatic versus non-adiabatic result

The dot-wire ring system (I)

$$\mathcal{H} \ = \ \mathcal{H}(\boldsymbol{r}, \boldsymbol{p};\ x_1, x_2, x_3)$$

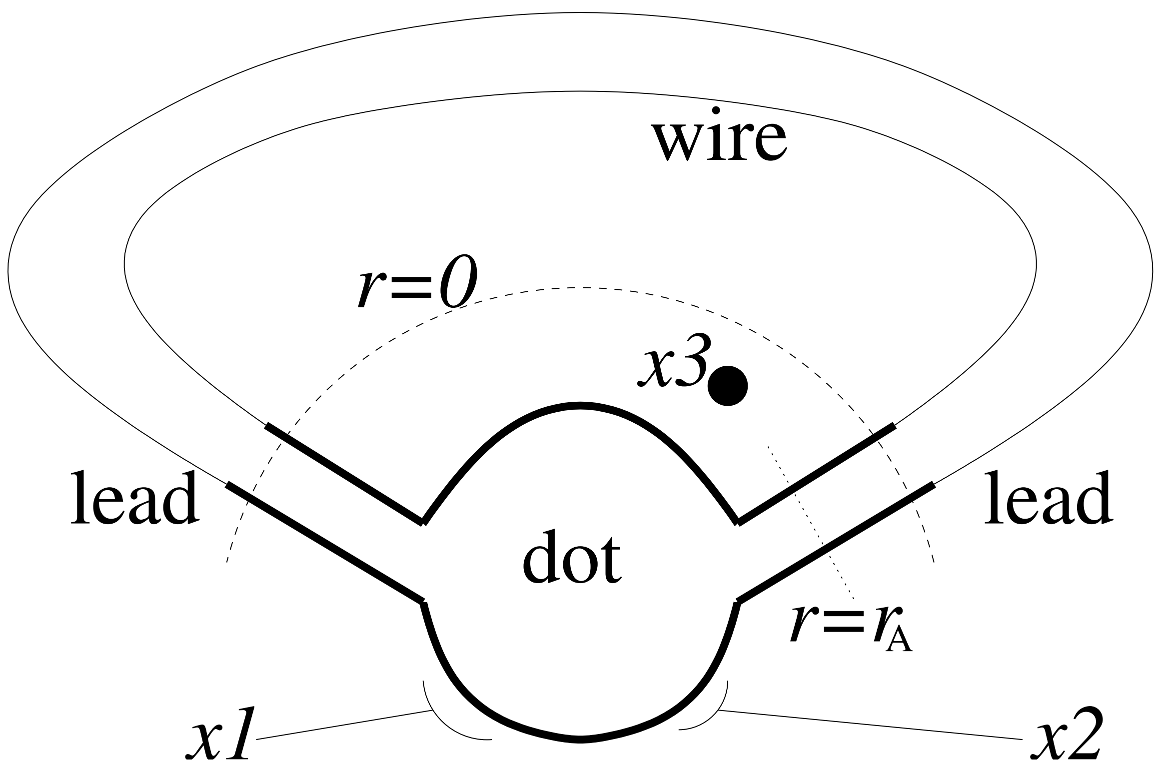
$$x_3 \ = \ \Phi \ = \ (\hbar/e)\phi \ = \ \text{magnetic flux}$$

$$-\dot{x}_3 \ = \ \text{electro motive force [Volt]}$$

$$\oint \vec{\mathcal{A}} \cdot \vec{dr} \ = \ \Phi$$

There is more than one way to put Φ into $\mathcal{H}$...

Conjugate current operator? Continuity?



The dot-wire ring system (II)

$$\mathcal{H} \;=\; \mathcal{H}(\boldsymbol{r},\boldsymbol{p};\; x_1, x_2, x_3)$$

$x_1,\ x_2 \ \ =\ \ $ shape parameters

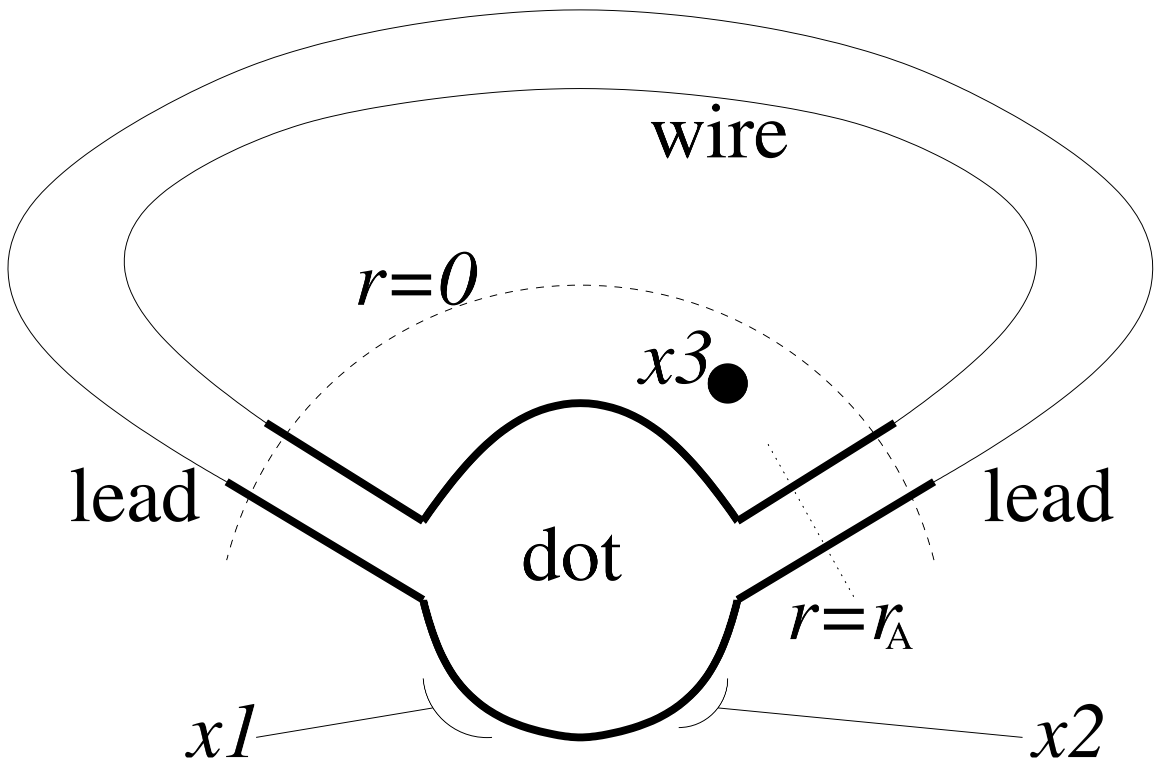
Possibilities:

$x =$ dot potential floor

$x =$ position of a wall element

$x =$ position of a scatterer inside the dot

$x =$ height of a barrier



Generalized forces / currents (I)

$$
\begin{aligned}
\mathcal{H} &= \mathcal{H}(\boldsymbol{r}, \boldsymbol{p}; x) \\
F &= -\frac{\partial \mathcal{H}}{\partial x}
\end{aligned}
$$

Example 1:

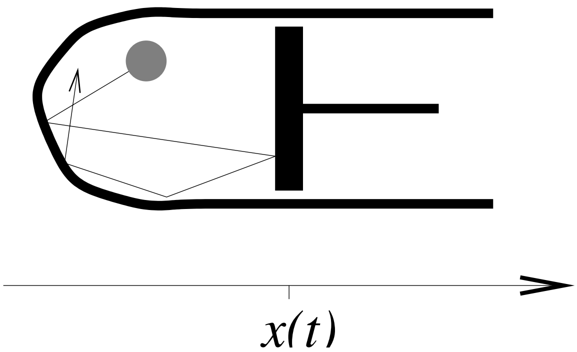
x = position of a wall element (or scatterer)

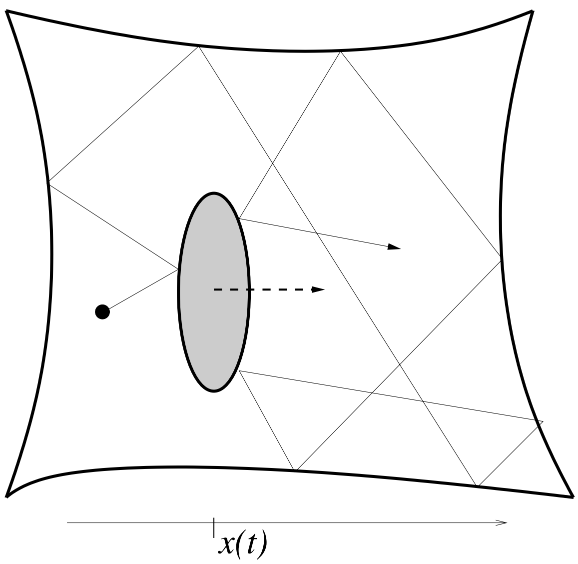
$\dot{x}$ = wall (or scatterer) velocity

F = Newtonian force

$\langle F \rangle = -\eta \dot{x}$ [friction law]

$\dot{\mathcal{W}} = \eta \dot{x}^2$ [rate of heating]





Generalized forces / currents (II)

$$\mathcal{H} = \mathcal{H}(\boldsymbol{r}, \boldsymbol{p}; x)$$
$$F = -\frac{\partial \mathcal{H}}{\partial x}$$

Example 2:

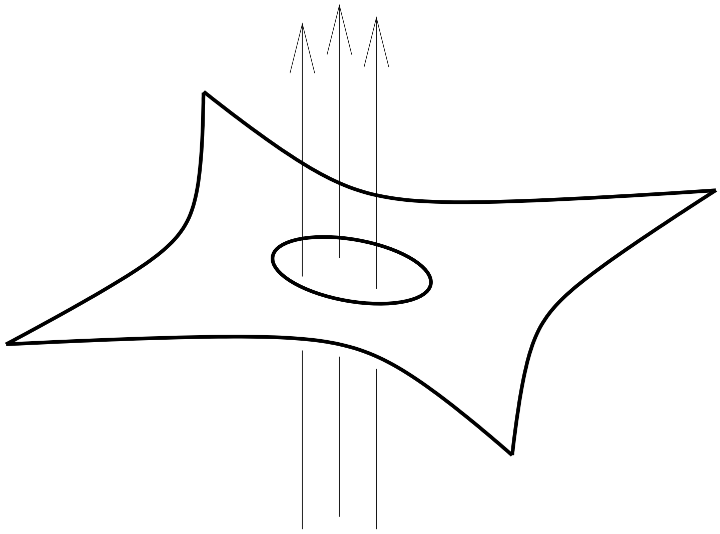
$x =$ magnetic flux through the ring

$\dot{x} = -\mathrm{EMF}$

$F =$ electrical current

$\langle F \rangle = -G\dot{x}$ [Ohm law]

$\dot{\mathcal{W}} = G\dot{x}^2$ [Joule law]



chaos!

Linear response theory

$$\langle \boldsymbol{F} \rangle_t \;=\; \int \boldsymbol{\alpha}(t-t')\; \delta\boldsymbol{x}(t')\; dt'$$

$$\begin{tikzcd}
\alpha^{kj}(t-t') \arrow[d] & & & \\
\chi^{kj}(\omega) \arrow[d] \arrow[rr] & & {} & \\
\mathrm{Re}[\chi^{kj}(\omega)] & & (1/\omega) \times \; \mathrm{Im}[\chi^{kj}(\omega)] \arrow[d] & \\
& & \boldsymbol{G}^{kj} \arrow[dl] \arrow[dr] & \\
& \begin{array}{c}\boldsymbol{\eta}^{kj} \\ \text{(dissipative)}\end{array} & & \begin{array}{c}\boldsymbol{B}^{kj} \\ \text{(non-dissipative)}\end{array}
\end{tikzcd}$$

$$\langle F^k \rangle \;\;=\;\; -\sum_j \boldsymbol{G}^{kj}\; \dot{x}_j$$

$$\langle F \rangle \;\;=\;\; -\boldsymbol{G} \cdot \dot{x} \;\;=\;\; -\boldsymbol{\eta} \cdot \dot{x} \;-\; \boldsymbol{B} \wedge \dot{x}$$

$$\dot{\mathcal{W}} \;\;=\;\; -\langle F \rangle \cdot \dot{x} \;\;=\;\; \sum_{kj} \boldsymbol{\eta}^{kj}\; \dot{x}_k\; \dot{x}_j$$

The Kubo Formula

$$\alpha^{kj}(\tau) \;=\; \Theta(\tau) \times \frac{i}{\hbar}\langle[F^k(\tau), F^j(0)]\rangle$$

$$\chi^{kj}(\omega) \;=\; \sum_{n,m} f(E_n)\left(\frac{-F^k_{nm}F^j_{mn}}{\hbar\omega-(E_m-E_n)+i0} + \frac{F^j_{nm}F^k_{mn}}{\hbar\omega+(E_m-E_n)+i0}\right)$$

$$\boldsymbol{G}^{kj} \;=\; \frac{1}{\omega} \times \mathrm{Im}[\chi^{kj}(\omega)] \;\Big|_{\omega\sim 0}$$

$$\boldsymbol{\eta}^{kj} = \pi\hbar \sum_{n,m} F^k_{nm}F^j_{mn}\ \delta(E_n - E_F)\ \overline{\delta(E_m - E_n)}$$

$$\boldsymbol{B}^{kj} \;=\; 2\hbar \sum_n f(E_n) \sum_{m(\neq n)} \frac{\mathrm{Im}\left[F^k_{nm}F^j_{mn}\right]}{(E_m-E_n)^2 + (\Gamma/2)^2}$$

The Kubo Formula and "quantum chaos"

τ_{cl} = classical correlation time

$\Delta \ \propto \ \hbar^d/L$ = mean level spacing

$\Delta_b \ \sim \ \hbar/\tau_{\text{cl}}$ = bandwidth

Effective width of the energy levels:

$$\Gamma = \left(\frac{\hbar\sigma}{\Delta^2}|\dot{x}|\right)^{2/3} \times \Delta \quad \sim \quad \Big(L\,|\dot{x}|\Big)^{2/3}\frac{1}{L}$$

$\Gamma \ll \Delta$	adiabatic regime
$\Delta < \Gamma < \Delta_b$	non-adiabatic regime
$\Delta_b < \Gamma$	non-perturbative regime

$L \to \infty$ is not the semiclassical limit!

The generalized FD relation

$$\begin{aligned} K^{kj}(\tau) &= (i/\hbar)\langle[F^k(\tau), F^j(0)]\rangle \\ C^{kj}(\tau) &= \tfrac{1}{2}(\langle F^k(\tau)F^j(0)\rangle + \mathrm{cc}) \end{aligned}$$

$$\alpha^{kj}(\tau) = \Theta(\tau)\ K^{kj}(\tau) \qquad \text{[“Kubo formula”]}$$

$$\boldsymbol{G}^{kj} = \lim_{\omega\to 0} \frac{\mathrm{Im}[\chi^{kj}(\omega)]}{\omega} = \int_0^\infty K^{kj}(\tau)\tau d\tau$$

$$\boldsymbol{G}^{kj} = \frac{1}{\Delta}\int_0^\infty C^{kj}(\tau)d\tau \qquad \text{[“FD relation”]}$$

$$\boldsymbol{B}^{kj} = \frac{-i}{\Delta}\int_{-\infty}^{\infty}\left[\frac{\tilde{C}^{kj}(\omega)}{\omega}\right]\frac{d\omega}{2\pi}$$

$$\boldsymbol{\eta}^{kj} = \frac{1}{2\Delta}\tilde{C}^{kj}(\omega\sim 0)$$

Kubo formula - Green functions - BPT formula

$$\eta^{3j} = \frac{\hbar}{\pi}\ \mathrm{trace}\left[F^3\ \mathrm{Im}[\mathsf{G}^+]\ F^j\ \mathrm{Im}[\mathsf{G}^+]\right]$$

$$= \frac{\hbar}{4\pi}\mathrm{trace}\left[\frac{\partial S^\dagger}{\partial x_3}\frac{\partial S}{\partial x_j}\right]$$

$$\boldsymbol{B}^{3j} = \frac{\hbar}{4\pi}\mathrm{trace}\left[\mathcal{F}^3\ \mathsf{G}^+\ \mathcal{F}^j\ \mathsf{G}^- - \mathcal{F}^3\ \mathsf{G}^-\ \mathcal{F}^j\ \mathsf{G}^+\right]$$

$$= \frac{e}{4\pi i}\mathrm{trace}\left[P_{\mathrm{A}}\left(\frac{\partial S}{\partial x_j}S^\dagger - \frac{\partial S^\dagger}{\partial x_j}S\right)\right] + \mathrm{intrf}$$

$$\boldsymbol{G}^{3j} = \frac{e}{2\pi i}\mathrm{trace}\left(P_{\mathrm{A}}\frac{\partial S}{\partial x_j}S^\dagger\right) \qquad \text{[BPT]}$$

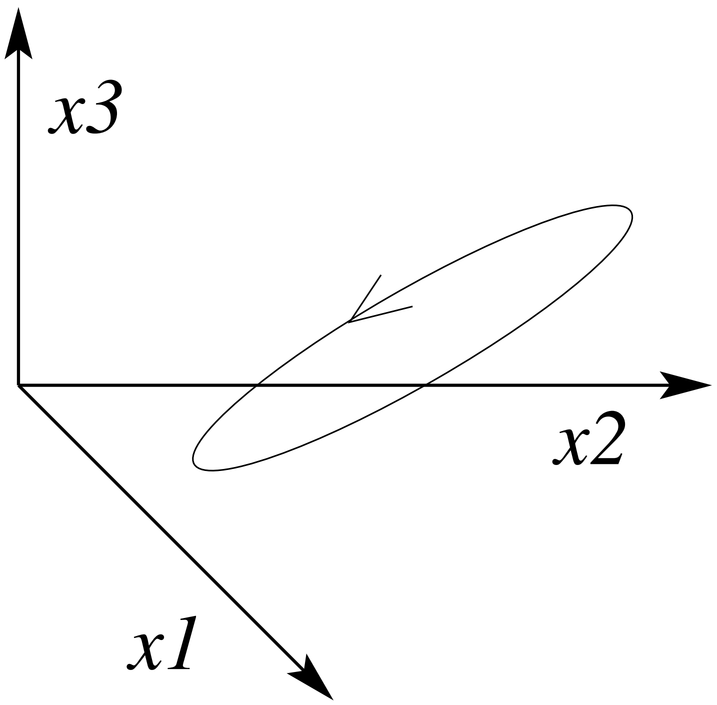
Driven Systems - pumping

Assume periodic ("AC") driving.

Does the current have a "DC" component?

Define charge transported per cycle:

$$Q = \oint I dt = ???$$



Linear response assumption $\Longrightarrow$
for one parameter driving $Q = 0$.

Ratchests are non-linear devices that use mixed or damped dynamics in order to pump with only one parameter.

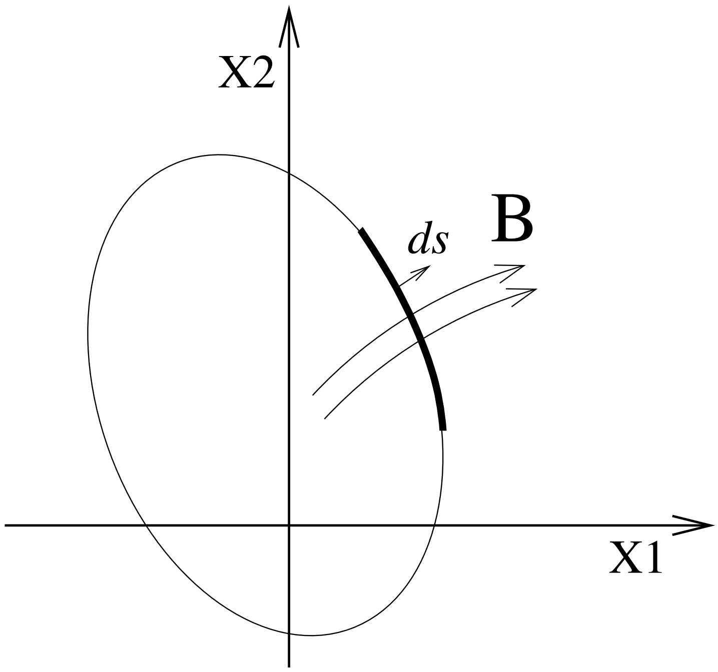
Pumping within the Kubo formulation

$$Q = \oint \langle F^3 \rangle dt$$

$$\langle F \rangle = -\boldsymbol{\eta} \cdot \dot{x} \quad - \boldsymbol{B} \wedge \dot{x}$$

$$Q = \left[-\oint \boldsymbol{\eta} \cdot dx \quad -\oint \boldsymbol{B} \wedge dx \right]_{k=3}$$

Consider a planar (x_1, x_2) pumping cycle.



$$Q = -\oint \boldsymbol{B} \cdot \; ds$$

No magnetic field. Onsager $\Longrightarrow$

$\boldsymbol{\eta}^{31} = \boldsymbol{\eta}^{32} = 0$ (no dissipative contribution)

$\boldsymbol{B}^{12} = 0$ (no vertical component)

The $\boldsymbol{B}$ field

$$Q \;=\; \left[-\oint \boldsymbol{B} \wedge dx\right]_{k=3}$$

$$\boldsymbol{B}^{ij} \;=\; \sum_n f(E_n)\boldsymbol{B}_n^{ij} \qquad\qquad \text{[geometric magnetism]}$$

$$\boldsymbol{B}_n^{kj} \;=\; 2\hbar \sum_{m(\neq n)} \frac{\mathrm{Im}\left[F_{nm}^{k} F_{mn}^{j}\right]}{(E_m - E_n)^2 + (\Gamma/2)^2}$$

This field is divergenceless (for $\Gamma = 0$)

A chain of degeneracies:

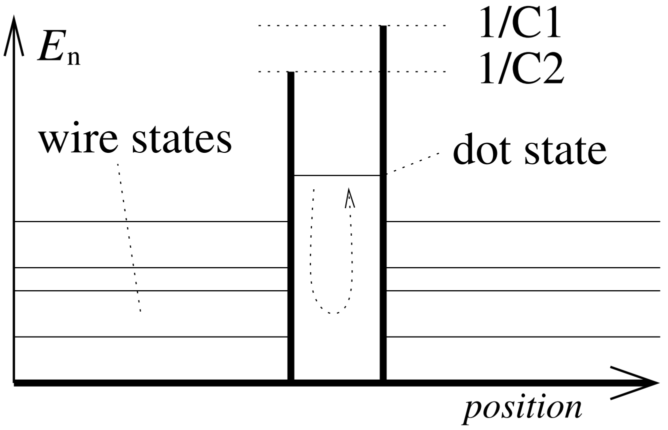
$$\left(x_1^{(0)}, \quad x_2^{(0)}, \quad \Phi^{(0)} + 2\pi\frac{e}{\hbar} \times \text{ integer}\right)$$

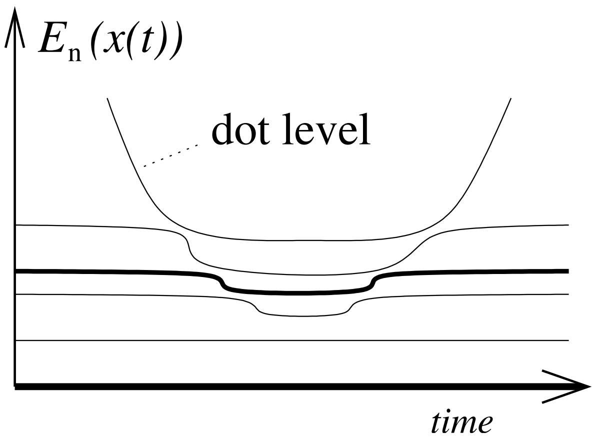
The degeneracies are like Dirac monopoles

- The issue of bandwidth

- The effect of screening

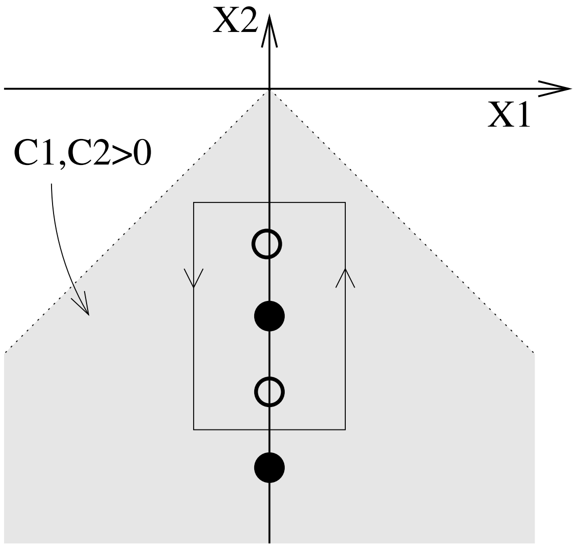
The two barrier model

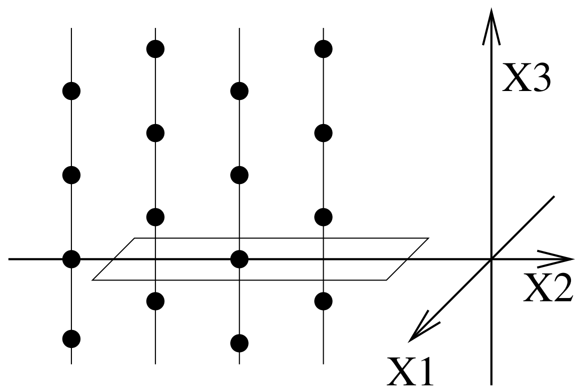




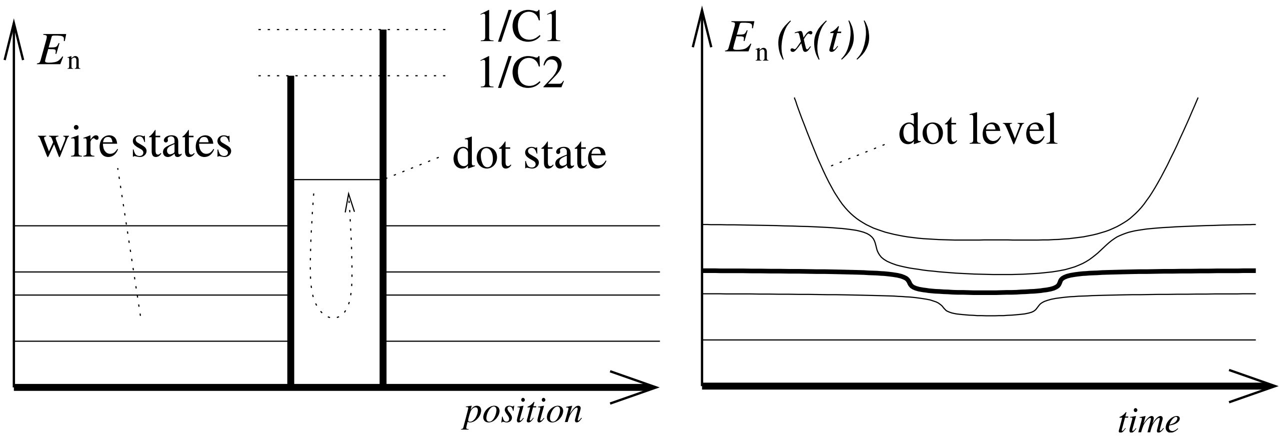
$$X_1 = \quad \tfrac{1}{2}(C_1 - C_2) \quad = \text{left-right bias}$$

$$X_2 = -\tfrac{1}{2}(C_1 + C_2) \quad = \text{dot potential floor}$$





Speculations...



For the open system, using BPT:

$$Q \approx 1 - g$$

- Is it due to non-adiabaticity?
- Is it a dissipative contribution?

What about strict adiabatic cycle in a closed system?

Shutenko, Aleiner, Altshuler (2000):

"If the system were closed [and strictly adiabatic], the charge distribution after each period of the perturbation would return to the original distribution, and therefore, the pumped charge would be *exactly quantized*."

Not correct!

Questions

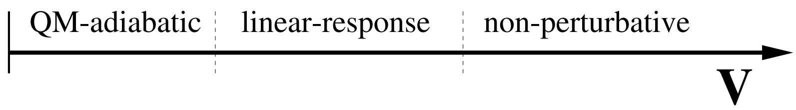
- Take the “two barrier model” as an example.
- Assume Fermi occupation.
- Adiabatic limit: Find the current of each level.
- Is there one level that carries most of the current?
- What is the effect of non-adiabaticity?
- What is the role of dissipation?
- Can we get in a closed system $Q > 1$ or even $Q \gg 1$
- Why in an open system always $Q = 1 - g$

Formalism:

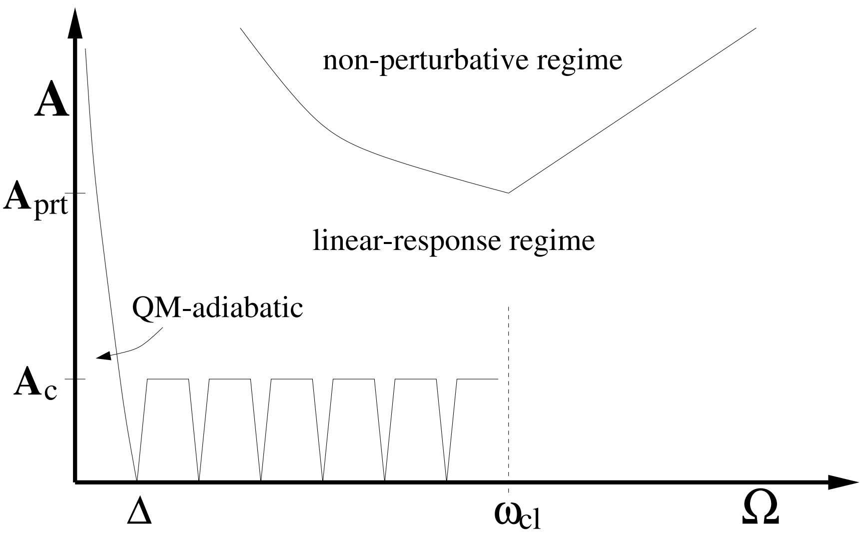
- Start with Kubo formula.
- Derive from it the adiabatic limit.
- Explain the implications of non-adiabaticity.
- Explain the emergence/role of dissipation.
- Take the limit of large L.
- Express the results using the S matrix.
- Does the result coincides with BPT?

Summary

- LRT gives a unified framework for the theory of pumping.
- Derivation of S matrix expressions for $\boldsymbol{\eta}$ and $\boldsymbol{B}$.
- Distinction between adiabatic, non-adiabatic and non-prt regimes.
- "Quantum chaos" considerations are essential (Γ).
- The emergence / relevance of dissipation.
- The $L \to \infty$ limit versus the $\hbar \to 0$ limit.
- Near-field versus far field pumping cycles around "Dirac chains".
- The analysis of deviations from "quantized" pumping.

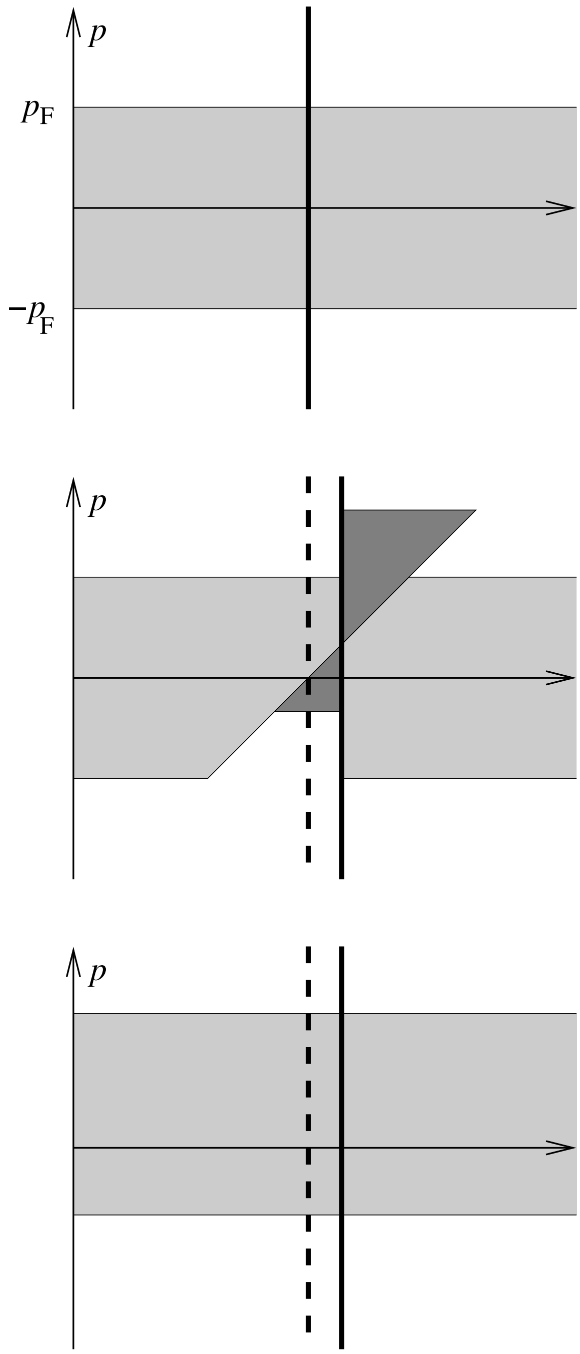


$$x(t) = Vt$$



$$x(t) = A\sin(\Omega t)$$

Digression - The 1D moving wall model



Strictly adiabatic:

$$dQ_n \;=\; \tfrac{1}{L}dX$$

$$dQ \;=\; \tfrac{p_F dX}{\pi\hbar}$$

$$N = \tfrac{2p_F L}{2\pi\hbar}$$

Non adiabatic:

$$dQ = (1-g) \times \tfrac{p_F dX}{\pi\hbar}$$