Concepts, problems and progress in quantum transport theory

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Questions and concepts

Background and basic questions:

"Fouriers Law: A challenge to theorists"
Lebowitz et al., *World Scientific* (2000)

"Fourier's law of heat conduction doesn't always hold - although precisely when it does, or doesn't, no one can say."
M. Buchanan, *nature physics* **2** (2005)

microscopic quantum dynamics:

$$i\hbar|\dot{\psi}\rangle = \hat{H}|\psi\rangle$$

$$\rho(x,t) := \langle\psi(t)|\hat{n}(x)|\psi(t)\rangle$$

macroscopic transport dynamics:

$$j = \kappa\nabla U \qquad j = D\nabla\rho$$

$$\dot{\rho} = D\Delta\rho$$

- *Does the diffusion equation "follow" from the Schrödinger equation ?*
- *If so, what are κ and D?*
- *Does the Einstein relation from Brownian motion, i.e., $\kappa \propto TG$ hold in general?*

Boltzmann equation:

$$\dot{f}(\mathbf{x}_1,\mathbf{v}_1,t)+\mathbf{v}_1\nabla f(\mathbf{x}_1,\mathbf{v}_1,t)=R_{\text{ext}}(\mathbf{v}_1'\to\mathbf{v}_1)f(\mathbf{x}_1,\mathbf{v}_1',t)+$$
$$\int d\mathbf{v}_2 d\mathbf{v}_1' d\mathbf{v}_2' R_{\text{int}}(\mathbf{v}_1,\mathbf{v}_2\to\mathbf{v}_1',\mathbf{v}_2')(f(\mathbf{x}_1,\mathbf{v}_1',t)f(\mathbf{x}_1,\mathbf{v}_2',t)-f(\mathbf{x}_1,\mathbf{v}_1,t)f(\mathbf{x}_1,\mathbf{v}_2,t))$$

Linearized form for spatially homogenous distributions

$$\dot{g}(\mathbf{v},t)=\int d\mathbf{v}' R(\mathbf{v}\to\mathbf{v}')g(\mathbf{v}',t)$$

$\Rightarrow$ diffusive dynamcis (may) exist $\Rightarrow$

$$D=\int \mathbf{v}R^{-1}(\mathbf{v}\to\mathbf{v}')\mathbf{v}' f^0(\mathbf{v})d\mathbf{v}'d\mathbf{v} \qquad \rho(\mathbf{x},t)=\int \mathbf{v}f(\mathbf{x},\mathbf{v},t)d\mathbf{v}$$

Do quantum systems map onto a classical Boltzmann equation at all?

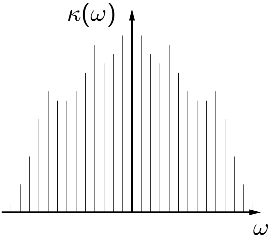
- Identify $f(\mathbf{x},\mathbf{v})$ from the quantum picture.
- Identify $R_{\text{ext}}, R_{\text{int}}$ from the quantum picture.
- Find $f^0(\mathbf{v})$, find, linearize and invert R

Kubo formula: derived for transport driven by external fields

$\hat{H} = \hat{H}_0 + \hat{U}(t) \quad E = -\nabla U \qquad \frac{\mathrm{d}}{\mathrm{d}t}\hat{U}_H = -E\,\hat{j}_H$

$$j(\omega) = \kappa(\omega)E(\omega) \quad \kappa(\omega) = \frac{1}{V}\int_0^\infty \mathrm{d}t\, \mathrm{e}^{-\mathrm{i}\omega t} \int_0^\beta \mathrm{d}\tau\, \mathrm{Tr}\{\hat{\rho}_0(T)\,\hat{j}(0)\,\hat{j}(t+\mathrm{i}\tau)\},$$

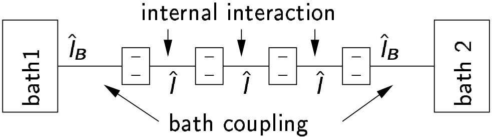
It is not entirely clear whether the conductivity κ always relates to the diffusion coefficient D in the way proposed by Einstein for Brownian motion



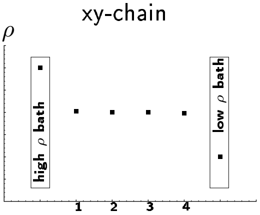
Trying to compute κ from a finite system one ends up with a set of singularities

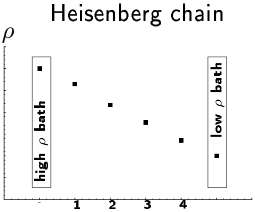
- diagonalize $\hat{H}$
- interpret the result for $\kappa(\omega)$

Modeling of coupled reservoirs:



$$i\hbar \frac{d}{dt}\hat{\rho} = \left[\hat{H}, \hat{\rho}\right] + \mathcal{L}(\mu_1, \mu_2)\hat{\rho}$$





- find some $\mathcal{L}$ that adequately models the reservoirs
- find the null-space ($\hat{\rho}_0$) of an non-Hermitian matrix of dimension d^2
- compute $j = \mathrm{Tr}\{\hat{\rho}_0 \hat{j}\}$ and $\nabla\rho = \mathrm{Tr}\{\hat{\rho}_0 \nabla\hat{n}\}$ to construct $D = j/\nabla\rho$

Direct projection onto (diffusive) modes:

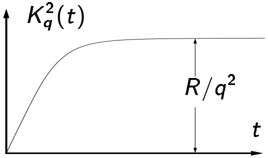
$$m(q,t) := \int \cos(qx)\rho(x,t)\mathrm{d}x \quad \Rightarrow \quad \text{diffusion eq.} \quad \Rightarrow \quad m(q,t) \propto e^{-\frac{D}{q^2}t}$$

construct "mode operator": $\hat{m}_q = \int \cos(qx)\hat{n}(x)\mathrm{d}x$

Diffusive transport? ⇒ Do the $m_q := \langle\psi(t)|\hat{m}_q|\psi(t)\rangle$ decay exponentially ?
Possibly the "time convolutionless projection operator method (TCL)" helps ⇒

$$\hat{H} = \hat{H}_0 + \lambda\hat{V}, \qquad [\hat{H}_0, \hat{m}_q] = 0 \qquad \Rightarrow \qquad \dot{m}_q = \sum_n \lambda^n K_q^n(t) m_q$$

If you strike it lucky $K_q^n(t) \approx 0$ except for $K_q^2(t)$, and $K_q^2(t)$ looks like this:



$$\Rightarrow \quad \dot{m}_q = -\frac{\lambda^2 R}{q^2} m_q$$

- divide $\hat{H}$ into $\hat{H}_0$ and $\hat{V}$
- diagonalize $\hat{H}_0$
- calculate $K_q^2(t)$ and estimate higher order terms

Models

Heisenberg chain: model and transported quantity

$$\hat{H} = \sum_{\mu} \hat{\sigma}^x_\mu \hat{\sigma}^x_{\mu+1} + \hat{\sigma}^y_\mu \hat{\sigma}^y_{\mu+1} + \Delta \hat{\sigma}^z_\mu \hat{\sigma}^z_{\mu+1} \qquad \hat{n}(x) = \hat{n}_\mu = \hat{\sigma}^z_\mu$$

Kubo formula:

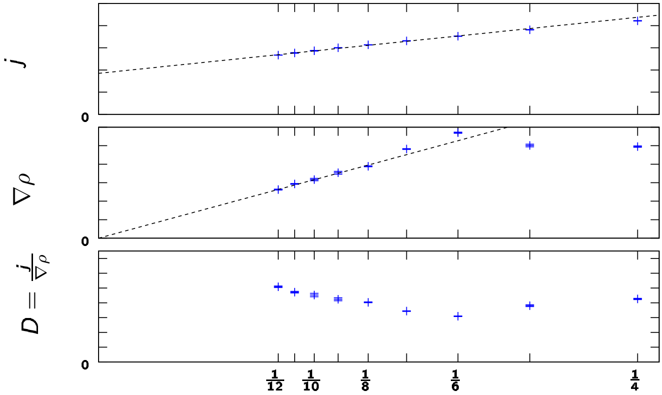
Mazur inequality: $\kappa(0) \geq \delta(0) \sum_n |\mathrm{Tr}\{\hat{C}_n \hat{j}\}|, \quad [\hat{H}, \hat{C}_n] = 0, \quad \mathrm{Tr}\{\hat{C}_n^2\} = 1$

$\Delta = 0 \Rightarrow$ defenitely very many $\mathrm{Tr}\{\hat{C}_n \hat{j}\} \neq 0 \Rightarrow$ ballistic
$\Delta = 1 \Rightarrow$ "integrable" (can be solved with a Bethe ansatz) $\Rightarrow$ ballistic

Boltzmann equation:
$\Delta = 0 \Rightarrow$ No scattering $\Rightarrow$ ballistic
$\Delta << 1 \Rightarrow$ scattering (Umklappprocess) $\Rightarrow$ if Boltzmann equation applies, diffusive
$\Delta \approx 1 \Rightarrow$ strongly correltated system $\Rightarrow$ Boltzmann equation inapplicable

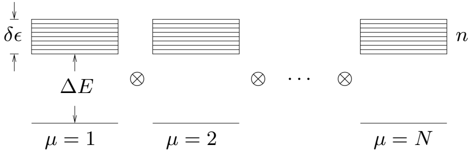
Projection onto modes
We're working on it!

Reservoirs coupled to the Heisenberg chain, $\Delta = 1$:



Find null-space of a $2^{24}x2^{24}$ non-Hermitian matrix? Here we used "stochastic unravelling". $\Rightarrow$ Probably ballistic transport in the limit of long chains.

Finite modular quantum system



$$\hat{H} = \sum_{\mu=1}^{N} \hat{h}_\mu + \hat{v}_\mu$$

$$\hat{h}_\mu = \sum_i h_i \, \hat{a}^\dagger_{\mu,i} \hat{a}_{\mu,i}, \quad h_i := \Delta E + i \frac{\delta\epsilon}{n}, \quad \hat{v}_\mu = \sum_{ij} c_{ij} \, \hat{a}^\dagger_{\mu,i} \hat{a}_{\mu+1,j} + \text{h.c.}$$

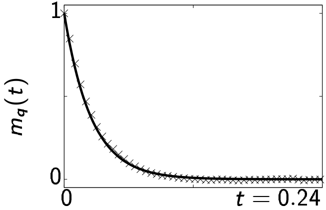
- This may be viewed as a model for: a particle moving on lattice sites, energy exchange between molecules, etc.
- The model features: no particle-particle interaction, nearest neighbor random interband hoppings, no disorder, a finite amount of sites
- The model may be directly numerically diagonalized for values up to, e.g., $n \approx 1000$, $N \approx 30$

What is the transport behavior of particles/energy ?

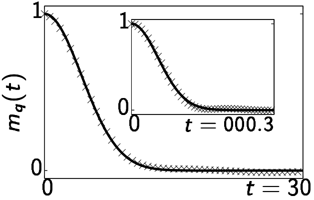
Results of the projection onto modes:

Dynamcis of modes $m_q(t)$:

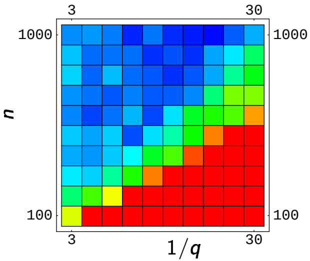
intermediate wavelength



long/short wavelength



Deviation from diffusion:



- diffusive transport occurs only on an intermediate (nano-) lengthscale
- the relevant dynamics are well described by TCL to 2. order

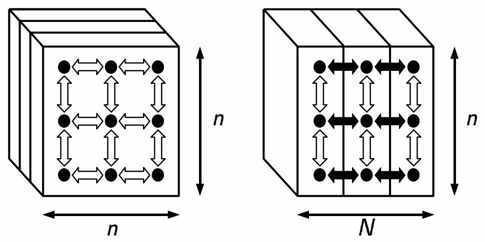
Application of other methods to fininte modular quantum systems:

Boltzmann equation:
Choose Bloch eigenstates as quasiparticle modes ⇒ no scattering ⇒ ballsitic transport. Misses the diffusive regime
Choose current eigenstates as quasiparticle modes ⇒ "scattering" for smaller systems exists but the quantum dynamcis do not map onto a Boltzmann equation.

Kubo formula:
Correct D results if one averages $\kappa(\omega)$ over small frequencies for the diffusive regime. But there is no clear transition to the ballistic regime

Reservoir coupling:
We're working on it!

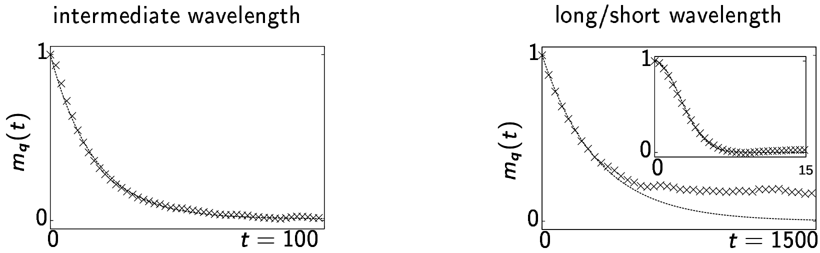
3d-Anderson models: projection onto modes



$$\hat{H} = \sum_{\mathbf{r}} \epsilon(\mathbf{r})\, \hat{a}^\dagger(\mathbf{r})\, \hat{a}(\mathbf{r}) + \sum_{\mathrm{NN}} \hat{a}^\dagger(\mathbf{r})\, \hat{a}(\mathbf{r}')$$

$\epsilon(\mathbf{r})$: Gaussian random numbers $\Rightarrow$

$$\hat{H} = \sum_{\mu=0}^{N-1} \hat{h}_0(\mu) + \sum_{\mu=0}^{N-1} \hat{v}(\mu, \mu+1)$$



The diffusive wavelength regime appears to be rather small.

Anderson models:

Projection: Relevant dynamics may be found from diagonalizing (some) *nxn* matrices rather than an *nxnxN* matrix.

Boltmann equation: Misses the localized and the ballsitic regime.

Kubo formula: Very hard to evaluate.

Reservoir coupling: We're working on it

The "take home message":
There are still rather fundamental open questions in the field of (regular) quantum transport. Nevertheless the quantitative determination of transport properties from first principles now appears feasible.

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