The limited validity of the Kubo formula for thermal conduction

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Transport phenomena and Kubo formula

Normal transport phenomena:

“field driven”	“gradient driven”
$\boldsymbol{j} = L_F \boldsymbol{F}$	$\boldsymbol{j} = -L_G \boldsymbol{\nabla} \rho$
electric current induced by an electric field	free diffusion, heat conduction, Brownian motion

How to compute the response coefficients (L’s)?

Linear response theory $\Rightarrow L_F(\omega)$:

$$j(\omega) = L_F(\omega)\boldsymbol{F}(\omega) \qquad \boldsymbol{F} = -\nabla V$$

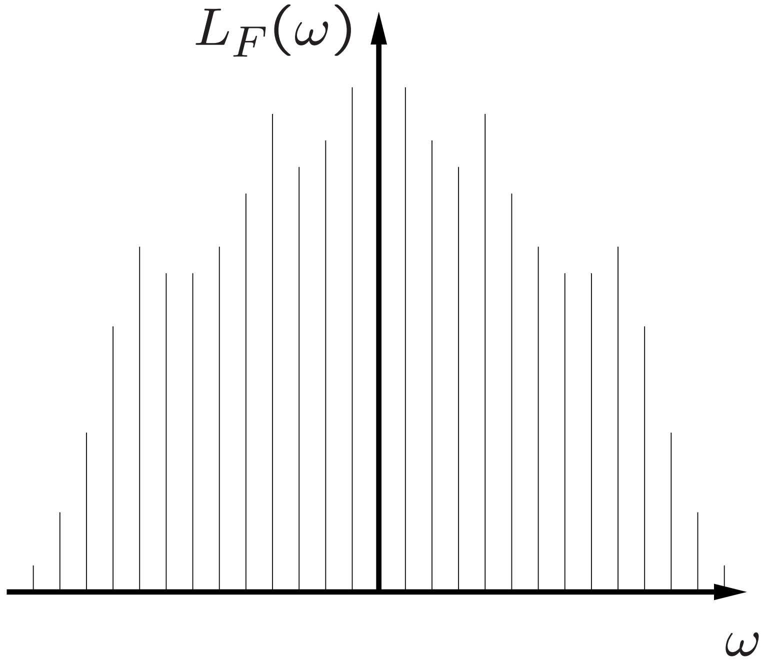
Kubo formula (KF):

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

Is the transport behvior of a given sytem normal or ballistic?

Does the KF apply to gradient driven phenomena like heat conduction?

Evaluation and Interpretation of the KF



δ-peak at $\omega = 0$: **"Drude peak"** $\Rightarrow$ **ballistic**
$L_F(\omega)$ **finite** at $\omega = 0$: $\Rightarrow$ **normal**

Finite quantum systems: discrete spectra $\Rightarrow L_F(\omega)$ is a sum of δ-peaks. $\Rightarrow$
Technically, the conductivity at some ω is either infinte (superconductor) or zero (isolator).

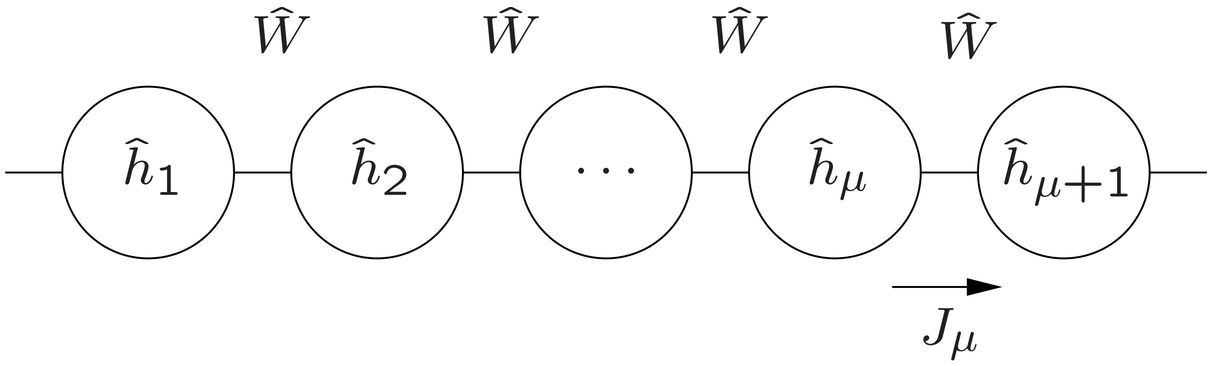
(Peak density at $\omega = 0$: $\bar{L}_F(0)$)

Does the Kubo formula apply to gradient driven transport ?

$L_F \propto L_G$ has been succesfully asserted by Einstein in the context of Brownian motion, but in general?

Gradient driven local current dynamics

"Modular system"

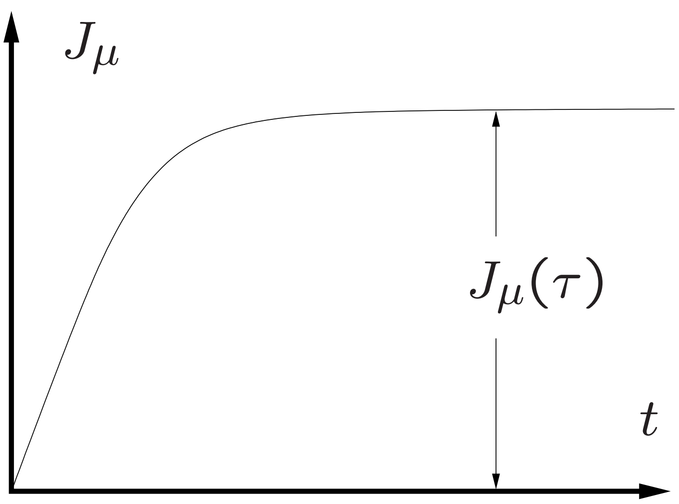


Energy (heat) current: $\quad J_n = \mathrm{Tr}\{\widehat{j}_\mu \, \widehat{\rho}_{\mu,\mu+1}\}$

Consider:

$$\widehat{\rho}_{\mu,\mu+1}(0) \propto \exp\left(\frac{-\widehat{h}_\mu}{T+\Delta T/2}\right) \otimes \exp\left(\frac{-\widehat{h}_{\mu+1}}{T-\Delta T/2}\right)$$

Short time dynamics under some model conditions:



$$J_\mu(\tau) = \bar{L}_F(0)\Delta T_\mu(0)$$

So far the Kubo formula applies!

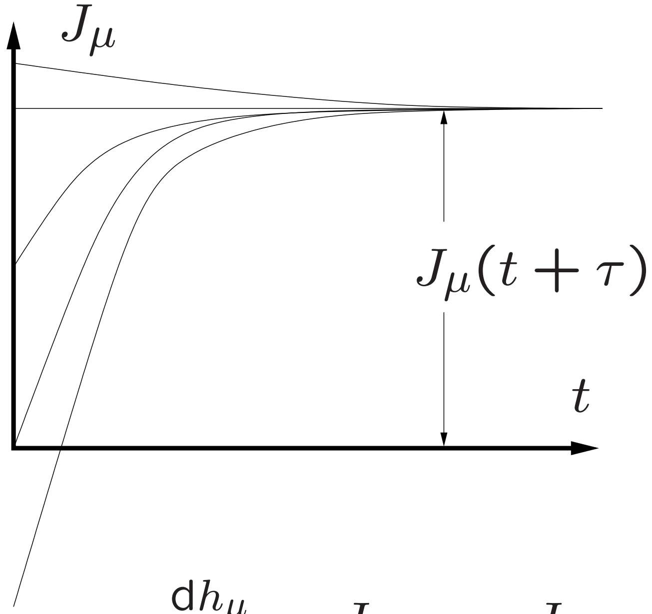
What happens after τ *?* $\Rightarrow$

Consider different (pure) initial states, classified according to

$$\Delta h_\mu = \mathrm{Tr}\{\widehat{\rho}_{\mu,\mu+1}(\widehat{h}_{\mu+1} - \widehat{h}_\mu)\}, \quad \Delta h_\mu = c\Delta T_\mu$$

HAM and current dynamics

The Hilbertspace Average Method (HAM) predicts for almost any initial state featuring a given Δh_μ



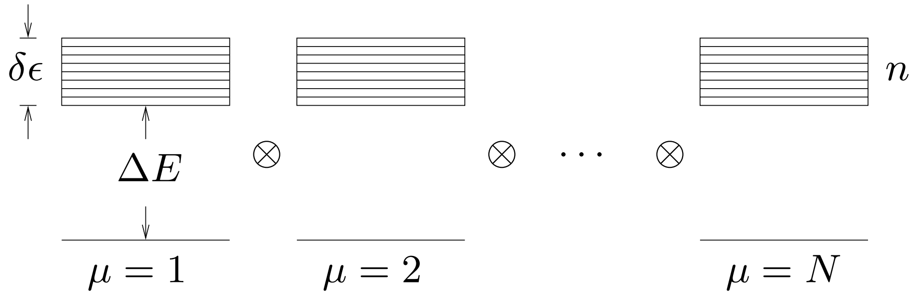
$$J_\mu(t+\tau) = \frac{\bar{L}_F(0)}{c}\Delta h_\mu(t)$$

$$\frac{\mathrm{d}h_\mu}{\mathrm{d}t} = J_{\mu-1} - J_\mu, \quad \text{for} \quad \tau \to 0 \Rightarrow$$

Discrete diffuison equation:

$$\frac{\mathrm{d}h_\mu}{\mathrm{d}t} = \frac{\bar{L}_F(0)}{c}\left(h_{\mu-1} + h_{\mu+1} - 2h_\mu\right),$$

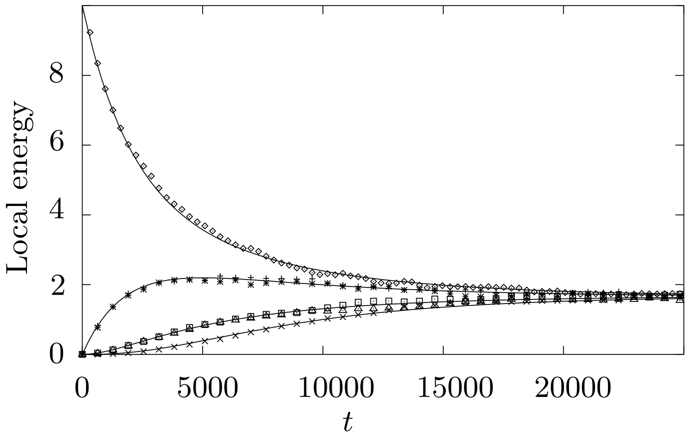
Design models:

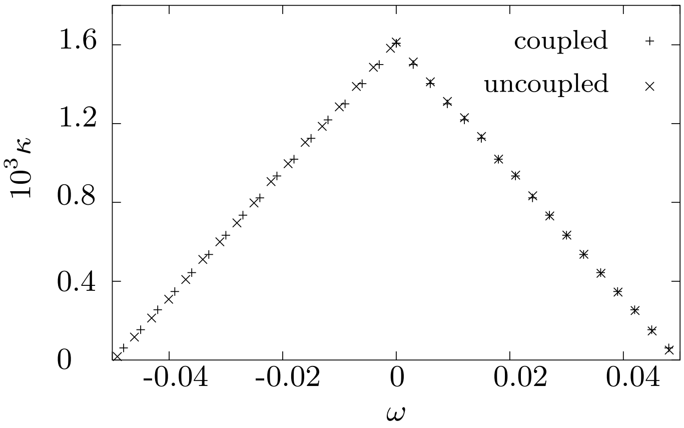


Local units coupled by random matrices

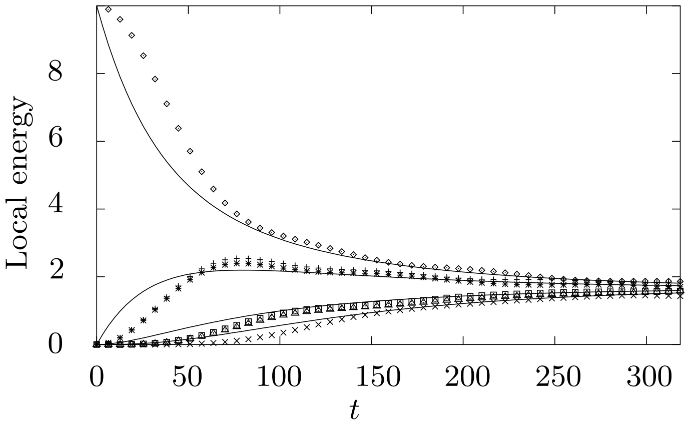
Transport behavior and Kubo spectra

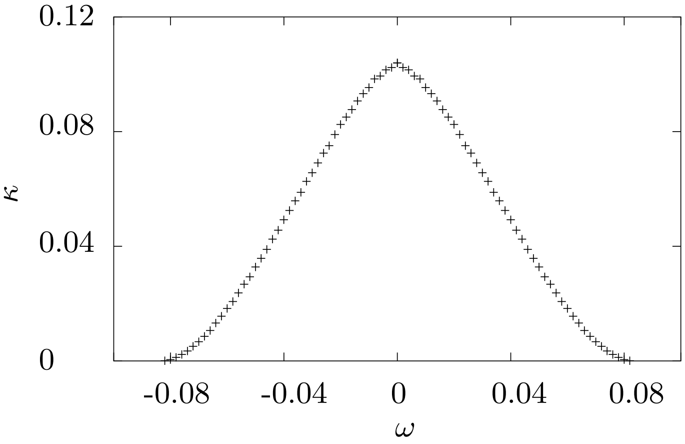
Intermediate coupling strength: diffusive transport, KF applies



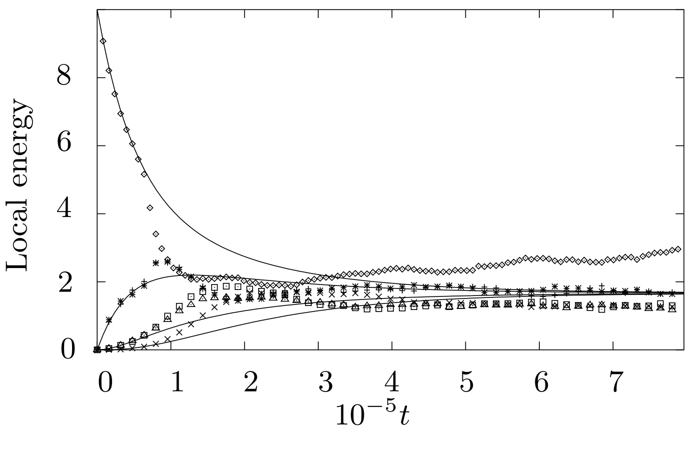


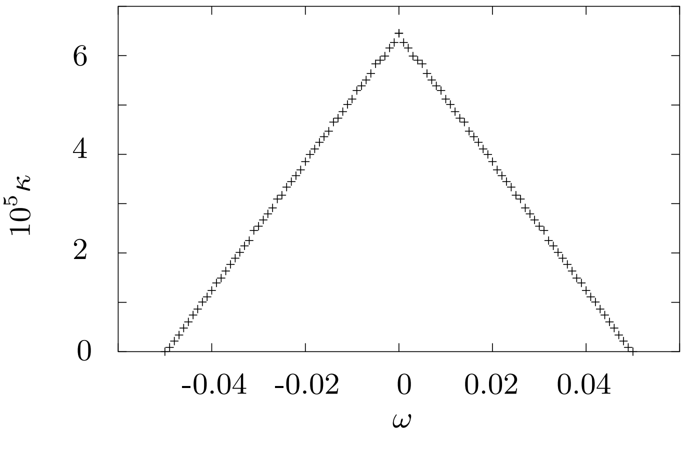
Strong coupling: no diffusive transport, KF does not apply





Weak coupling: no diffusive transport, KF does not apply





There always is a finite Drude weight!

The bottom line

If the system exhibits normal heat transport the conductivity is correctly described by the Kubo formula.

Whether or not the system exhibits diffusive transport cannot be judged only from evaluating the Kubo formula at $\omega = 0$

More about this:

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Thank you for your attention!