Kubo formula and ac conductance of open systems

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Brief review

- Transport coefficients diverge in many low dimensional systems
- Integrable systems treated individually
- Nonintegrable momentum conserving systems have universal properties
- Analytical techniques: RG, mode coupling
- Universality class(es): $L^{1/3}$, $L^{1/2}$
- Rely on Kubo formula

Standard proof of Kubo formula

$$\kappa_{\sigma\rho} = \lim_{\omega\to 0}\lim_{L\to\infty}\frac{\beta}{L^d}\int_{t=0}^{\infty} e^{i\omega t} < J^{\sigma}(t)\, J^{\rho}(0) > \; dt$$

where $J^{\sigma,\rho}$ are currents for the conserved charges σ,ρ and $\kappa_{\sigma\rho}$ is the linear response function

- Assumes system in thermal equilibrium as $t \to -\infty$
- Assumes Hamiltonian dynamics thereafter
- Order of limits important, otherwise RHS depends on boundary conditions.
- $\kappa \to \infty$ as $L \to \infty$ for low dimensional momentum conserving systems. Proof fails.

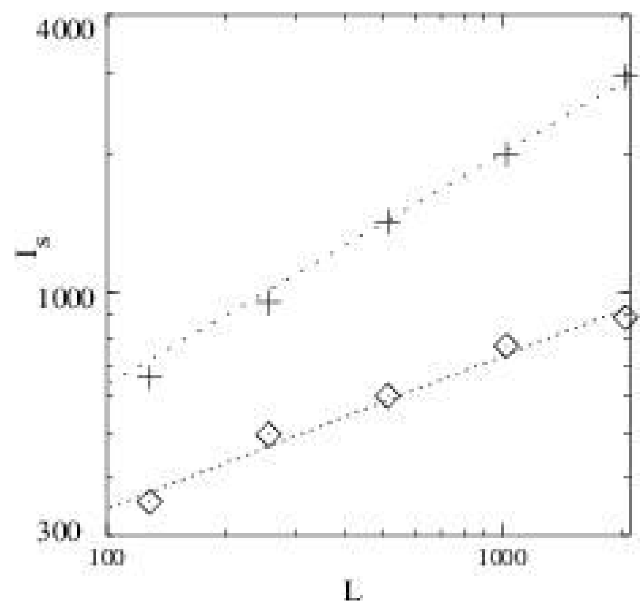
Importance of boundary conditions

Integrable (finite) systems

- Periodic bc: <J(t)J(0)> finite as t→∞; Kubo integral diverges
- Hard wall bc: Kubo integral is zero
- Open bc with reservoirs: Kubo integral is finite.

Non-integrable (finite) momentum conserving systems

- Hard wall bc: Kubo integral is zero
- Periodic & open bc: integral finite, but not same for both



Kubo formula for open systems: prior work

- Quantum dots: Hamiltonian for system + leads

  Can only handle very simple reservoirs

  (Fisher & Lee, Allen & Ford, Szafer & Stone)

- Open classical systems: Fluctuation theorem

  Only $\omega = 0$

  (Andrieux & Gaspard)

Kubo formula for open systems

(Abhishek Dhar, Anupam Kundu)

P(x, v, t) is phase space density of system.

k'th reservoir at temperature $T_k = T + \Delta T_k$

Fokker Planck equation:

$$\partial_t P = [L_0 + L_{\Delta T}]\, P$$

Assume system at temperature T as $t \to -\infty$

Linear response:

$$P(x,v,t) = P_0(x,v) + \int_{-\infty}^{t} \exp[(t - t')\, L_0]\, L_{\Delta T(t')} P_0(x,\ v)\, dt'$$

For any observable,

$$< A(t) > \;=\; < A>_{eq} + \int_{-\infty}^{t} A \;\exp[(t - t')\, L_0]\; L_{\Delta T(t')} P_0 \, dt'$$

$L_{\Delta T(t')}$ depends on the type of heat bath. For several examples, show explicitly that

$$L_{\Delta T(t')}\, P_0 \;=\; - \sum_k \Delta\beta_k(t')\, {J^e}_{b;k}\, P_0$$

${J_{b;k}}^e$ is the energy current flowing in from k'th reservoir

$$< A(t) > \;=\; < A>_{eq} - \int_{-\infty}^{t} < A(t)\, {J^e}_{b;\,k}(t')>_{eq} \Delta\beta_k(t')\, dt'$$

$$< {J^e}_{b;\,j}(t)>_{\Delta T} \;=\; - \int_{-\infty}^{t} < {J^e}_{b;\,j}(t)\, {J^e}_{b;\,k}(t')>_{eq} \Delta\beta_k(t')\, dt'$$

Each heat bath different. Other conserved currents?

General reservoir, any conserved current:

$\lambda^k_{N,N'}$ transition rate from N' particle state to N particle state due to k'th reservoir. In equilibrium,

$$0 = \partial_t P_{0;N}(x,\ v) = \sum_{k,N'} \int [\lambda^k_{N,N'} P_{0;\,N'}(x', v') - \lambda^k_{N',N}\, P_{0;\,N}(x,\ v)]\, dx' dv'$$

Out of equilibrium,

$$\partial_t P_N = \sum_{k,N'} \Delta(\beta\mu)_k\, [(\partial_{\beta\mu} \lambda^k_{N,N'}) P_{0;N'} - (\partial_{\beta\mu} \lambda^k_{N',N})\, P_{0;N}]$$

$$\partial_t P_N = -\sum_{k,N'} \Delta(\beta\mu)_k\, [N' \lambda^k_{N,N'} P_{0;N'} - N\, \lambda^k_{N',N} P_{0;N}]$$

$$\partial_t P_N = \sum_{k,N'} \Delta(\beta\mu)_k\, (N - N')\, \lambda^k_{N,N'} P_{0;N'} = \sum_k \Delta(\beta\mu)_k J_{b;k} P_{0;N}$$

Proof applies to any conserved quantity (discretize if continuous, e.g. energy).

$$< A(t) >_{\Delta\Phi} = \; < A >_{eq} \; + \; \sum_{k,\rho} \int_{-\infty}^{t} < A(t)\, J^{\rho}{}_{b;k}(t') >_{eq} \Delta\Phi^{\rho}{}_{k}(t')\, dt'$$

where J^{ρ} is current and $\Delta\Phi^{\rho}$ is thermodynamic potential for conserved quantity ρ. ($\Phi^{e} = -\beta$, $\Phi^{n} = \beta\mu$)

DC and AC cases

Zero frequency:

Pipe of length L, same current for any cross section at ω = 0

$$\kappa_{\sigma\rho}(L) = \frac{1}{L} \int_{t'=-\infty}^{t'=t} < j^{\sigma}(x,t)\, j^{\rho}(y,t') >_{eq} dx\,dy\,dt'$$

Finite system

(same expression as Andrieux & Gaspard)

Finite frequency:

$$< J^{\sigma}{}_{b;m}(\omega) > \; = \sum_{k,\rho} \Delta\Phi^{\rho}{}_{k}(\omega) \int_{0}^{\infty} < J^{\sigma}{}_{b;m}(t)\, J^{\rho}{}_{b;k}(0) >_{eq} e^{-i\omega t}\, dt$$

Not expressed in terms of currents in interior of system

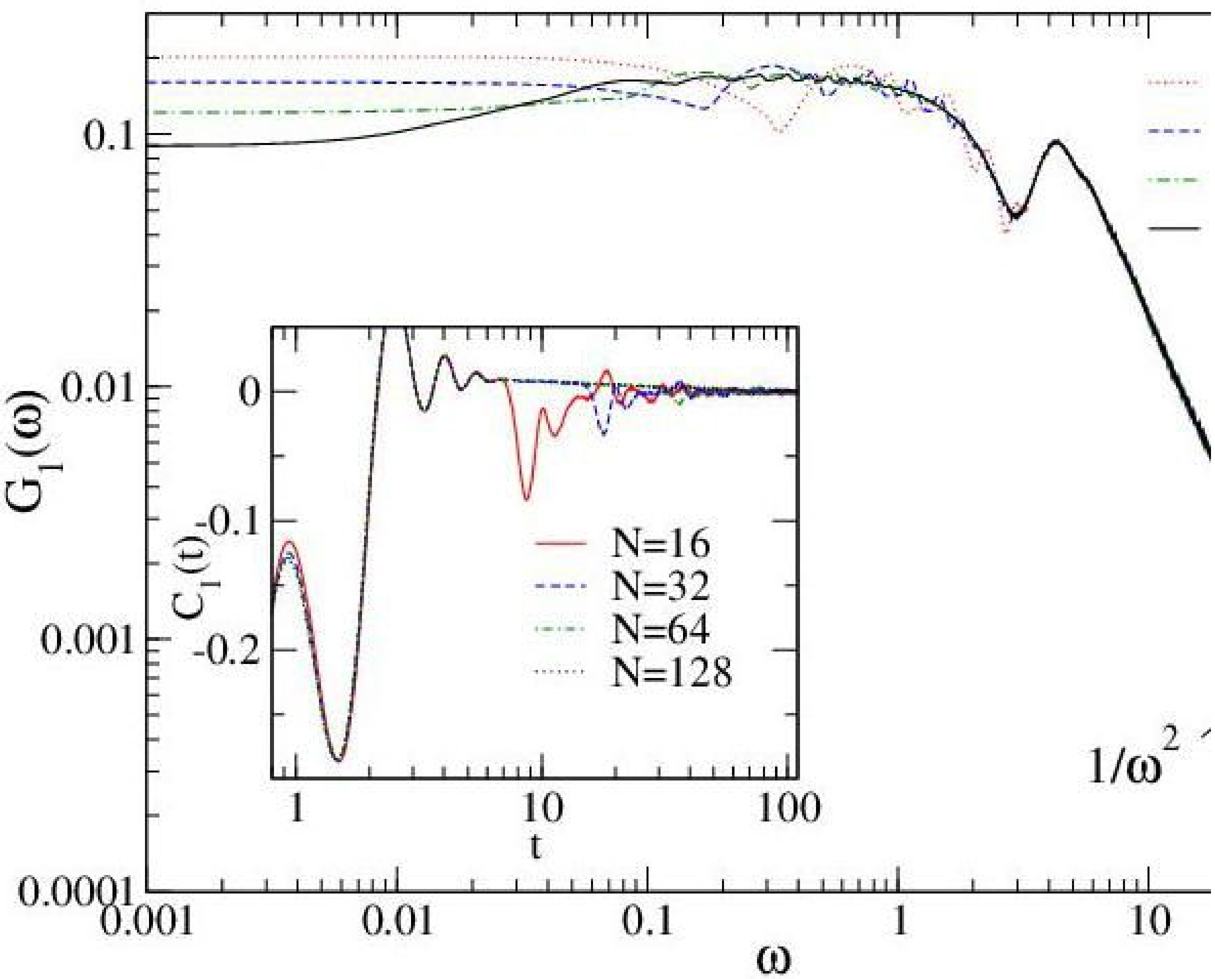
$\omega \neq 0$ *heat conductance: numerics*

FPU quartic chain. Current between first two particles.

Resonance at frequency of sound waves across system, ~ 1/N

Higher than ω=0 for large N.

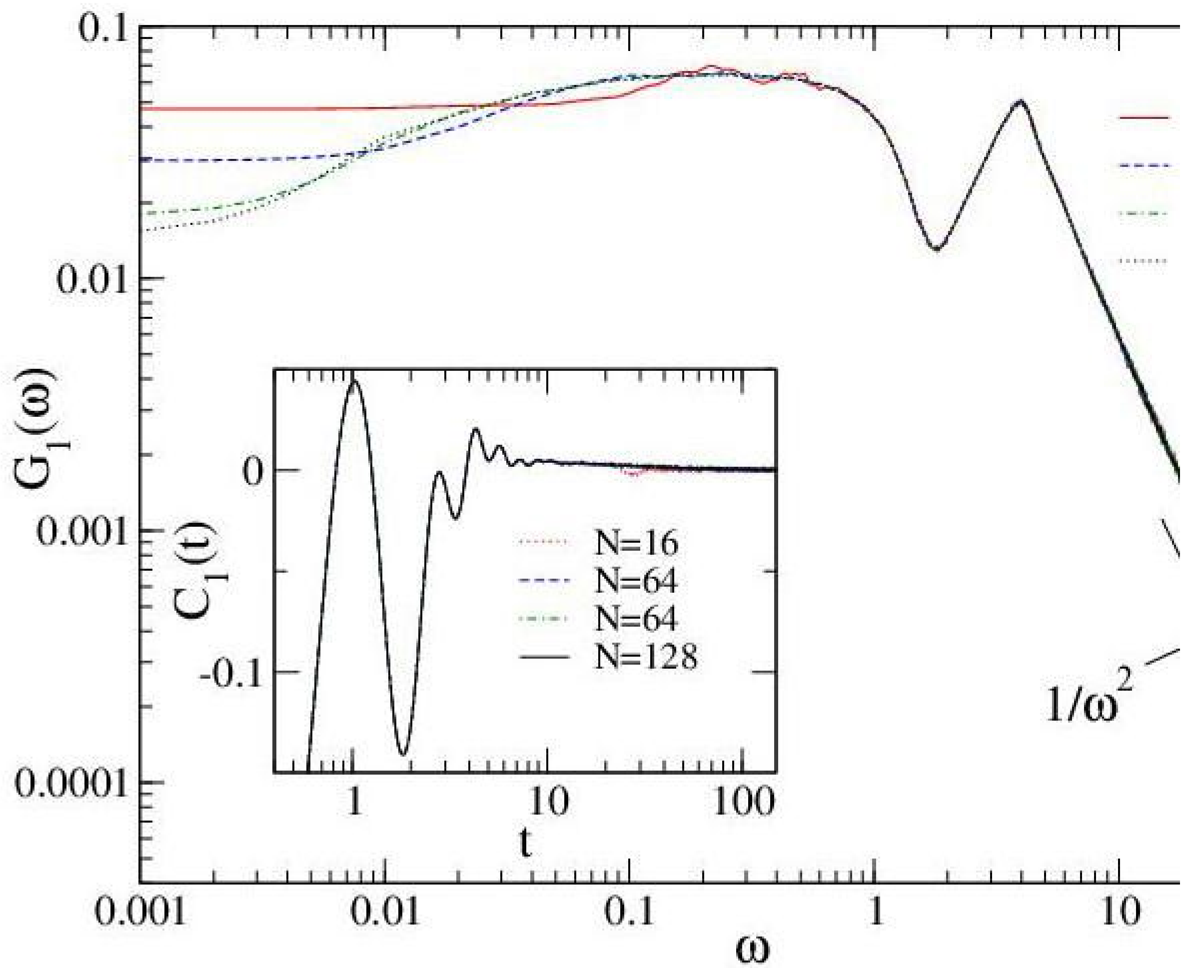
Oscillators?



$\omega \neq 0$ *heat conductance (contd.)*

Harmonic oscillator chain, additional tethering for each particle.

No low frequency peak because no low frequency sound

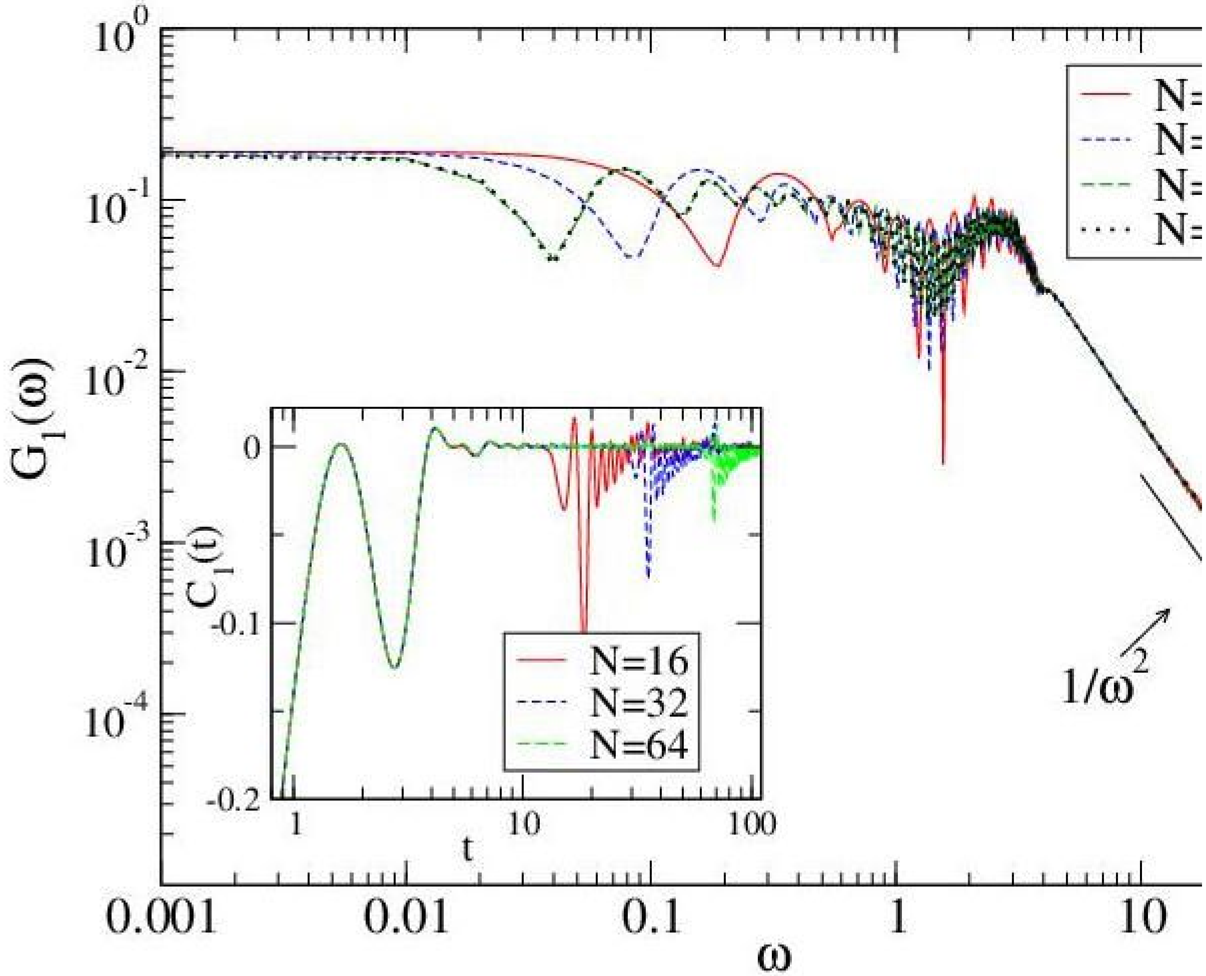


$\omega \neq 0$ *heat conductance (contd.)*

Harmonic oscillator chain

Clear peak ω ~ 1/N, many harmonics

Analytical solution



Conclusions

- Correlation functions depend on boundaries when singular
- Prove Kubo-like formula for open classical systems with reservoirs
- Reduces to standard result for $\omega = 0$, one dimension
- Numerics: Low frequency $\omega \sim 1/L$ peak in conductance, can be higher than $\omega = 0$