Aspects of Thermal and Electrical Transport in Nearly Integrable systems.

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Abstract:

Thermal and Electrical transport in nearly integrable systems can be studied through the finite frequency conductivities of charge and heat currents in 1 dimension. I will summarize recent analytical results including a novel sum rule for the thermal conductivity. Also presented is our recent work on the t-t'-V model in 1-d. The role of boundary conditions in defining various stiffnesses is commented upon.

- Finite ω response functions: Motivation and formalism New sum rule, and two new fundamental operators: Thermal operator ϑ and thermoelectric operator Φ.
- Problems with Kubo- identity for dissipative systems

- Hydrodynamics of thermal transport in a lattice model: Second sound velocity and thermal stiffness

- 1-dimensional examples
    - t-t'-V model with PBCs
    - Open BC's
    - Toda lattice energy current persistence

Finite frequency thermal response functions:

Needed in many contexts, e.g. imagine a Si chip at 20 GHZ and its power dissipation. Neglected area with rather surprising new results. SS Phys Rev 2006

Need to use Luttinger's formalism.

$$
\begin{aligned}
\frac{1}{\Omega}\langle \hat{J}_x \rangle &= L_{11}E_x + L_{12}(-\nabla_x T/T) \\
\frac{1}{\Omega}\langle \hat{J}_x^Q \rangle &= L_{21}E_x + L_{22}(-\nabla_x T/T),
\end{aligned}
$$

where $(-\nabla_x T/T)$ is regarded as the *external driving thermal force*, and $\hat{J}_x^Q$ is the heat current operator.

$$
\kappa_{zc} = \frac{1}{TL_{11}}(L_{22}L_{11} - L_{12}L_{21}).
$$

We want finite frequency versions of these…..Turn to Luttinger

$$
K_{tot} = K + \sum_x K(\vec{x})\psi(\vec{x},t).
$$

Here $K = \sum_x K(\vec{x})$, and $K(\vec{x}) = H(\vec{x}) - \mu n(\vec{x})$ is the *grand canonical* Hamiltonian

We can define the local temperature through

$$\delta T(\vec{x},t) = \frac{\delta\langle K(\vec{x},t)\rangle}{C(T)}.$$

Luttinger writes

$$\begin{aligned}
\frac{1}{\Omega}\langle \hat{J}_x\rangle &= L_{11}E_x + L_{12}(-\nabla_x T/T) + \hat{L}_{12}(-\nabla_x \psi(\vec{x},t)) \\
\frac{1}{\Omega}\langle \hat{J}^Q_x\rangle &= L_{21}E_x + L_{22}(-\nabla_x T/T) + \hat{L}_{22}(-\nabla_x \psi(\vec{x},t)),
\end{aligned}$$

Let $\psi(\vec{x},t) = \psi_q \exp\{-i(q_x x + \omega t + i0^+ t)\}$, (adiabatic switching implied) and the electric potential $\phi(\vec{x},t) = \phi_q \exp\{-i(q_x x + \omega t + i0^+ t)\}$ thus write

$$\delta J(q) = (iq_x)L_{11}(q_x,\omega)\phi_q + (iq_x)\left[L_{12}(q_x,\omega)\frac{\delta T_q}{T} + \hat{L}_{12}(q_x,\omega)\ \psi_q\right],$$

In equilibrium (i.e. static inhomogeneous limit) there is no net current therefore

$$0 = L_{12}(q,0)\frac{\delta T_q}{T} + \hat{L}_{12}(q,0)\psi_q.$$

However,

$$\lim_{\vec{q}\to 0}\psi(\vec{q},0) = -\lim_{\vec{q}\to 0}\frac{\delta T_q}{T}.$$

Hence We conclude that:

$$\lim_{q\to 0}\left[L_{12}(q,0) - \hat{L}_{12}(q,0)\right] = 0$$

Luttinger's identity

$$L_{ij}(q,\omega) = \hat{L}_{ij}(q,\omega)$$

Basic assumption of our work:

Generalized Luttinger's identity

Can compute RHS mechanically. Extension satisfies Causality, Onsager reciprocity and also Hydrodynamics at small q, w

$$\hat{J}_x^Q = \hat{J}_x^E - \frac{\mu}{q_e}\hat{J}_x,$$

where $\hat{J}_x^E$ is the *energy current* and $\hat{J}_x$ the charge current.

$$\hat{J}_x^Q = \lim_{q_x \to 0} \frac{1}{q_x}\left[K, K(q_x)\right].$$

$$\hat{J}_x^Q(\vec{q}) = \sum_x \hat{J}_x^Q(\vec{x}) \exp(i\vec{q}.\vec{x}), \quad \text{so that } \hat{J}_x^Q = \lim_{q \to 0} \hat{J}_x^Q(\vec{q}).$$

$$\begin{aligned}
\delta \hat{J}_x &= L_{11}(q_x, \omega)(iq_x\phi_q) + L_{12}(q_x, \omega)(iq_x\psi_q) \\
\delta \hat{J}_x^Q &= L_{21}(q_x, \omega)(iq_x\phi_q) + L_{22}(q_x, \omega)(iq_x\psi_q).
\end{aligned}$$

$$K_{tot} = K + \left[\rho(-q_x)\phi_q + K(-q_x)\psi_q\right] \exp\left(-i\omega t + 0^+ t\right),$$

We can reduce the calculations of all L_{ij} to essentially a single one, with the help of some notation. Keeping q_x small but non zero, we define currents, densities and forces in a matrix notation as follows:

	i=1	i=2
	Charge	Energy
$\mathcal{I}_i$	$\hat{J}_x(q_x)$	$\hat{J}^Q_x(q_x)$
$\mathcal{U}_i$	$\rho(-q_x)$	$K(-q_x)$
$\mathcal{X}_i$	$E^x_q = iq_x\phi_q$	$iq_x\psi_q$.

The perturbed Hamiltonian can then be written as

$$K_{tot} = K + \sum_j Q_j e^{-i\omega_c t}, \quad \text{where} \quad Q_j = \frac{1}{iq_x}\mathcal{U}_j\mathcal{X}_j.$$

$$\langle \mathcal{I}_i \rangle = -\sum_j \chi_{\mathcal{I}_i, Q_j}(\omega_c),$$

$$\begin{aligned}
\chi_{A,B}(\omega_c) &= -i \int_0^\infty dt\; e^{i\omega t - 0^+ t} \langle [A(t), B(0)] \rangle \\
&= \sum_{n,m} \frac{p_m - p_n}{\varepsilon_n - \varepsilon_m + \omega_c} A_{nm} B_{mn} \\
&= -\frac{1}{\omega_c} \left[\langle [A, B] \rangle + \sum_{n,m} \frac{p_m - p_n}{\varepsilon_n - \varepsilon_m + \omega_c} A_{nm} ([B, K])_{mn} \right].
\end{aligned}$$

$$L_{ij}(q_x, \omega) = \frac{i}{\Omega \omega_c} \left[-\langle [\mathcal{I}_i, \mathcal{U}_j] \rangle \frac{1}{q_x} - \sum_{n,m} \frac{p_m - p_n}{\varepsilon_n - \varepsilon_m + \omega_c} (\mathcal{I}_i)_{nm} (\mathcal{I}_j^\dagger)_{mn} \right].$$

For arbitrary frequencies the Onsager functions read as

$$L_{ij}(\omega) = \frac{i}{\Omega\omega_c}\left[\langle\mathcal{T}_{ij}\rangle - \sum_{n,m}\frac{p_m - p_n}{\varepsilon_n - \varepsilon_m + \omega_c}(\mathcal{I}_i)_{nm}(\mathcal{I}_j)_{mn}\right],$$

$$\langle\mathcal{T}_{ij}\rangle = -\lim_{q_x\to 0}\langle[\mathcal{I}_i,\mathcal{U}_j]\rangle\frac{1}{q_x}.$$

The operators $\mathcal{T}_{ij}$ are not unique, since one can add to them a ‘gauge operator” $\mathcal{T}_{ij}^{gauge} = [P, K]$ with arbitrary P. These fundamental operators play a crucial role in the subsequent analysis, since they

These important operators are written in a more familiar as follows:

Stress tensor	Thermal operator	Thermoelectric operator
$\mathcal{T}_{11}$	$\mathcal{T}_{22}$	$\mathcal{T}_{12} = \mathcal{T}_{21}$
τ^{xx}	Θ^{xx}	Φ^{xx}
$-\frac{d}{dq_x}\left[\hat{J}_x(q_x), \rho(-q_x)\right]_{q_x\to 0}$	$-\frac{d}{dq_x}\left[\hat{J}_x^Q(q_x), K(-q_x)\right]_{q_x\to 0}$	$-\frac{d}{dq_x}\left[\hat{J}_x(q_x), K(-q_x)\right]_{q_x\to 0}$
The thermoelectric operator	can also be written as	

$$\Phi^{xx} = \mathcal{T}_{21} = -\frac{d}{dq_x}\left[\hat{J}_x^Q(q_x), \rho(-q_x)\right]_{q_x\to 0},$$

$$
\begin{aligned}
L_{ij}(\omega) &= \frac{i}{\omega_c}\mathcal{D}_{ij} + \frac{1}{\Omega}\int_0^{\infty} dt\; e^{i\omega_c t} \int_0^{\beta} d\tau\; \langle \mathcal{I}_i(t - i\tau)\mathcal{I}_j(0)\rangle \\
\mathcal{D}_{ij} &= \frac{1}{\Omega}\left[\langle \mathcal{T}_{ij}\rangle - \sum_{nm} \frac{p_n - p_m}{\varepsilon_m - \varepsilon_n}(\mathcal{I}_i)_{nm}(\mathcal{I}_j)_{mn}\right]
\end{aligned}
$$

Generalized Kubo formulas for non dissipative systems. Contain a stiffness term that is interesting and non trivial.

Comment [1]: D terms is nonzero for supersystems- including integrable models. (No additional hypothesis needed as in Luttinger's paper on Superfluids.

Comment[2]: Sum rule for thermal conductivity is new.

``Sum rule for thermal conductivity and dynamical thermal transport coefficients in condensed matter '', B Sriram Shastry, Phys. Rev. B 73, 085117 (2006)

$$\int_{-\infty}^{\infty} \frac{d\nu}{2} \Re e\sigma(\nu) = \frac{\pi \langle \tau^{xx} \rangle}{2\Omega}$$

F sum rule

$$\int_{-\infty}^{\infty} \frac{d\nu}{2} \Re e\kappa(\nu) = \frac{\pi \langle \Theta^{xx} \rangle}{2T\Omega}, .$$

Thermal sum rule

$$\int_{-\infty}^{\infty} \frac{d\nu}{\pi} \Re e\kappa_{zc}(\nu) = \frac{1}{T\Omega} \left[\langle \Theta^{xx} \rangle - \frac{\langle \Phi^{xx} \rangle^2}{\langle \tau^{xx} \rangle} \right].$$

Zero current thermal conductivity where explicit value of μ is not needed.

$$L_{ij}(\omega) = L_{ji}(\omega).$$

Onsager reciprocity requires the "heavy usage" of Jacobi's identity to my surprise!!

$$\begin{aligned}
\langle \mathcal{T}_{12} \rangle &= -\left(\frac{d}{dq} \frac{1}{q} \left[\langle [K, \rho(q)], K(-q)] \rangle \right] \right)_{q \to 0} \\
&= \left(\frac{d}{dq} \frac{1}{q} \langle [[\rho(q), K(-q)], K] + [K(-q), K], \rho(q)]] \rangle \right)_{q \to 0} \\
&= \left(\frac{d}{dq} \langle \left[[\hat{J}^Q_x(-q), \rho(q)] \right] \rangle \right)_{q \to 0} \\
&= \langle \mathcal{T}_{21} \rangle .
\end{aligned}$$

Thermo power operator for Hubbard model

$$
\begin{aligned}
\Phi^{xx} &= -\frac{q_e}{2}\sum_{\vec{\eta},\vec{\eta'},\vec{r}}(\eta_x+\eta'_x)^2 t(\vec{\eta})t(\vec{\eta'})c^\dagger_{\vec{r}+\vec{\eta}+\vec{\eta'},\sigma}c_{\vec{r},\sigma} - q_e\mu\sum_{\vec{\eta}}\eta_x^2 t(\vec{\eta})c^\dagger_{\vec{r}+\vec{\eta},\sigma}c_{\vec{r},\sigma} + \\
&\quad \frac{q_e U}{4}\sum_{\vec{r},\vec{\eta}} t(\vec{\eta})(\eta_x)^2(n_{\vec{r},\bar{\sigma}}+n_{\vec{r}+\vec{\eta},\bar{\sigma}})(c^\dagger_{\vec{r}+\vec{\eta},\sigma}c_{\vec{r},\sigma}+c^\dagger_{\vec{r},\sigma}c_{\vec{r}+\vec{\eta},\sigma}).
\end{aligned}
$$

This object can be expressed completely in Fourier space as

$$
\begin{aligned}
\Phi^{xx} &= q_e\sum_{\vec{p}}\frac{\partial}{\partial p_x}\left\{v_p^x(\varepsilon_{\vec{p}}-\mu)\right\}c^\dagger_{\vec{p},\sigma}c_{\vec{p},\sigma} \\
&\quad +\frac{q_e U}{2\mathcal{L}}\sum_{\vec{l},\vec{p},\vec{q},\sigma,\sigma'}\frac{\partial^2}{\partial l_x^2}\left\{\varepsilon_{\vec{l}}+\varepsilon_{\vec{l}+\vec{q}}\right\}c^\dagger_{\vec{l}+\vec{q},\sigma}c_{\vec{l},\sigma}c^\dagger_{\vec{p}-\vec{q},\bar{\sigma}'}c_{\vec{p},\bar{\sigma}'}.
\end{aligned}
$$

$$
\begin{aligned}
\tau^{xx} &= \frac{q_e^2}{\hbar}\sum\eta_x^2\, t(\vec{\eta})\, c^\dagger_{\vec{r}+\vec{\eta},\sigma}c_{\vec{r},\sigma} \quad \text{or} \\
&= \frac{q_e^2}{\hbar}\sum_{\vec{k}}\frac{d^2\varepsilon_{\vec{k}}}{dk_x^2}\,c^\dagger_{\vec{k},\sigma}c_{\vec{k},\sigma}
\end{aligned}
$$

$$
\Theta^{xx} = \sum_{p,\sigma} \frac{\partial}{\partial p_x} \left\{ v^x_{\vec{p}} (\varepsilon_{\vec{p}} - \mu)^2 \right\} \; c^\dagger_{\vec{p},\sigma} c_{\vec{p},\sigma} + \frac{U^2}{4} \sum_{\eta,\sigma} t(\vec{\eta}) \eta_x^2 (n_{\vec{r},\bar{\sigma}} + n_{\vec{r}+\vec{\eta},\bar{\sigma}})^2 c^\dagger_{\vec{r}+\vec{\eta},\sigma} c_{\vec{r},\sigma}
$$
$$
- \mu U \sum_{\vec{\eta},\sigma} t(\vec{\eta}) \eta_x^2 (n_{\vec{r},\bar{\sigma}} + n_{\vec{r}+\vec{\eta},\bar{\sigma}}) c^\dagger_{\vec{r}+\vec{\eta},\sigma} c_{\vec{r},\sigma}
$$
$$
- \frac{U}{8} \sum_{\vec{\eta},\vec{\eta}',\sigma} t(\vec{\eta}) t(\vec{\eta}') (\eta_x + \eta'_x)^2 \left\{ 3 n_{\vec{r},\bar{\sigma}} + n_{\vec{r}+\vec{\eta},\bar{\sigma}} + n_{\vec{r}+\vec{\eta}',\bar{\sigma}} + 3 n_{\vec{r}+\vec{\eta}+\vec{\eta}',\bar{\sigma}} \right\} c^\dagger_{\vec{r}+\vec{\eta}+\vec{\eta}',\sigma} c_{\vec{r},\sigma}
$$
$$
+ \frac{U}{4} \sum_{\vec{\eta},\vec{\eta}',\sigma} t(\vec{\eta}) t(\vec{\eta}') (\eta_x + \eta'_x) \eta'_x c^\dagger_{\vec{r}+\vec{\eta},\sigma} c_{\vec{r},\sigma} \left\{ c^\dagger_{\vec{r}+\vec{\eta},\bar{\sigma}} c_{\vec{r}+\vec{\eta}+\vec{\eta}',\bar{\sigma}} + c^\dagger_{\vec{r}-\vec{\eta}',\bar{\sigma}} c_{\vec{r},\bar{\sigma}} - h.c. \right\} . \quad (1)
$$

Where does the Kubo identity make a mistake?

$$\mathcal{K}(A) \equiv [\rho_0, A] - \int_0^\beta \rho_0[A(-i\tau), H]d\tau,$$

where

$$\rho_0 = 1/Z \exp(-\beta H)$$

It is (incorrectly) claimed that

$$\mathcal{K}(A) = 0$$

for any operator A. (Books refer to this as the Kubo identity). Let $p_n = 1/Z \exp -\beta\varepsilon_n$. Inserting complete states we see that

$$A_{nm}(p_n - p_m) = p_n \int_0^\beta d\tau A_{nm}(\varepsilon_m - \varepsilon_n) \exp -\tau((\varepsilon_m - \varepsilon_n))$$

Theorem: (SS-2006).

Kubo identity is only true for a class of operators of the type A-> [H,B] which have vanishing diagonal matrix elements in the energy eigenbasis!! It is infact false if diagonal elements in this basis are non zero!

$$\mathcal{K}([B, H]) = 0$$

Hydrodynamics of energy and charge transport in a band model:

This involves the fundamental operators in a crucial way:

$$\left\{\frac{\partial}{\partial t}+\frac{1}{\tau_c}\right\}\delta J(r)=\frac{1}{\Omega}\langle\tau^{xx}\rangle\left[\frac{1}{q_e^2}\frac{\partial\mu}{\partial n}(-\nabla\rho)-\nabla\phi(r)\right]+\frac{1}{\Omega}\langle\Phi^{xx}\rangle\left[\frac{1}{C(T)}(-\nabla K(r))-\nabla\Psi\right]$$

$$\left\{\frac{\partial}{\partial t}+\frac{1}{\tau_E}\right\}\delta J^Q(r)=\frac{1}{\Omega}\langle\Phi^{xx}\rangle\left[\frac{1}{q_e^2}\frac{\partial\mu}{\partial n}(-\nabla\rho)-\nabla\phi(r)\right]+\frac{1}{\Omega}\langle\Theta^{xx}\rangle\left[\frac{1}{C(T)}(-\nabla K(r))-\nabla\Psi\right]$$

$$\frac{\partial\rho}{\partial t}+\nabla J(r)=0$$

Einstein diffusion term of charge

Energy diffusion term

$$\frac{\partial K(r)}{\partial t}+\nabla J^Q(r)=p_{ext}(r)$$

Continuity

Input power density

These eqns contain energy and charge diffusion, as well as thermoelectric effects. Potentially correct starting point for many new nano heating expts with lasers.

Integrable systems are ``weak superconductors''

They possess temporal persistence in current, without the Meissner effect! Giamarchi, Giamarchi+SS (1992)

$$D_Q = 0 = D_M$$ **Isothermal stiffnesses vanish**

$$\kappa(\omega) = \frac{i}{T(\omega + i0^+)} D_Q + \frac{1}{T\mathcal{L}} \int_0^\infty dt e^{i\omega t} \int_0^\beta d\tau \langle \hat{J}_x^Q(t - i\tau) \hat{J}_x^Q(0) \rangle.$$

$$\sigma(\omega) = \frac{i}{T(\omega + i0^+)} D_M + \frac{1}{T\mathcal{L}} \int_0^\infty dt e^{i\omega t} \int_0^\beta d\tau \langle \hat{J}_x(t - i\tau) \hat{J}_x(0) \rangle.$$

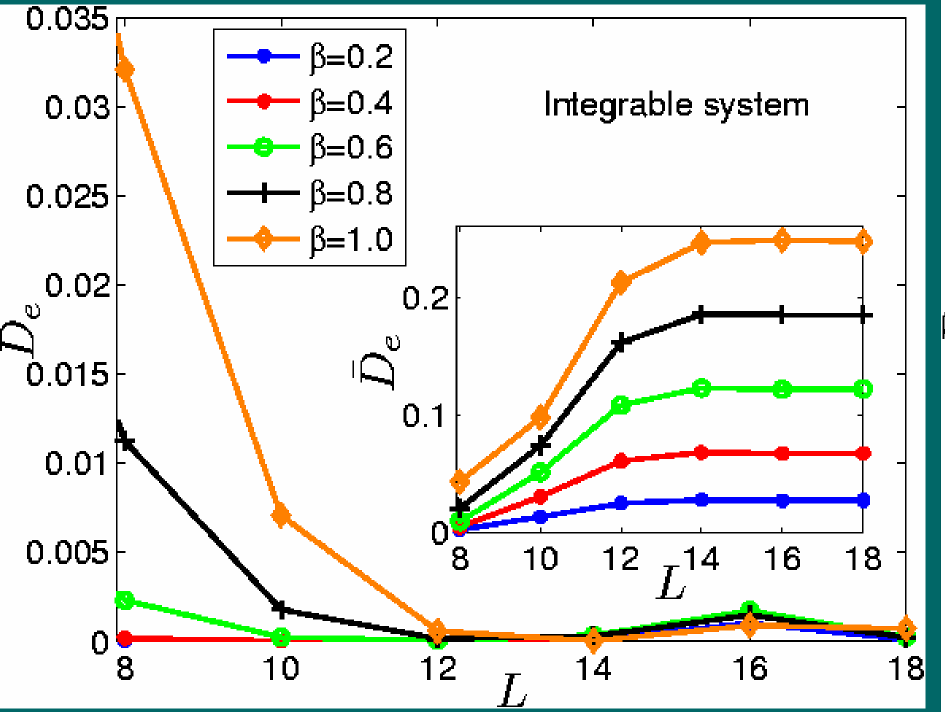
As $t \rightarrow \infty$ the current correlators do not decay to zero but are finite: temporal persistence. Therefore:

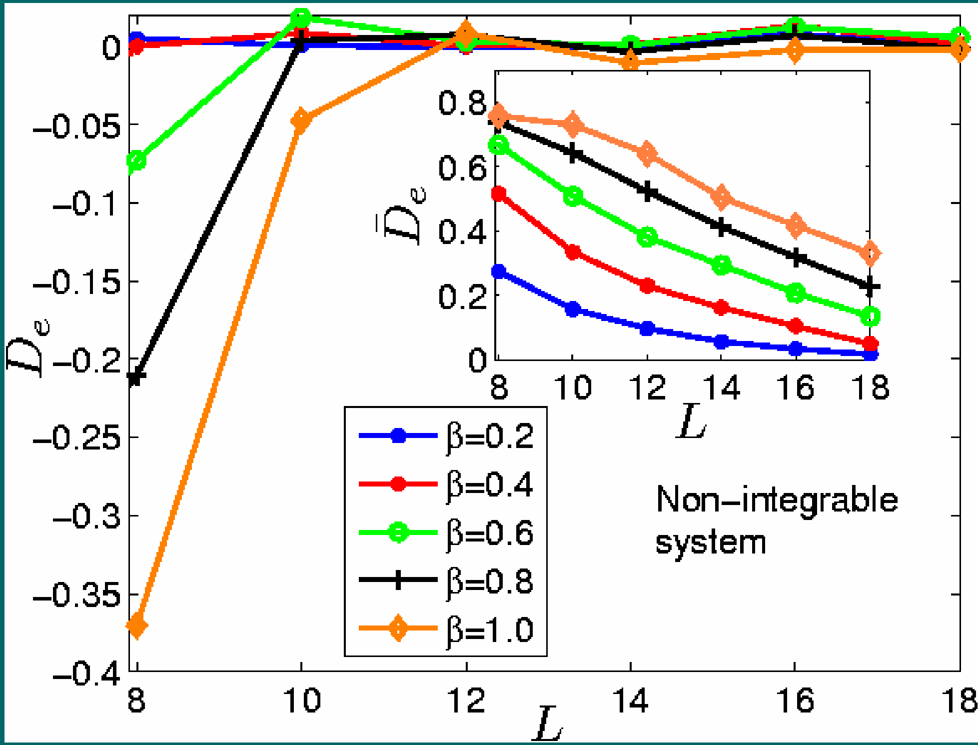
$$\sigma(\omega) \rightarrow D_c \; \delta(\omega) + \sigma_{reg}(\omega)$$

Adiabatic stiffness from persistence

Prelovsek,Zotos…..

T-t'-V model: i.e. perturbed Heisenberg model at Isotropic point (Fermi representation)





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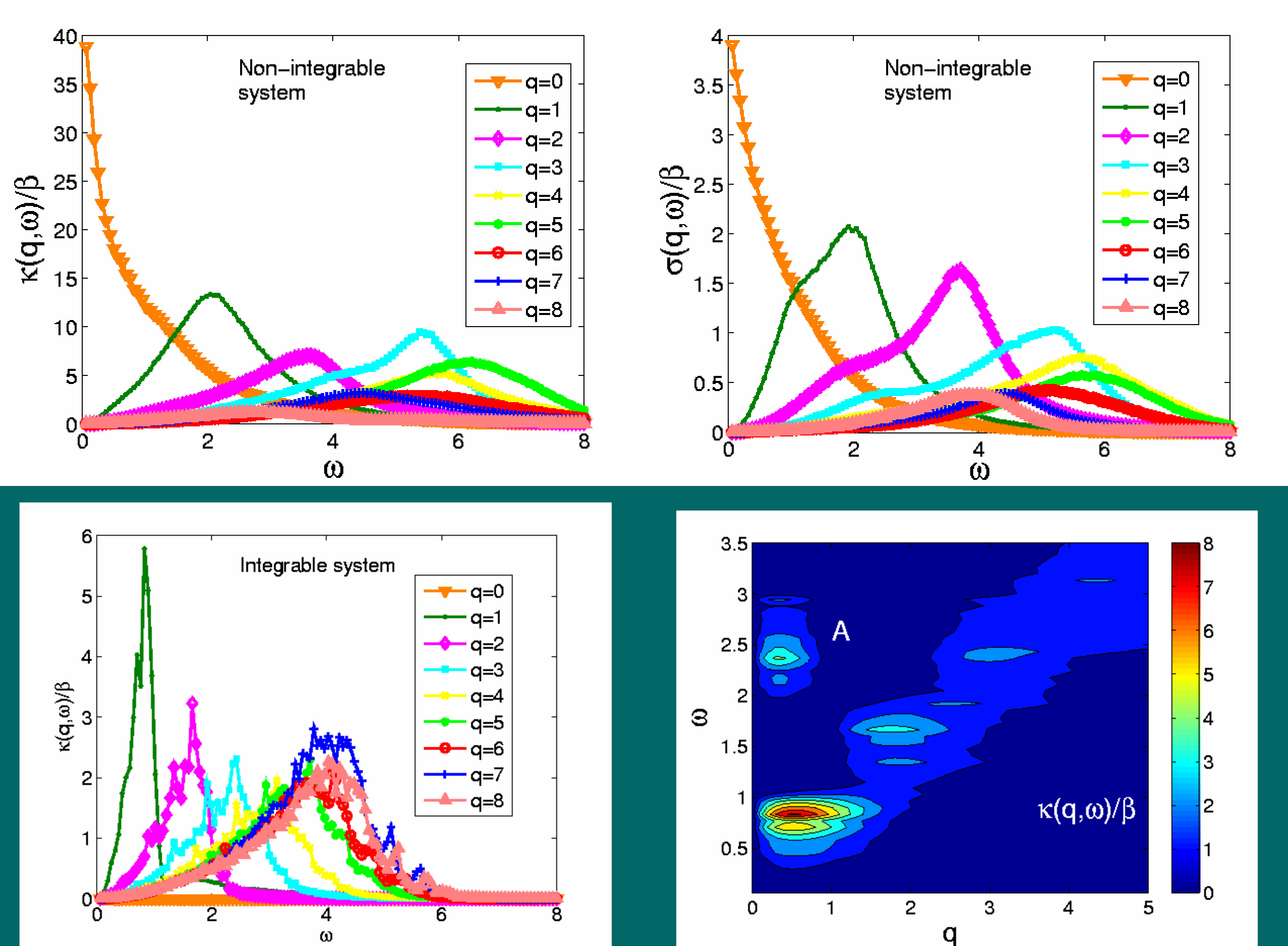
arXiv:0705.3791 : Signatures of integrability in charge and thermal transport in 1D quantum systems

Subroto Mukerjee, and SS



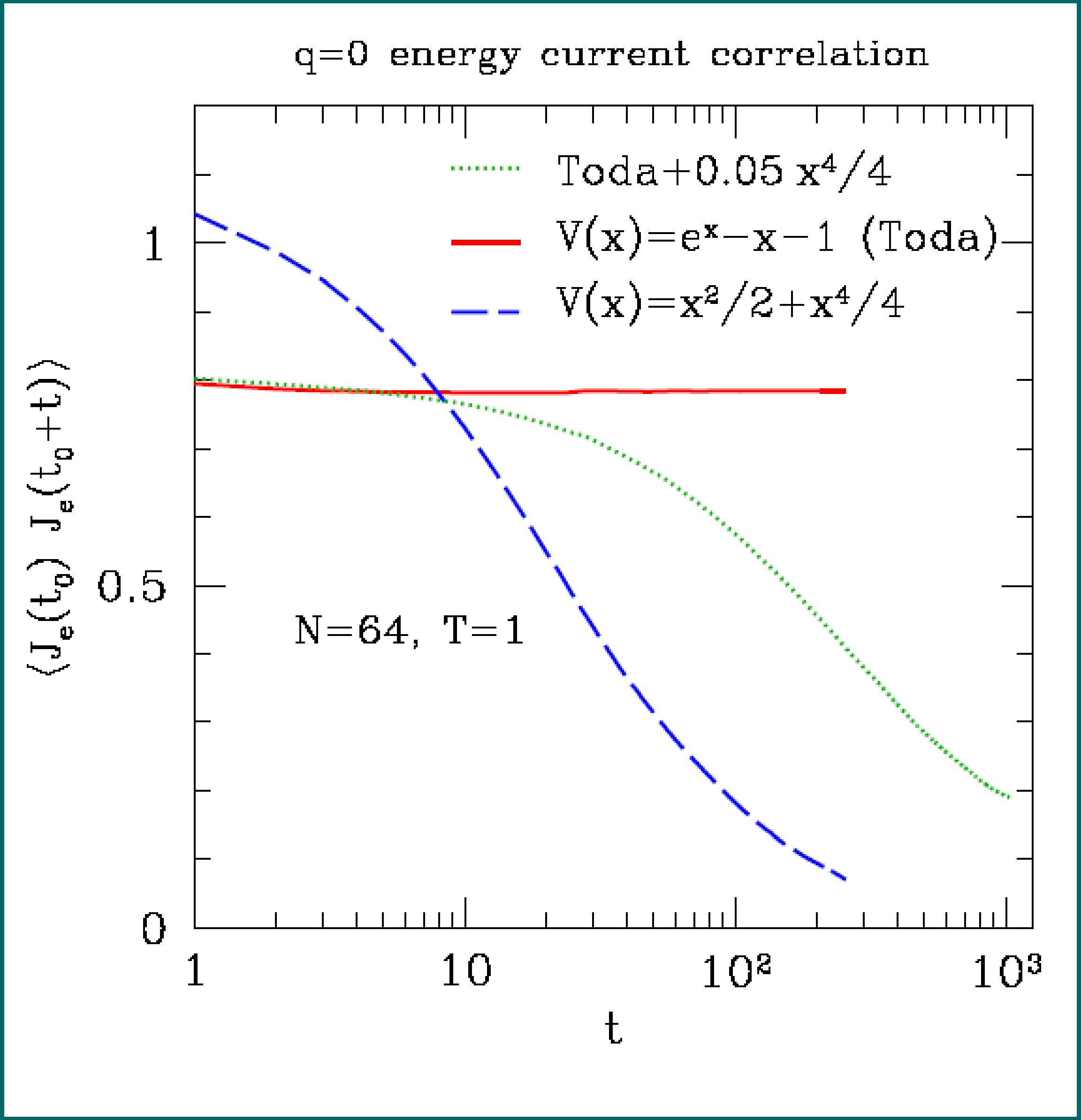
Non−integrable system
q=0
q=1
q=2
q=3
q=4
q=5
q=6
q=7
q=8
κ(q,ω)/β
ω
σ(q,ω)/β
Integrable system
A
q

Severely limited by size constraints.

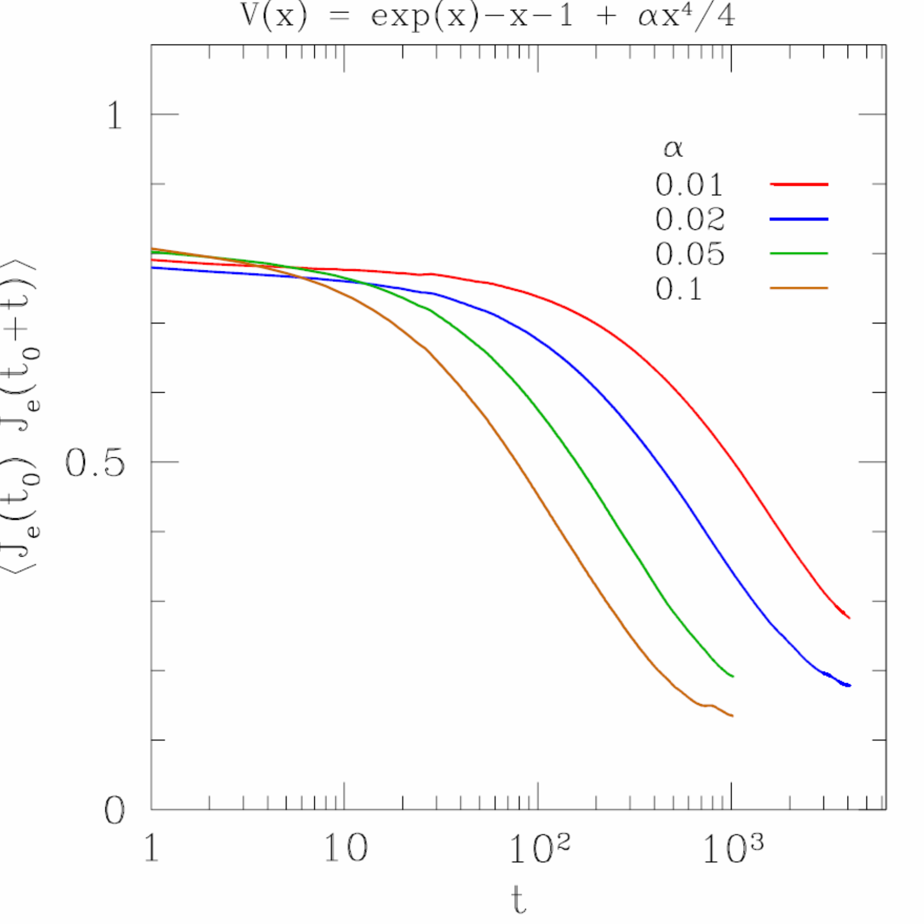
Hence change system

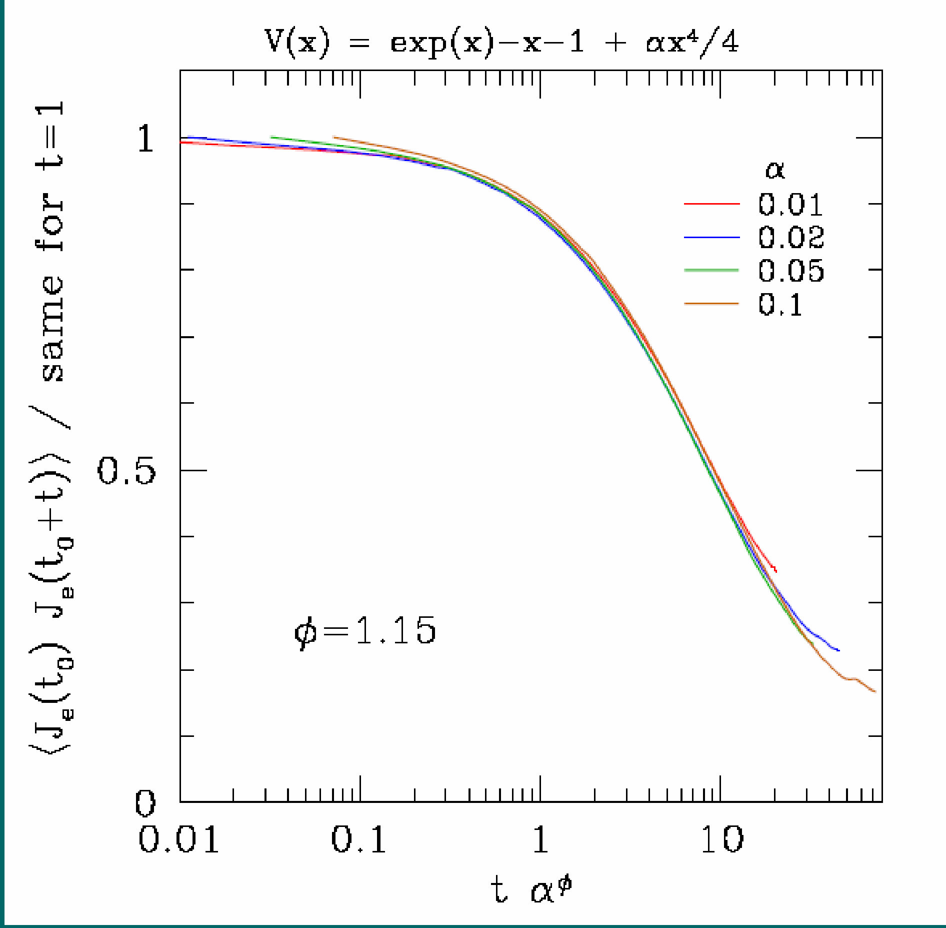
Study perturbed Toda lattice using cfs.

Peter Young and SS (to be published)



q=0 energy current correlation
Toda+0.05 x⁴/4
V(x)=eˣ−x−1 (Toda)
V(x)=x²/2+x⁴/4
N=64, T=1
⟨Jₑ(t₀) Jₑ(t₀+t)⟩
t
0
0.5
1
1
10
10²
10³

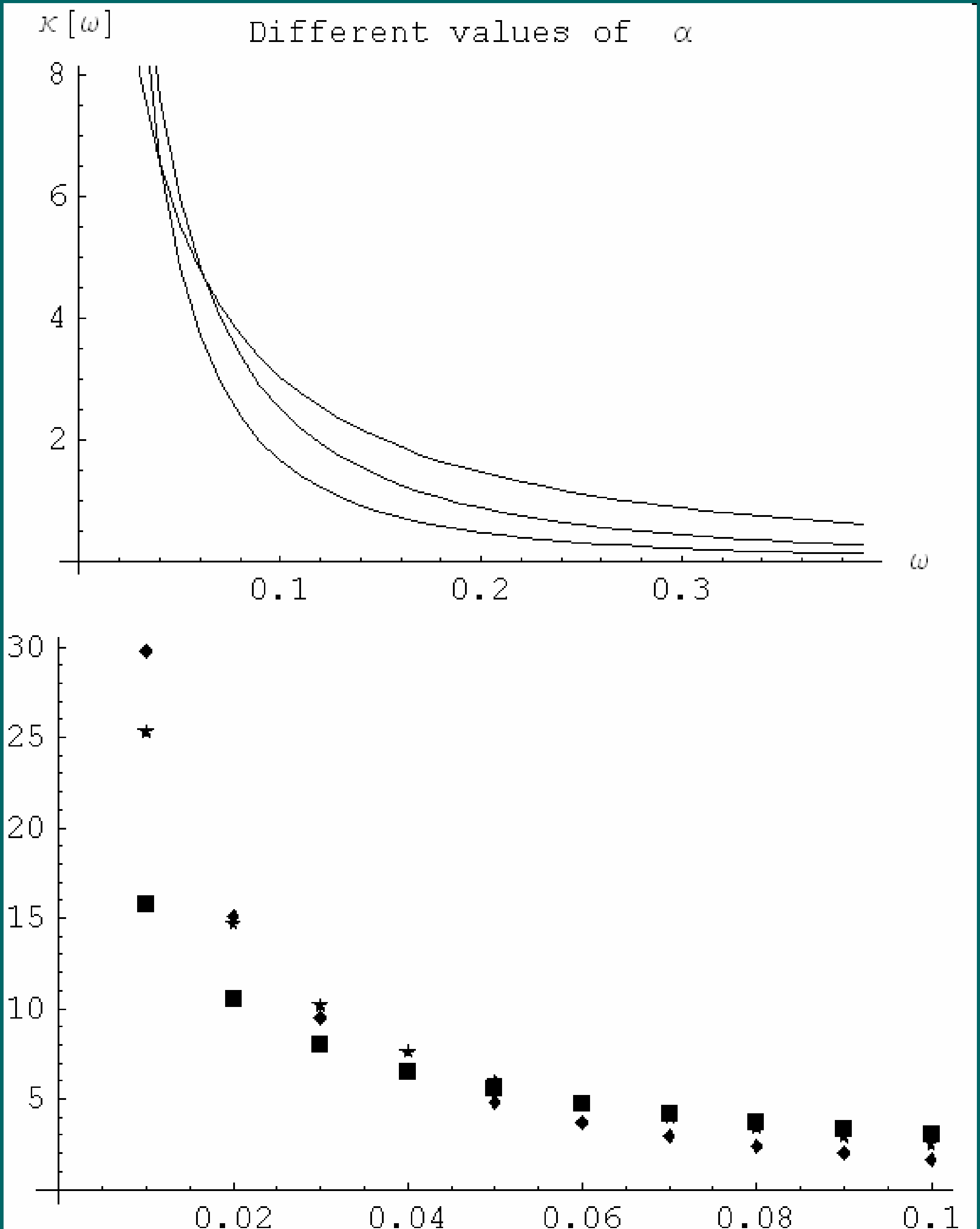




Perturbed Toda lattice energy current correlations for different values of parameter α.

Remarkable collapse of data on suitable scaling. The scaling exponent is ϕ ~1.15

We may think of α as the integrability destruction parameters



Visualizing the loss of integability through the conductivity function.

Conclusions:

•Kubo type formulas are non trivial at finite frequencies, and have much structure

•Destruction of integrability: KAM in classical mechanics. In QMBT we feel CF’s are the way to go.

•Universality classes, exponents are similar to Critical phenomena, with Integrable systems as generalized “critical points” .

Useful link for this kind of work:

http://physics.ucsc.edu/~sriram/sriram.html