Anomalous transport in spin 1/2 chains: AC conductivity

Ramsés Sánchez (Bonn), Vipin Varma (ICTP→CUNY)

and

Vadim Oganesyan(CUNY)

arxiv (soon)

What is this talk about?

- Frequency dependent diffusivity near $T=\infty$ in certain lattice models

$$D(\omega, T=\infty) \sim T\,\sigma(\omega, T)|_{T\to\infty} \sim |\omega|^{\alpha}$$

- Exponent α appears to depend on interactions, can be positive or negative; in integrable chains this form extends to $\omega=0$, but remains observable in intermediate dynamic range otherwise. Is this a sort of criticality?

- $\alpha\to-1^{+}$ near free-fermion limits

(why) is this interesting? General comments

- Specific examples of anomalous AC transport (let alone with adjustable exponents) are not common; AC response is not easy to compute and has been neglected by "integrable models" aficionados

- As with other difficult problems (e.g. non-fermi liquids/fractionalization) we try to gain intuition/confidence by working in 1D with hope of learning something non-trivial AND generalizable.
  Or be content with explaining a few experiments on spin chains and/or cold atoms
- Quite generally -- equilibrium statmech near $T=\infty$ is trivial.
  High temperature dynamics is NOT (e.g. MBL, NMR echoes, entanglement spread etc), also no general purpose theoretical tools for studying this regime.
- Unlike Spivak's talk, where high T was "trivial", here we do NOT have Maxwell-Boltzmann stats as $T\to\infty$ (lattice is crucial), also assume no phonons

Models and observables

- $H = H_0 + H_{nnn}$
- XXZ model (integrable): $H_0 = J_1 \sigma_i^{\pm} \sigma_{i+1}^{\mp} + 2\Delta \sigma_i^z \sigma_{i+1}^z$
- Next near neighbor flips: $\mathrm{H}_{nnn} = J_2 \sigma_i^{\pm} \sigma_{i+2}^{\mp}$
- Fermions or assisted flips $H_{nnn} = t_2 \sigma_i^{\pm} \sigma_{i+1}^z \sigma_{i+2}^{\mp}$
- Linear response conductivity:

$$\sigma(\omega, T) = \pi \frac{1 - e^{-\beta\hbar\omega}}{\omega Z} \sum_{n,m} e^{-\beta E_n} |J_{nm}|^2 \delta(E_n - E_m - \hbar\omega)$$

$\sigma(\omega, T \to \infty) = f_0(\omega)/T + \ldots.$

$f_0(\omega) = N^{-1} \sum |\langle m | j_{q=0} | n \rangle|^2 \delta(\omega - E_{mn})$

What is “integrability”?

- Infinite towers of conserved quantities, $[Q_m ,H]=0$

$$D \geq \frac{\beta}{2L} \sum_m \frac{\langle \hat{j}\, Q_m \rangle^2}{\langle Q_m^2 \rangle}$$

- “Drude” amplitude of $\sigma(\omega)=D\delta(\omega)+\ldots$
- Lower bound via Mazur’s inequality, which maybe thought of as a statement about post-quench dynamics with residual current “at” $t=\infty$. D is not required to be finite in integrable models but usually is.

- Super- and sub-diffusive relaxation toward $t=\infty$?

How do we compute?

- Match educated guesses (ansatzes) for $\sigma(\omega)$ to manualy calculated moments (short time series)

Not quite a variational approach but similar in spirit

- "Predict" evolution of $\sigma(\omega)$ with Hamiltonian parameters – look for quantitative and qualitative trends

- Compare against exact diagonalization

Anomalous and ergodic anzatzes for $\sigma(\omega)$

- "legacy" Gaussian Ansatz with low freq. anomaly (3 parameters)

$$\sigma(\omega)=(A/\omega_0)|\omega/\omega_0|^{\alpha}\exp[-(\omega/\omega_0)^2]\rightarrow\langle\delta x^2\rangle\sim t^{1-\alpha}$$

- "maximally" hydrodynamic 2 parameter ansatz (Mukerjee etal, 2006)

$$\langle j(t)j(0)\rangle=A/(\tau^2+t^2)^{-3/4}$$

- 5 parameter diffusive ansatz for "atomic" (zz-dominated) limit

$$\sigma(\omega)=(A/\omega_0)\exp[-(\omega/\omega_0)^2]+(B/\omega_1)\sum_{\pm}\exp[-((\omega\pm\Omega)/\omega_1)^2]$$

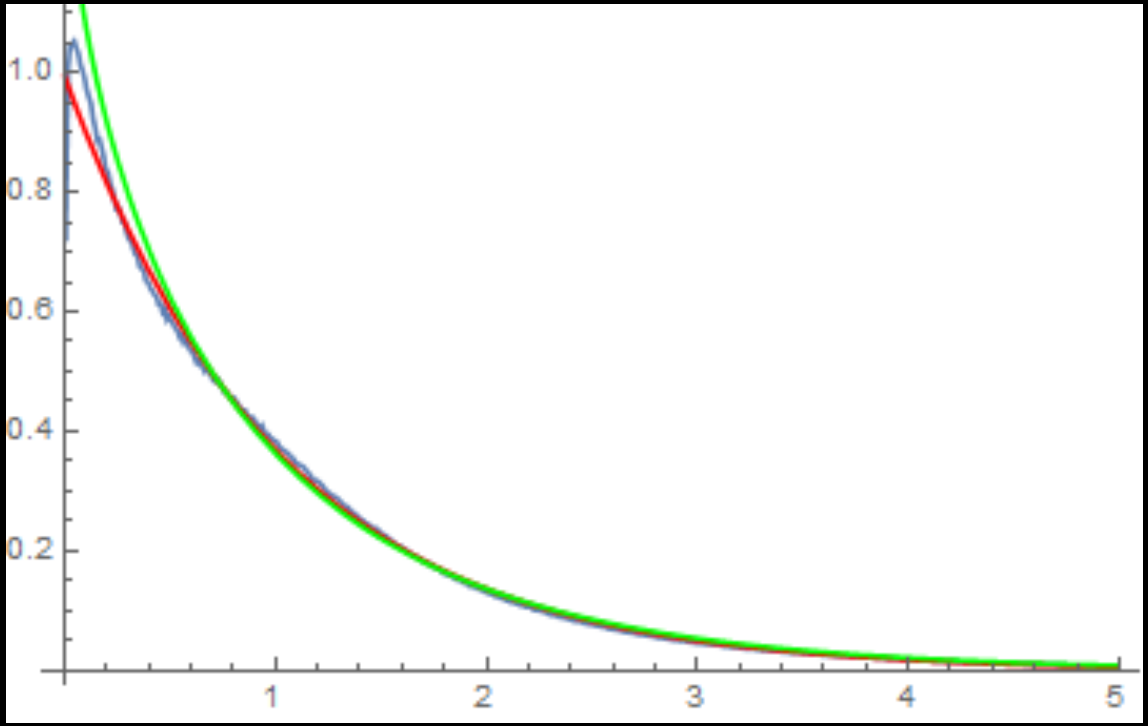
Warmup #1– strongly nonlinear hydro (Mukerjee etal 2006)

- $H=\sum_j c_j^{+} c_j c_{j+1}^{+} c_{j+1} + c_j^{+} c_{j+1} + c_j^{+} c_{j+2} + h.c.$
- $\langle j(t)j(0)\rangle \approx A/(t^2+\tau^2)^{3/4}$
- $\sigma \sim \omega^{1/4}\ K(-1/4, \omega\tau)$

- Or try 3 parameter ansatz

$\sigma(\omega)=a\exp(-b\sqrt{\omega}-c\omega)$

$\sigma \approx const-\sqrt{\omega}$ form should be "universal" as $\omega\rightarrow 0$



Warmup #2 – atomic limit (zz-dominated)

$H_0 = J_1 \, \sigma_i^{\pm} \, \sigma_{i+1}^{\mp} + 2\Delta \sigma_i^z \, \sigma_{i+1}^z$

$\Delta = \infty \rightarrow \sigma = A\delta(\omega) + B\delta(\omega - \Omega) + B\delta(\omega + \Omega)$

Finite Δ, replace with 3 Gaussians → 5 parameters.

Matching to moments gives diffusion constant $\sim 1/\Delta$

Consistent with some existing TDMRG (no ED available there)

Matching moments for the anomalous ansatz

Restrict analysis to representation with equal number of moments and parameters, i.e. no fitting/optimizing whatsoever.

$$\sigma(\omega)=\frac{2\pi\mu_1}{\omega_0\,\Gamma\left(\frac{1+\alpha}{2}\right)}\left|\frac{\omega}{\omega_0}\right|^{\alpha}\exp\left[-\left(\frac{\omega}{\omega_0}\right)^{2}\right]\rightarrow$$

$$\mu_n\equiv\int d\omega\,\omega^{2n}\,\sigma(\omega)$$

$$\mu_1 = \frac{1}{2}J_1^2+2J_2^2, \tag{20}$$

$$\mu_2 = \frac{1}{4}J_1^2\Delta^2+J_2^2\Delta^2-\frac{3}{2}J_1^2J_2\Delta+\frac{5}{2}J_1^2J_2^2, \tag{21}$$

$$\begin{aligned}\mu_3 = {} & \frac{1}{4}J_1^2\Delta^4+J_2^2\Delta^4+\frac{5}{16}J_1^4\Delta^2+\frac{3}{2}J_2^4\Delta^2+10J_1^2J_2^2\Delta^2\\ & -\frac{11}{4}J_1^2J_2\Delta^3-\frac{5}{2}J_1^4J_2\Delta-\frac{27}{8}J_1^2J_2^3\Delta+\frac{7}{2}J_1^2J_2^4\\ & +\frac{85}{16}J_1^4J_2^2,\end{aligned} \tag{22}$$

$\leftrightarrow$

$$\frac{\mu_n}{\mu_1}=\omega_0^{2n-2}\frac{\Gamma\left(\frac{2n-1+\alpha}{2}\right)}{\Gamma\left(\frac{1+\alpha}{2}\right)}$$

Solution:

$$\alpha(J_2,\Delta) = \frac{3\,\mu_2(J_2,\Delta)^2 - \mu_1(J_2)\mu_3(J_2,\Delta)}{\mu_1(J_2)\mu_3(J_2,\Delta) - \mu_2(J_2,\Delta)^2}$$

$$\omega_0(J_2,\Delta)^2 = \frac{2}{\alpha(J_2,\Delta)+1}\frac{\mu_2(J_2,\Delta)}{\mu_1(J_2)}$$

Integrable chains ($J_2 = 0$):

$$\alpha(0,\Delta) = \frac{2\Delta^2 - 5}{2\Delta^2 + 5}$$

- closely captures a recently computed result for $\Delta = 1$, $\alpha = -3/7 \approx -0.43$ compared to ~ -0.33 from recent TDMRG (Ljubotina/Varma/Znidaric/Prosen) or much earlier ED results by Fabrizio/McCoy -0.41
- Is this an accident or good luck?
- If $\sigma(\omega)$ is sufficiently featureless then we might not be too far off re: coarse features and trends.
- The formula for $\Delta < 1$ is likely valid, qualitatively

Results -- $J\downarrow 2$ dependence

- Asymmetry near $J\downarrow 2 = 0$: interplay between $J\downarrow 2$ and Δ

$$\mu_1 = \frac{1}{2}J_1^2 + 2J_2^2, \tag{20}$$

$$\mu_2 = \frac{1}{4}J_1^2\Delta^2 + J_2^2\Delta^2 - \frac{3}{2}J_1^2J_2\Delta + \frac{5}{2}J_1^2J_2^2, \tag{21}$$

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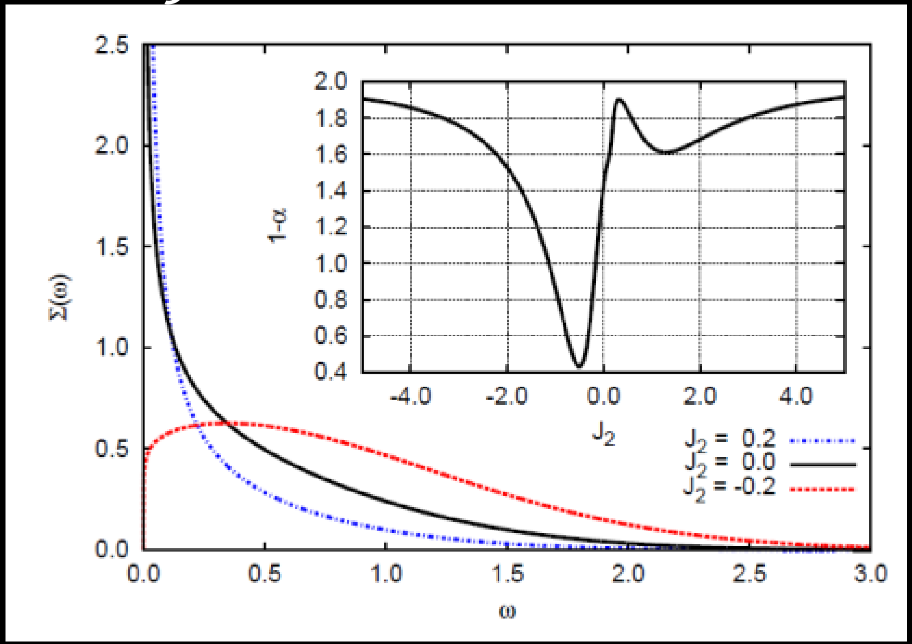
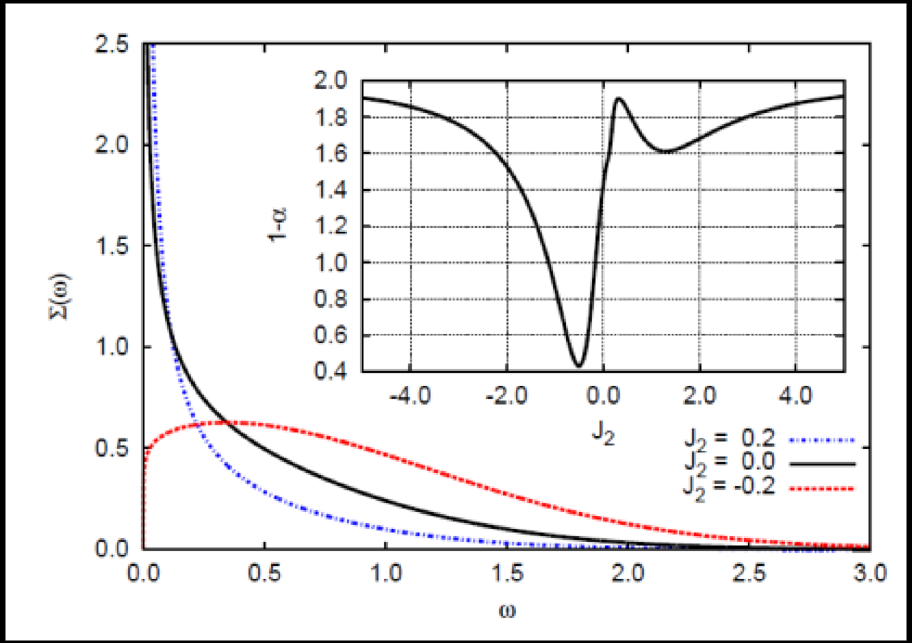
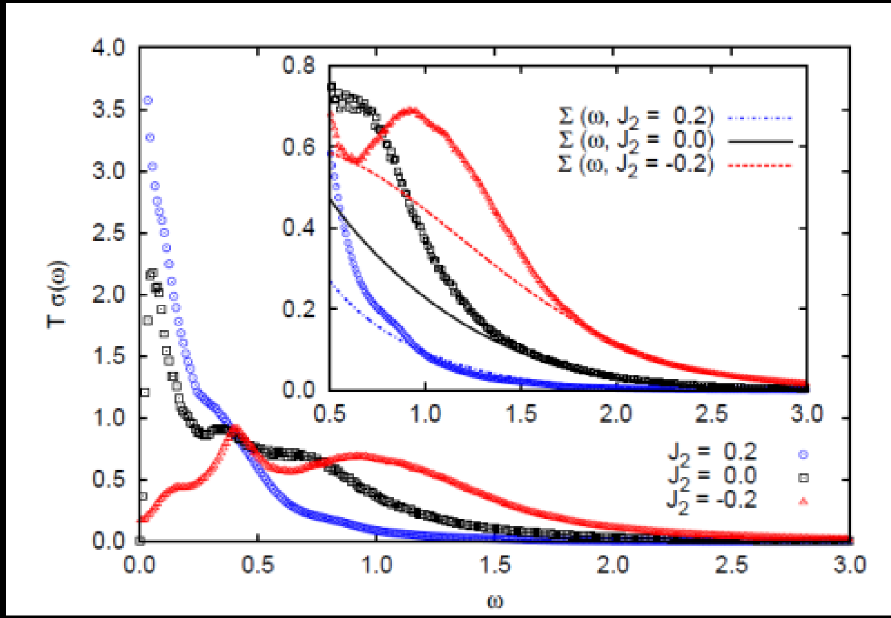


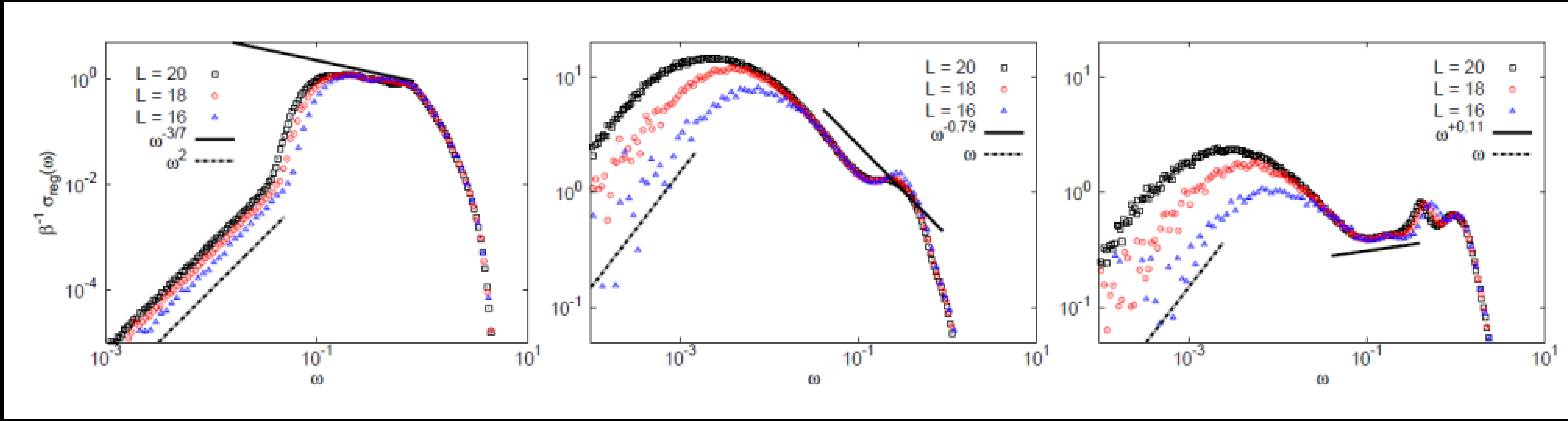
- Predicts SUB-diffusion left of the Heisenberg point (?!)
- Predicts $\alpha = -1$ near free fermion limits $J\downarrow 2 \to \pm\infty$ limit

Aside – high frequency behavior is also interesting (ask me later) and is tracked by the approximation





Comparing to ED with $J/2 = 0, +0.2, -0.2$



Comments:

- ED is VERY difficult to interpret along the integrable XXZ line
- Super-diffusion at $J/2 = +0.2$ is there over at least 2 decades. There should be diffusion eventually at lower ω
- Sub-diffusion is noticeable over some dynamical range but eventually gives way to a new peak.

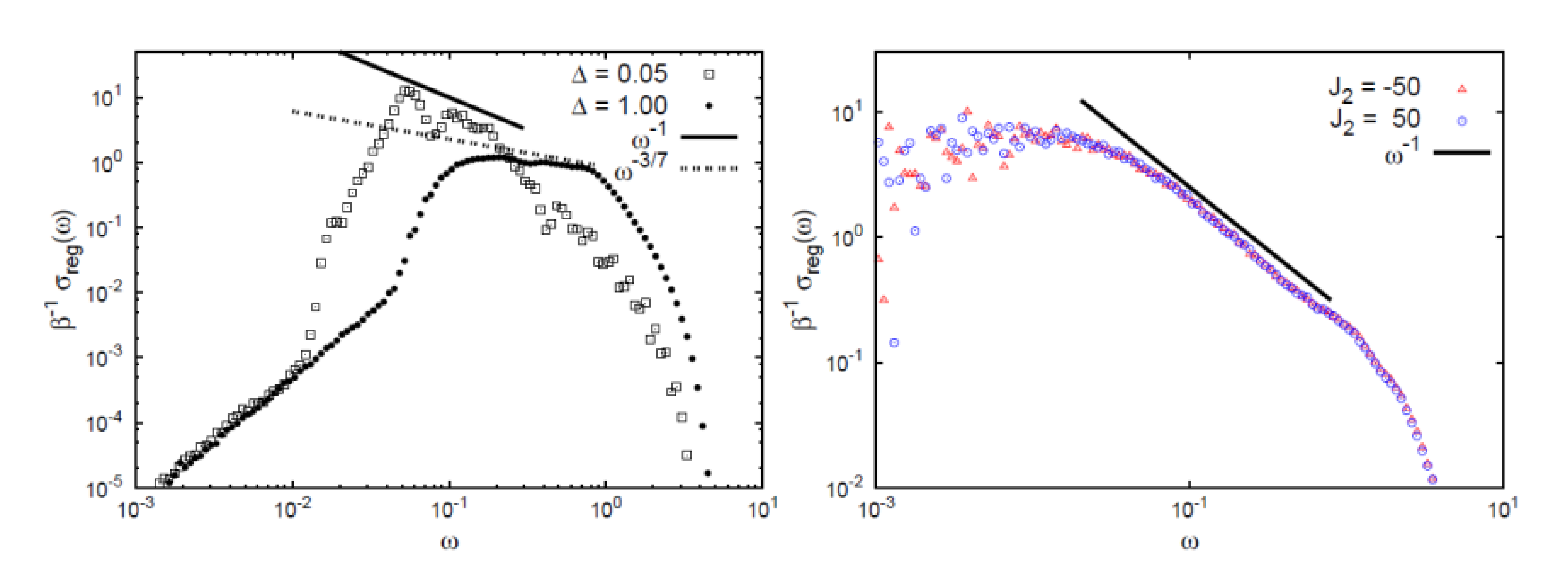
Simple microscopic insights? 3 sites

Consider a small cluster e.g. of 3 sites – conductivity has response at two frequencies

$$\omega_{\pm} = \frac{1}{2}\left(\Delta - 3J_2 \pm \sqrt{(\Delta + J_2)^2 + 8}\right)$$

This correctly captures the cross term in the moments and downward/upward shift of weight vs. *J↓2*

Free fermion limits: $\Delta = J_2 = 0$ and $J_2 \to \pm\infty$



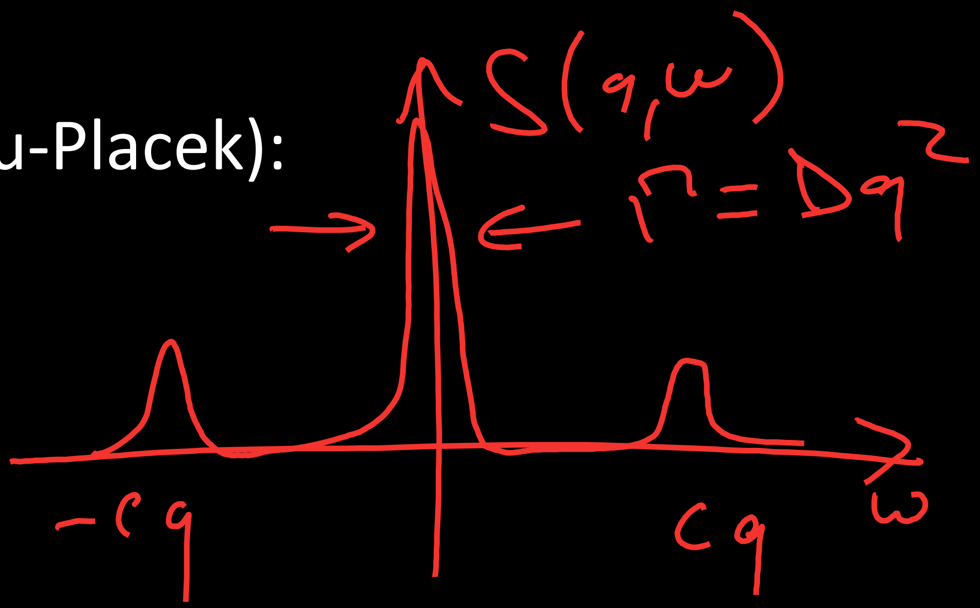
- Conductivity exponent drifts towards -1 for both integrable and non-integrable weakly interacting problems (as predicted by the moments)
- Somewhat surprising, but maybe shouldn't be – the current operator at q=0 has non-conserved pieces that decay slowly near non-interacting limits

summary/outlook

- Low freq. anomalies in AC conductivity that appear to drift akin to marginal perturbations on a conventional critical surface.
  We expect this behavior to give way to ordinary diffusion as $\omega \to 0$
  What is the model space where this behavior extends to $\omega = 0$?
- Can we connect this with “generalized hydrodynamics”?
- Extension to thermal and thermoelectric phenomena, long-range interactions, higher spin, nonlinear response,…
- How does one detect this behavior in “realistic” experiments? AC conductivity is difficult to measure.

Dynamic structure factor

- How do we avoid the $\delta(\omega)$ peak in conductivity? It is a nuisance if trying to observe $\sigma_{reg}(\omega)$
- Light scattering in conventional fluids (Landau-Placek):



- Coherent features (phonons) move out to “high” frequency ~c*q, while ordinary diffusion occupies low freq.
- $T=\infty$ XY chain has a quasi phonon peak

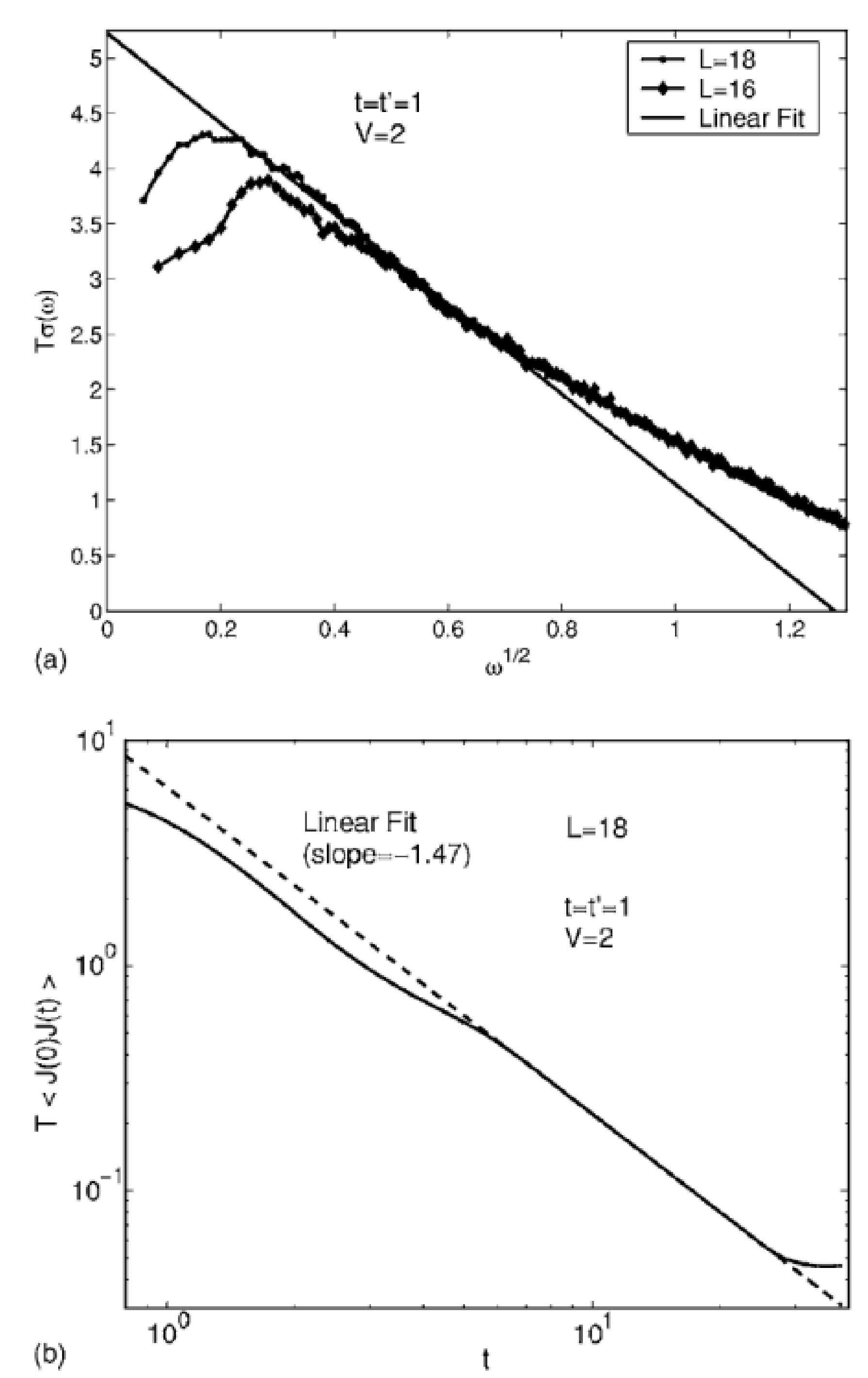
but no diffusion $$S(k,\omega)=\frac{1}{\sqrt{16J^2\sin^2(\frac{k}{2})-\omega^2}}$$

- Using memory functions can re-compute S(q,w) with interactions:

<u>Super-diffusion → 4 peak profile with a dip at $\omega=0$!</u>

- Different from T=0 structure factor (Imambekov etal RMP)

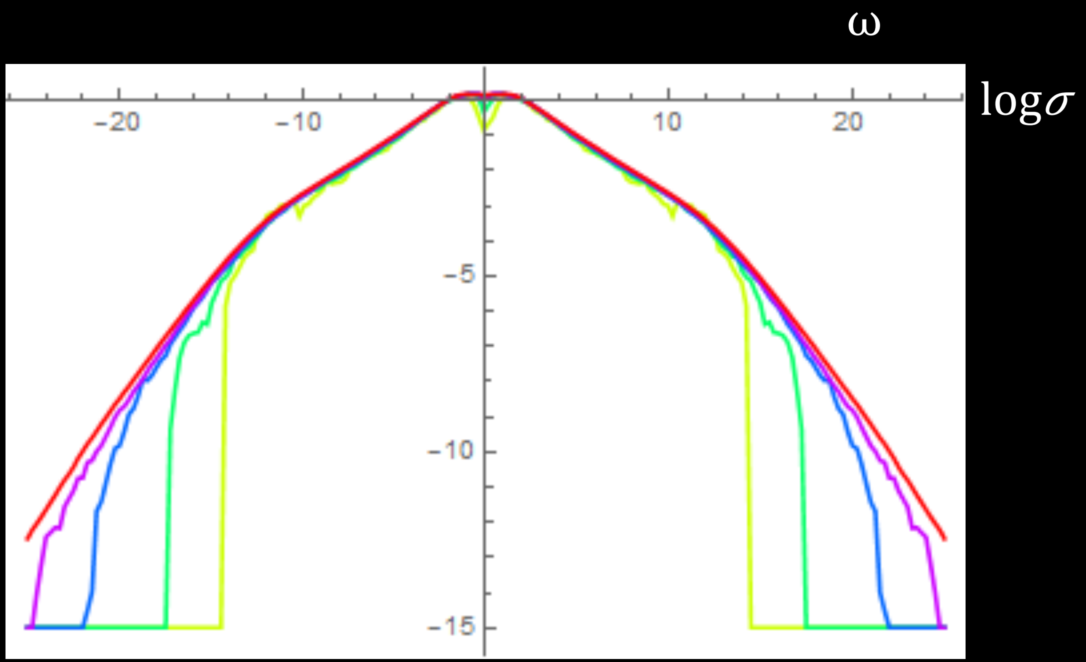
More low freq plots



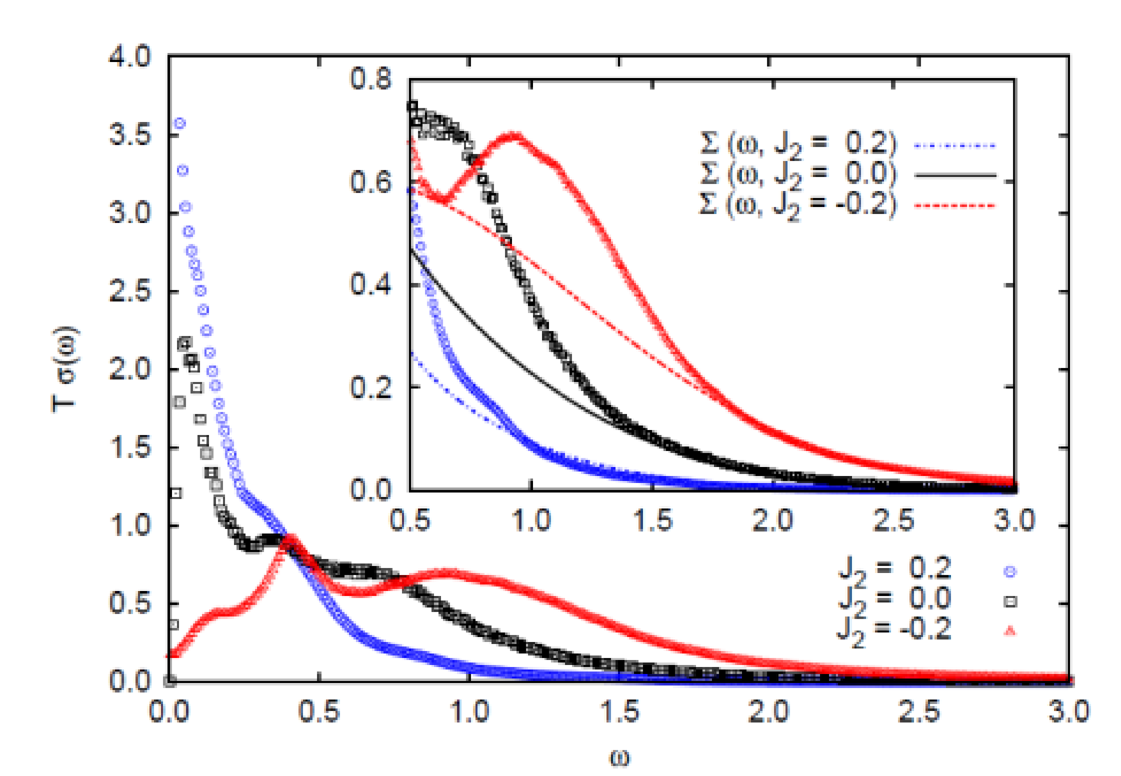
Asymptotics of $\sigma(\omega\to\infty)$? $\sim\exp[-\omega/\omega^{*}]$?

- Most (all?) high temperature series in lattice models have finite radii of convergence

- What about short time expansions? If the same "folk" theorem holds then radius of conv. near t=0 is $1/\omega^{*}$
- A handle on finite size effects?



tails also help “understand” other gross features, e.g. strong variation vs. J_2 at “medium” frequencies?”



Memory function formalism (Woelfle/Goetze, Forster's book)

$$\partial_t C(k,t) + k^2 \int_0^t d\tau \Sigma(k,t-\tau) C(k,\tau) = 0 \quad (t>0)$$

$$\tilde{C}(k,z) = \frac{i}{z + ik^2 \tilde{\Sigma}(k,z)} C(k,t=0), \quad (\mathrm{Im}z > 0)$$

$$\int \frac{d\omega}{2\pi} \omega^{2n} \frac{C(k,\omega)}{C(k)} = k^2 \int \frac{d\omega}{2\pi} \omega^{2n-2} \Sigma(k,\omega)$$

=

$$\mu_n = \sum_{j,j'} (4/L) e^{-ik(j-j')} \langle [\ldots[[\hat{S}^z_j, H], H], \ldots, H] \hat{S}^z_{j'} \rangle$$

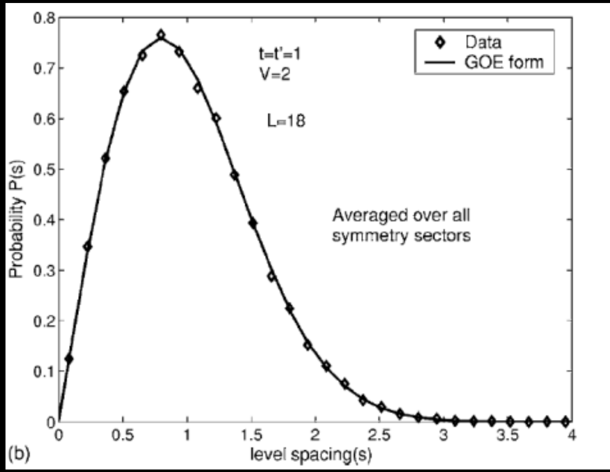
And

$$\lim_{k\to 0} C(k,0)\Sigma(k,t) = \sigma_{\mathrm{reg}}(t)$$

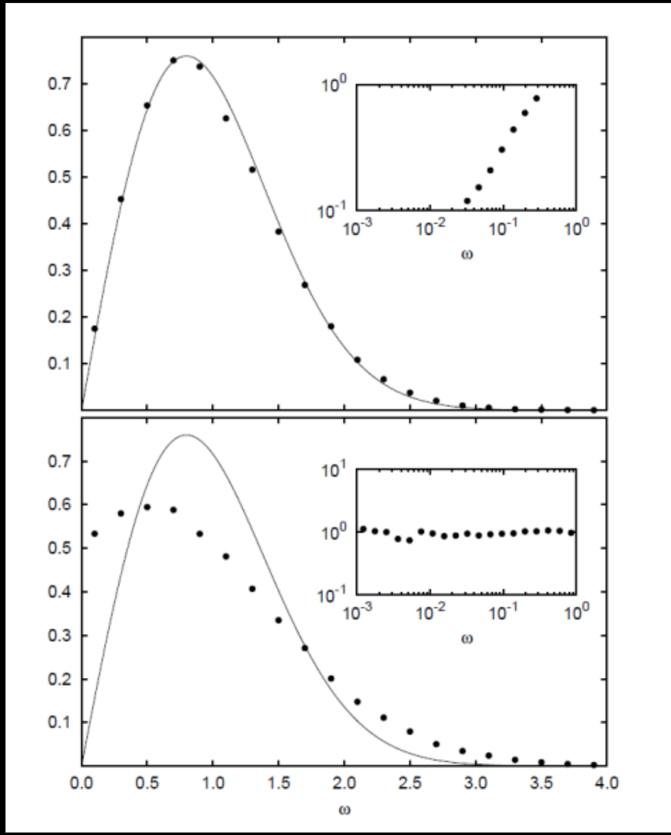
RMT perspective?

$t_2 = 1$

all matrix elements of current are comparable



$J_2 = 0.2$



all levels

levels connected by current