Magnetic transport: from Heisenberg to Kitaev chains

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Rev. Lett. 112, 120601 (2014)
Phys. Rev. B 91, 104404 (2015)
arXiv:1503.03871

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Thanks to: X. Zotos UoC, J. Herbrych UoC, C. Karrasch UCB, F. Heidrich-Meisner LMU

SFB 1143

SEVENTH FRAMEWORK PROGRAMME

nth nano school for contacts in nanosystems

Transport what

- spin S_m^α
- energy $E_m \sim \sum_{n,\alpha\beta} J_{mn}^{\alpha\beta} S_m^\alpha S_n^\beta$

spin current $j_{Spin} \sim \sum_{lm} J_{lm} \vec{S}_l \times \vec{S}_m$

energy current $j_{Energy} \sim \sum_{lmn} J_{lm} J_{mn} \vec{S}_l \cdot (\vec{S}_m \times \vec{S}_n)$

(magnetothermal $j = j_{Energy} - h \cdot j_{Spin}$)

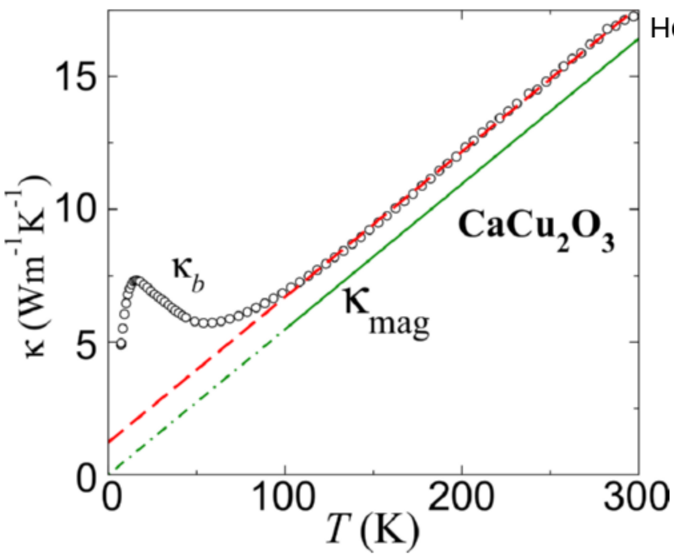
Transport why

- Energy / heat conductivity: kinetic approach

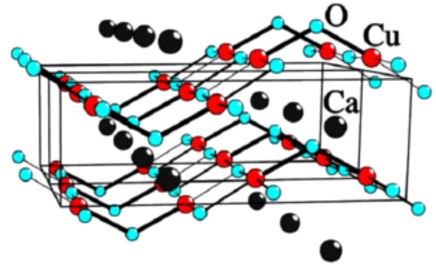
$$\kappa_{mag} \sim \underbrace{C_{mag} v_{QP}}_{\text{elementary excitations}} \underbrace{l_{mag}}_{\text{scattering}}$$

elementary excitations scattering

Elementary Excitations in Heat Transport



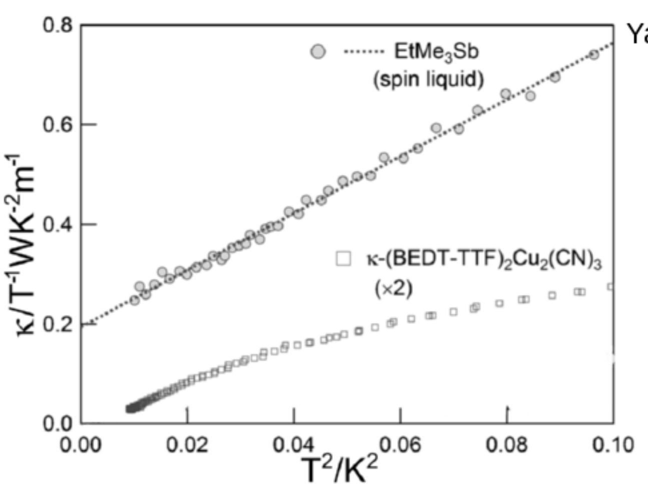
Hess, Büchner, WB, et al., PRL 98, 027201 (07)



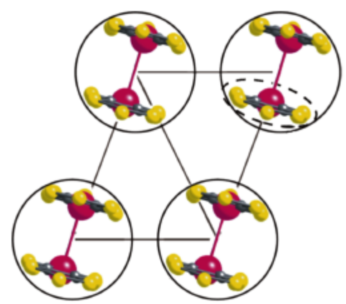
~ CuO chains

$\kappa_{mag} \sim T$

spinons



Yamashita, Nakata, Kasahara, et al., Nature Phys. 5, 44 (09)



~ molecular Δ lattice

U(1)-liquid, spinons: $\sim T^{3/2}$

+ impurities: $\sim T$

Nave, Lee, PRB 76, 235124 (07)

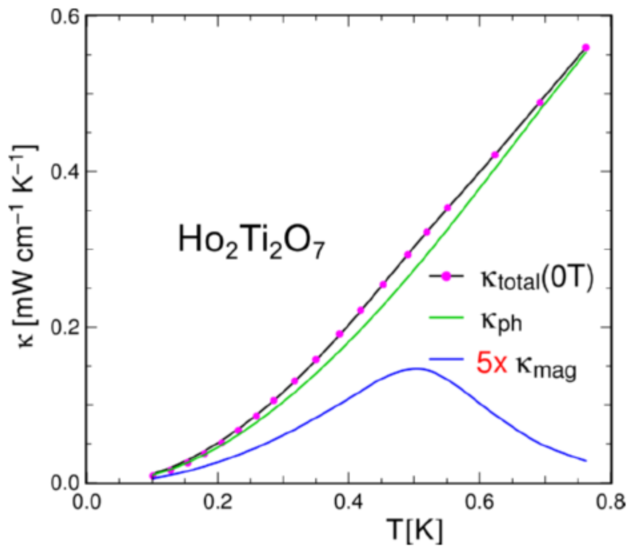
nodal-Z_2 d-wave, spinons: $\sim T$

Grover, Trivedi, Senthil, et al.
PRB 81, 245121 (10)

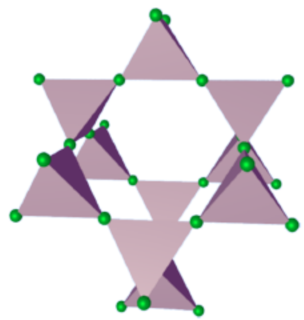
Z_2-liquid, visons: $\sim e^{-\Delta/T}$

Qi, Xu, Sachdev, PRL 102, 176401 (09)

Elementary Excitations in Heat Transport



Kolland, Breunig, Valldor, et al. PRB 86, 060402(R) (12)
Toews, Zhang, Ross, et al., PRL 110, 217209 (13)

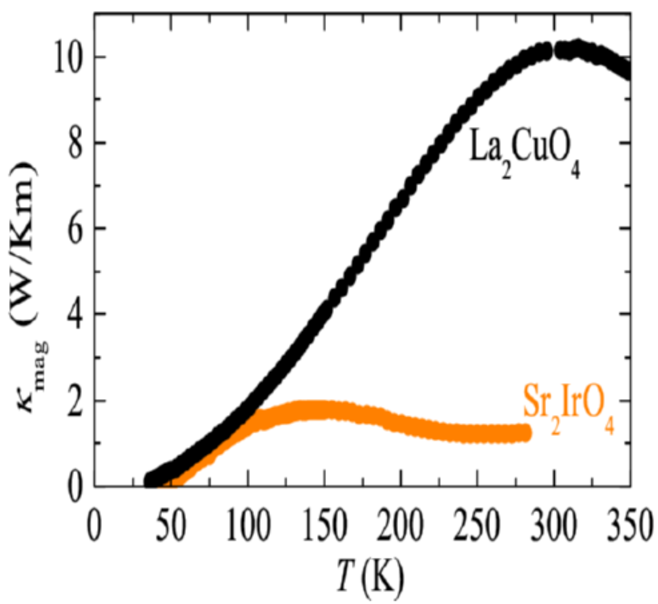


Kagome, spin ice

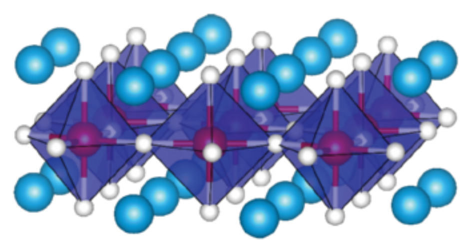
gap

$$\kappa_{mag} \sim T^2/[c_1 + c_2 e^{-\Delta/T}]$$

monopoles



Hess, et al. PRL 90, 197002 (2003),
Steckel, Tagaki, Hess, et al., arXiv:1507.04252



2D { real / pseudo } σ-AFMs

$$\kappa_{mag} \sim T^2$$

magnons

Beyond Kinetic Approaches

- correlation functions

$$C_{S/E}(t) = \mathrm{Re}\langle j_{S/E}(t)\, j_{S/E}\rangle$$

Drude weight & regular conductivity

$$\sigma_{S|E}(\omega)=\beta^{1|2}\int_0^\infty dt\, C_{S|E}(t)e^{i\omega t}$$

$$=\beta^{1|2}\bar{C}_{S|E}\delta(\omega)+\kappa_{S|E}(\omega)$$

- Tools

ED: tJ arbitray, but $N\sim 20$

tDMRG: $N\sim 200$ but $tJ\lesssim 15$

Quantum Typicality: tJ arbitrary & N~36...

(... QMC, TMRG, perturbation theory)

- $\bar{C}_{S|E}$ finite → perfect conductor

$$H=J\sum_l (S_l^x S_{l+1}^x + S_l^y S_{l+1}^y + \Delta S_l^z S_{l+1}^z)$$

$$[H, j_E]=0$$

$$\bar{C}_{S|E} \geqslant \frac{\sum_{Q_{cons}} \langle j_{S|E} Q_{cons}\rangle^2}{\langle Q_{cons}^2\rangle}$$

Mazur, Physica 43, 533 (69)

XXZ: infinite heat conductivity

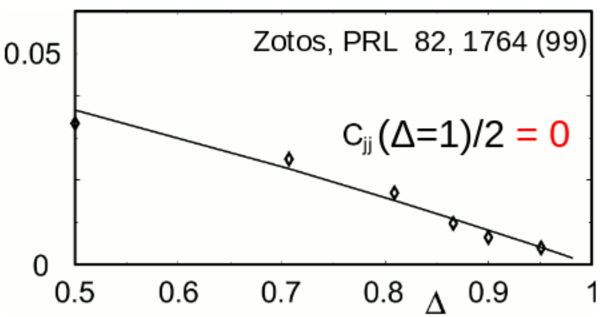
but spin Drude weight nontrivial

all tDMRG data: Karrasch, Moore, Heidrich-Meisner, et al.
PRL 108, 227206 (12), PRB 87, 245128 (13), 89, 075139 (14)

Spin Drude Weight

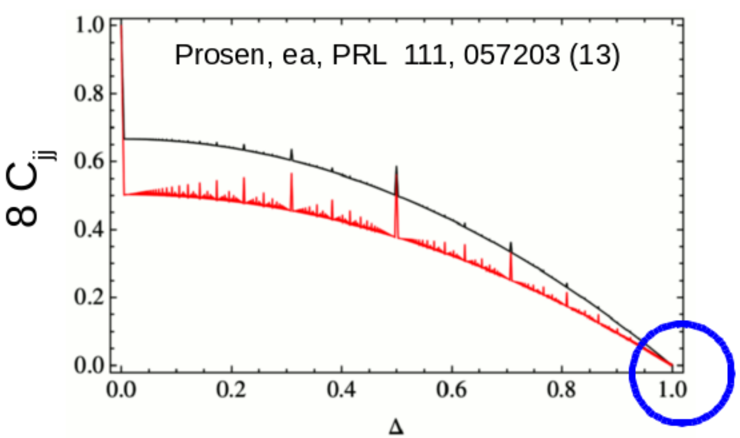
- Bethe A T=0 ✓ Shastry, Sutherland, PRL 65, 243 (90)

High-T Spin Drude Weight



Benz, ea, JPSJ 74, 181 (05)

$$C_{jj} = \frac{\Delta^2+2}{32} \neq 0$$



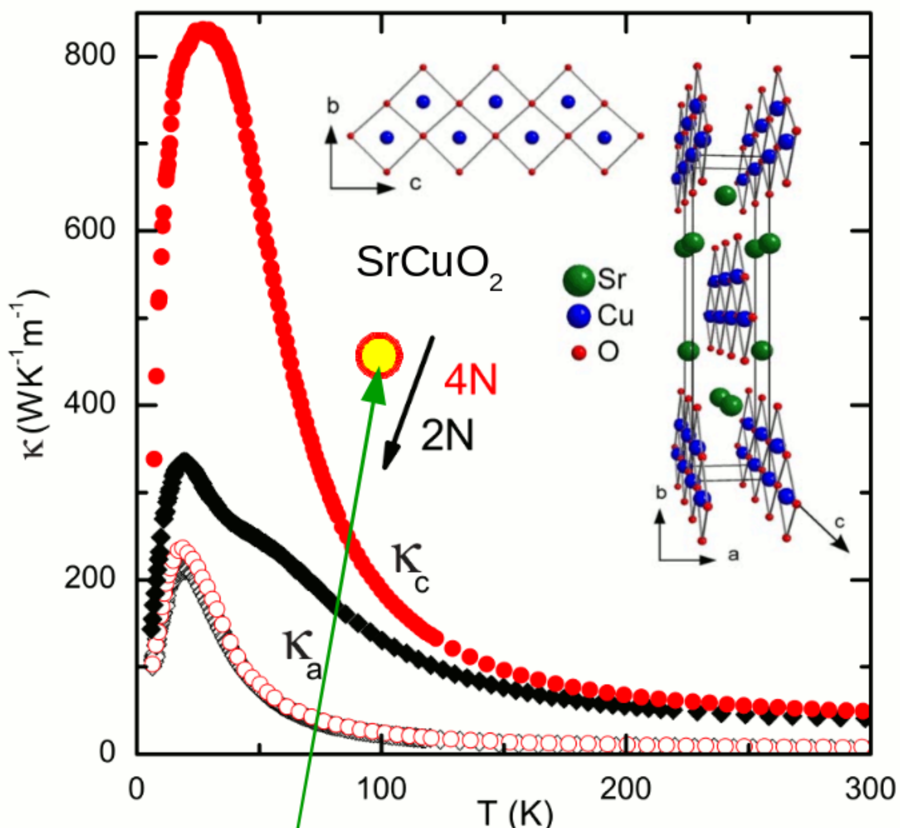
- Bethe A T=0 ✓
  $\Delta=1$ $T\neq0$ ⚡
  - Shastry, Sutherland, PRL 65, 243 (90)
  - Zotos, PRL 82, 1764 (99)
  - Benz, ea, JPSJ 74, 181 (05)
- NEES bounds
  - Prosen, PRL 106, 217206 (11)
  - Prosen, ea, PRL 111, 057203 (13)
  - Carmelo, ea, arXiv:1407.0732 (14)
- ED
  - Narozhny, ea, PRB 58, 2921R (98)
  - Fabricius, ea, PRB 57, 8340 (98)
  - Heidrich-Meisner, WB, ea, PRB 68, 134436 (03)
  - Heidrich-Meisner, WB, et al. EPJ 151, 135 (07)
  - Steinigeweg, ea, PRB 80, 184402 (09)
  - Herbrych, ea, PRB 84, 155125 (11)
  - Steinigeweg, WB, PRL 107, 250602 (11)
  - Steinigeweg, ea, PRE 87, 012118 (13)
- QMC
  - Alvarez, ea, PRL 88, 077203 (02)
  - Heidarian, ea, PRB 75, 241104R (07)
  - Grossjohann, WB, PRB 81, 012404 (10)
- tDMRG
  - Langer, ea, PRB 79, 214409 (09)
  - Prosen, ea, JSM (09), P02035.
  - Jesenko, ea, PRB 84, 174438 (11)
  - Karrasch, ea, PRL 108, 227206 (12)
  - Karrasch, ea, PRB 87, 245128 (13)
  - Huang, ea, PRB 88, 115126 (13)
  - Karrasch, ea, PRB 88, 195129 (13)
  - Karrasch, ea, PRB 89, 075139 (14)
  - Karrasch, ea, PRB 90, 155104 (14)
- Master eqn
  - Bonfim, ea, PRL 69, 367 (92); PRL 70, 249 (93)
  - Znidaric, PRL 106, 220601 (11)
- Bosonization
  - Sirker, ea, PRL 103, 216602 (09)
  - Sirker, ea, PRB 83, 035115 (11)

$C_{jj}(\Delta=1)$ = zero / non-zero ~ 50 / 50

incomplete: ~ ×3

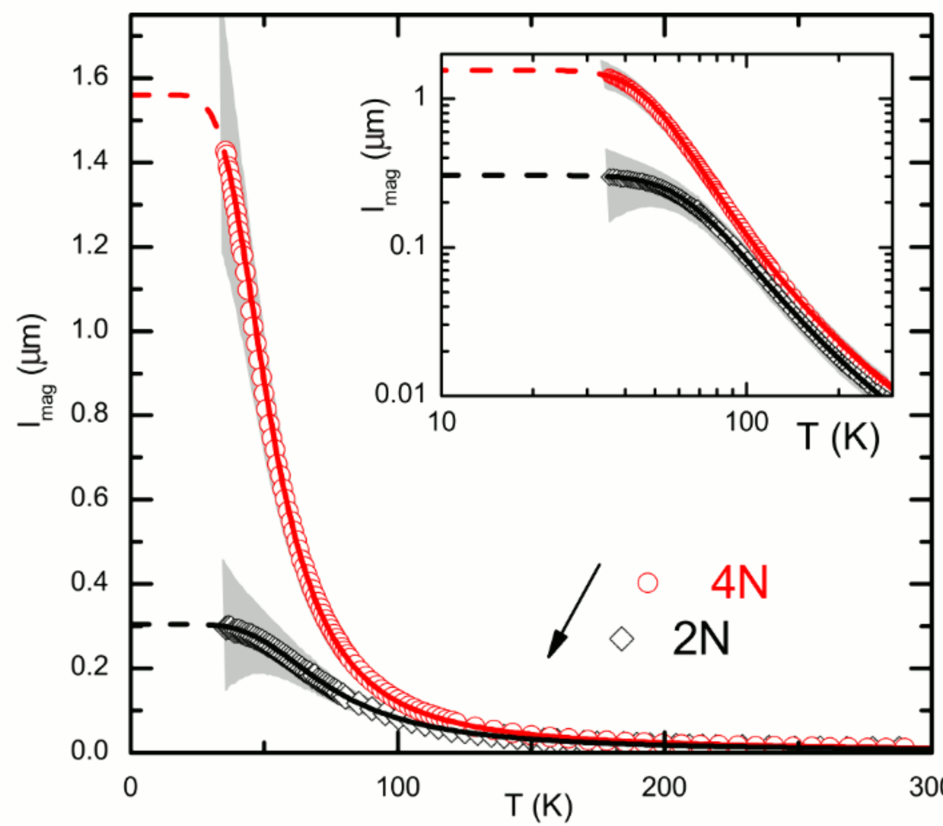
Heat Transport in Heisenberg Chains: Large Mean Free Paths

N. Hlubek, C. Hess, et al. PRB **81**, 020405R (2010)



~simple metals:
Cu, Ag @ 100K

- Purely magnetic mean free path

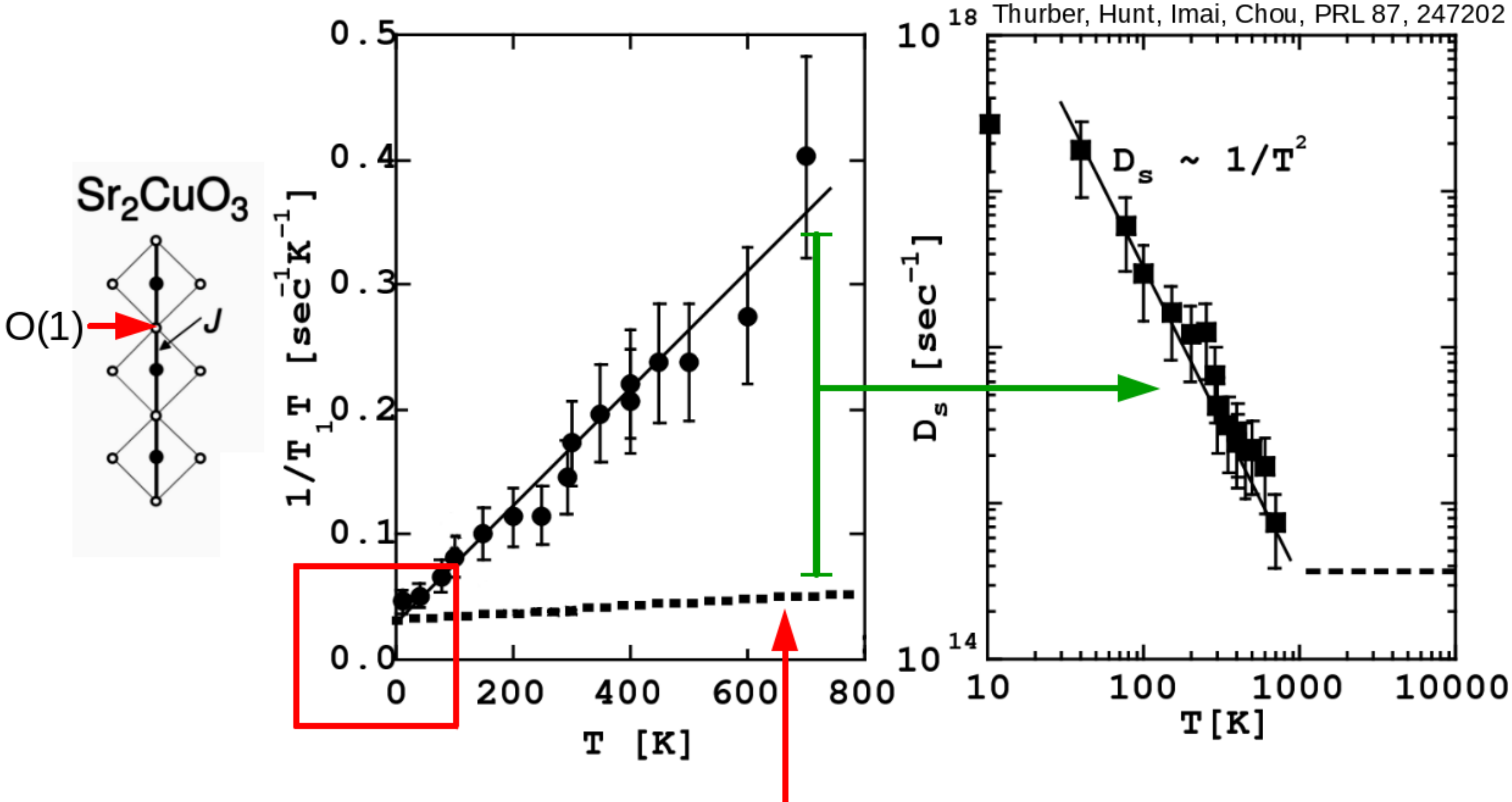


ballistic

Spin Transport in Heisenberg chains: indirect

- Indirect access of spin-current correlations: O(1)-NMR on Sr_2CuO_3

Thurber, Hunt, Imai, Chou, PRL 87, 247202 (2001)



T=0 ballistic + T≠0 diffusive

..., Sachdev, PRB 50, 13 006 (94), ...

Outline

- Magnetic transport in spin chains
- Quantum typicality
- High-T spin-Drude weight of the XXZ-chain
- Energy dissipation in the XXZ-chain: staggered fields
- Kitaev-XXZ-chain: connecting integrable points

break integrability

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break integrability

Quantum Typicality I

Goldstein, et al., PRL 96, 050403 (06)
Popescu, et. al., Nat. Phys. 2 (06)

- Concept: "properties" of a single pure state
  = "properties" of the full statistical ensemble

$$C(t) = \langle j(t) j \rangle = \frac{\mathrm{Tr}\{e^{-\beta H} j(t) j\}}{\mathrm{Tr}\{e^{-\beta H}\}} = \frac{\sum_n \langle n | e^{-\beta H} j(t) j | n \rangle}{\sum_n \langle n | e^{-\beta H} | n \rangle}$$

$$= \frac{\langle \psi | e^{-\beta H/2}\, j(t) j\, e^{-\beta H/2} | \psi \rangle}{\langle \psi | e^{-\beta H} | \psi \rangle} + E(|\psi\rangle)$$

random pure state $|\psi\rangle$

$$|\psi\rangle = \sum_{k=1}^{\dim} a_k |k\rangle$$

$$P(|a_k|^2) = N e^{-N|a_k|^2}$$

unitarily invariant distribution
~equipartition dim.-sphere surface

phase random $\in [0, 2\pi)$

$$E(|\psi\rangle) = O\left(\frac{\sqrt{\langle |j(t) j|^2 \rangle}}{\sqrt{\mathrm{Tr}\{e^{-\beta(H - E_0)}\}}} \right)$$

$\sqrt{d_{eff}}$: effective dimension

$\beta \to \infty$: $d_{eff} = 2^N$

Controlled
- draw several states
- increase dimension

Quantum Typicality II

- Rewrite

$$\left.\begin{array}{l} 1^{st} \text{ pure state: } |\Phi_\beta(t)\rangle = e^{-iHt-\beta H/2}|\psi\rangle \\ 2^{nd} \text{ pure state: } |\varphi_\beta(t)\rangle = e^{-iHt} j e^{-\beta H/2}|\psi\rangle \end{array}\right\} \qquad C(t) = \frac{\langle\Phi_\beta(t)|\, j\, |\varphi_\beta(t)\rangle}{\langle\Phi_\beta(0)|\Phi_\beta(0)\rangle} + E$$

- Numerical gain
  - exact diagonalization unnecessary
  - time & temperature dependence generated by eg. Runge-Kutta
  - memory required for only 2 states and j, H sparse matrices

increase Hilbert-space dimensions

- by several orders of magnitude w.r.t ED
- without restrictions

current dim ~10^{10} = ~33...36 spins
increase ~ 10^4

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- … in pursuit since 1990[1]: is $\bar{C}_S(\beta=0)$ for the isotropic Heisenberg chain finite?

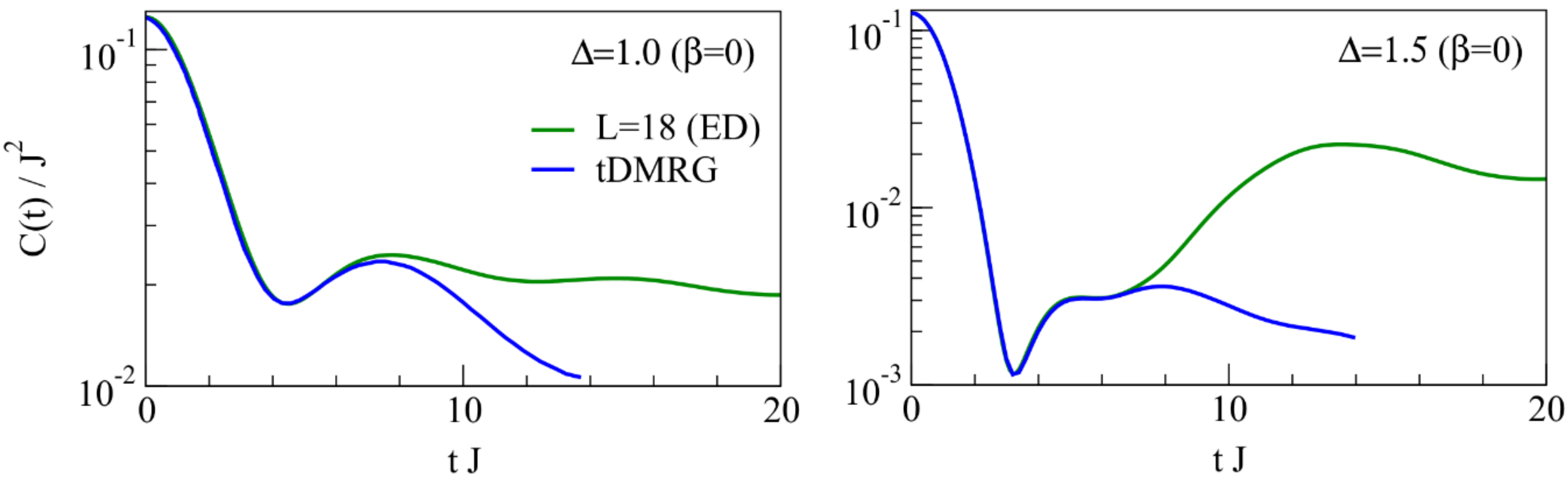
[1] Shastry, Sutherland, PRL 65, 243 (90)
+ ~85 papers up to 2015

BA ↯ ED ↯ tDMRG ↯ QMC...

$$H=J\sum_l \left(S_l^x S_{l+1}^x + S_l^y S_{l+1}^y + \Delta S_l^z S_{l+1}^z\right)$$

Quantum typical way

isotropic point | above isotropic point

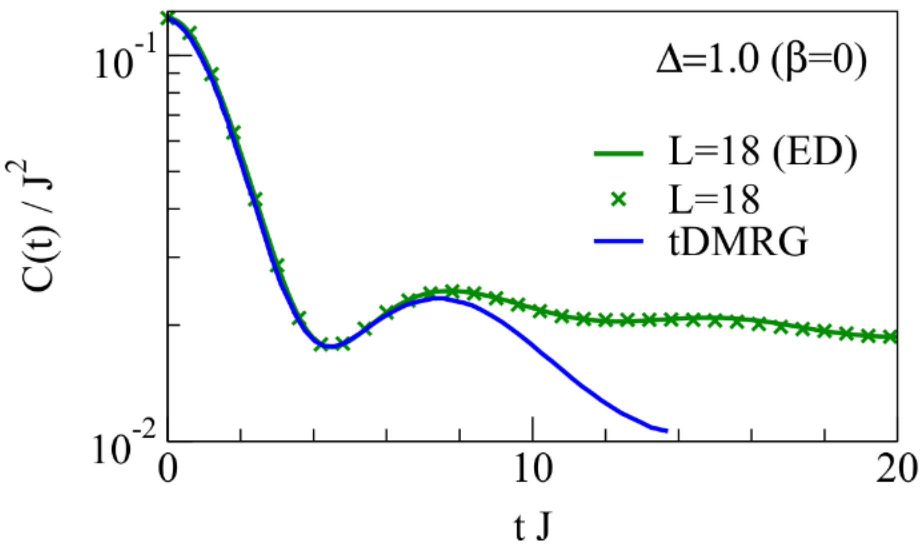


- ED cannot reproduce tDMRG

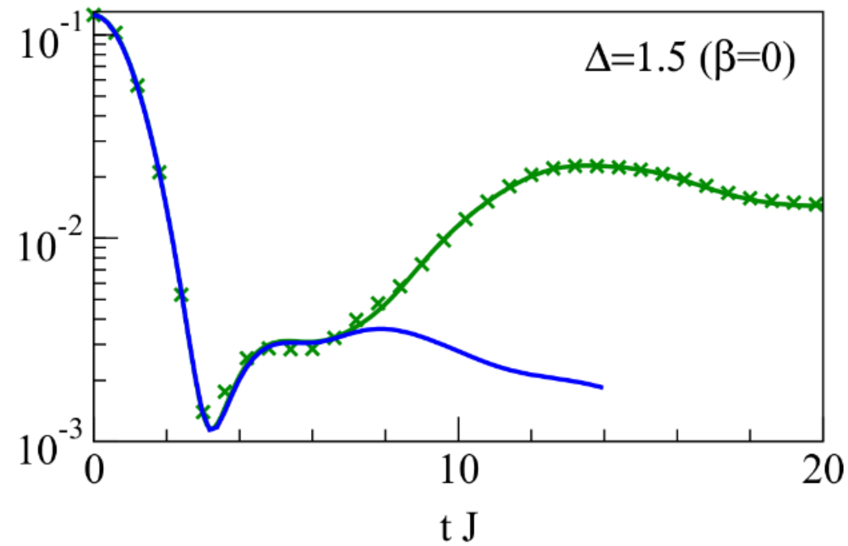
tDMRG data: courtesy of Karrasch, Heidrich-Meisner, Moore, et al. PRL 108, 227206 (12), PRB 87, 245128 (13), 89, 075139 (14)

Quantum typical way

isotropic point



above isotropic point

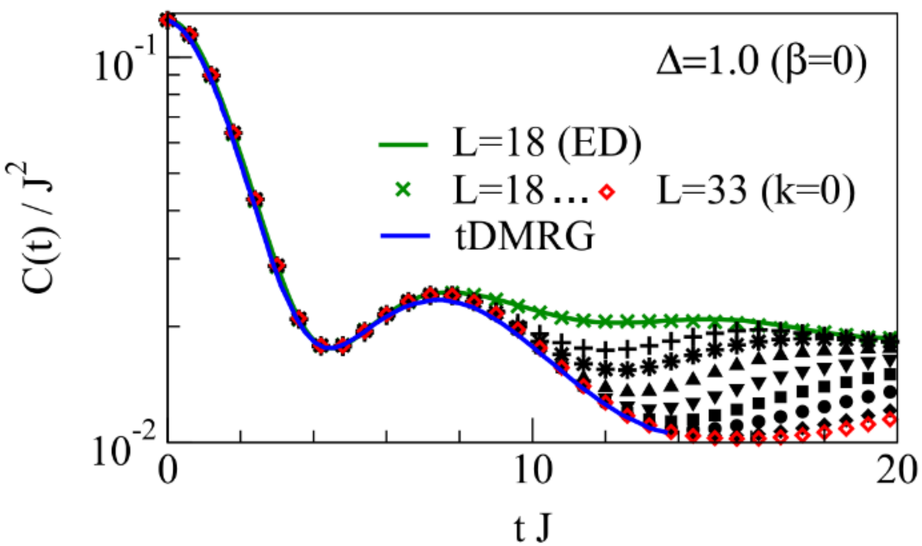


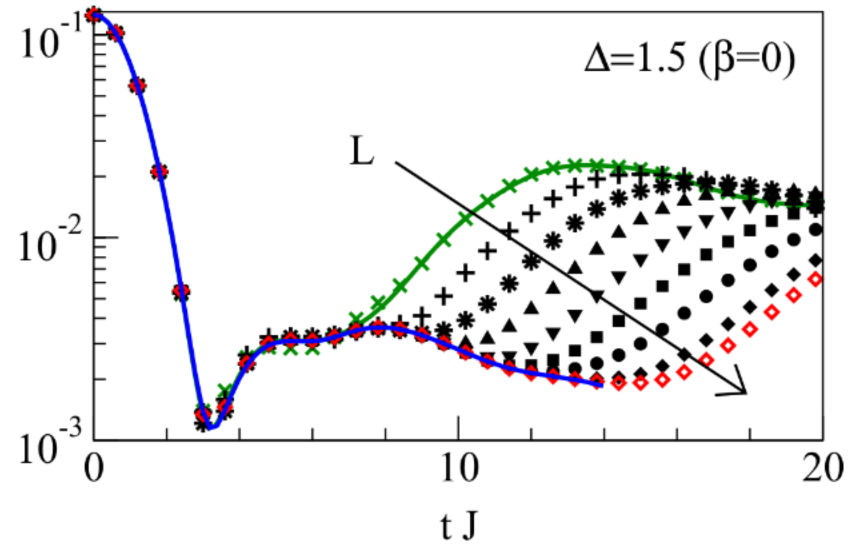
- single pure state reproduces ED
- need 'small' systems to observe error
- less interaction ↔ larger error
- (error can be reduced by average over small number of pure states)

Quantum typical way

isotropic point

above isotropic point

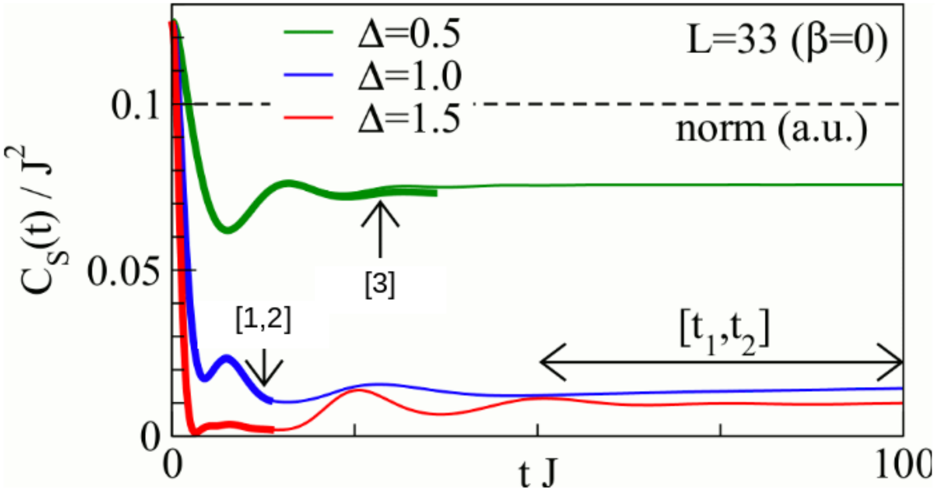




- single pure state reproduces tDMRG
- proof of concept for QTY
- note log scale

Long Time Limit

- below and above isotropic point



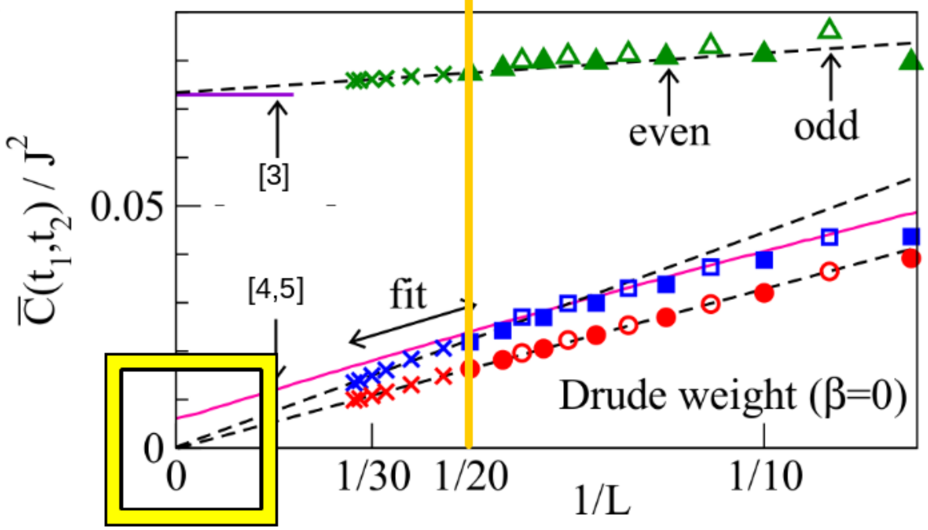
- norm = const. → RK4 works
- long time limit: not reached by tDMRG
- long time limit: finite size cotrolled
- define Drude weight

$$D := \frac{1}{t_2 - t_1}\int_{t_1}^{t_2} C(t)\,dt = \overline{C}(t_1, t_2)$$

[1] Karrasch, et al., PRL 108, 227206 (12)
[2] " PRB 89, 075139 (14)
[3] Karrasch, et al. PRB 90, 155104 (14)

full ρ ED

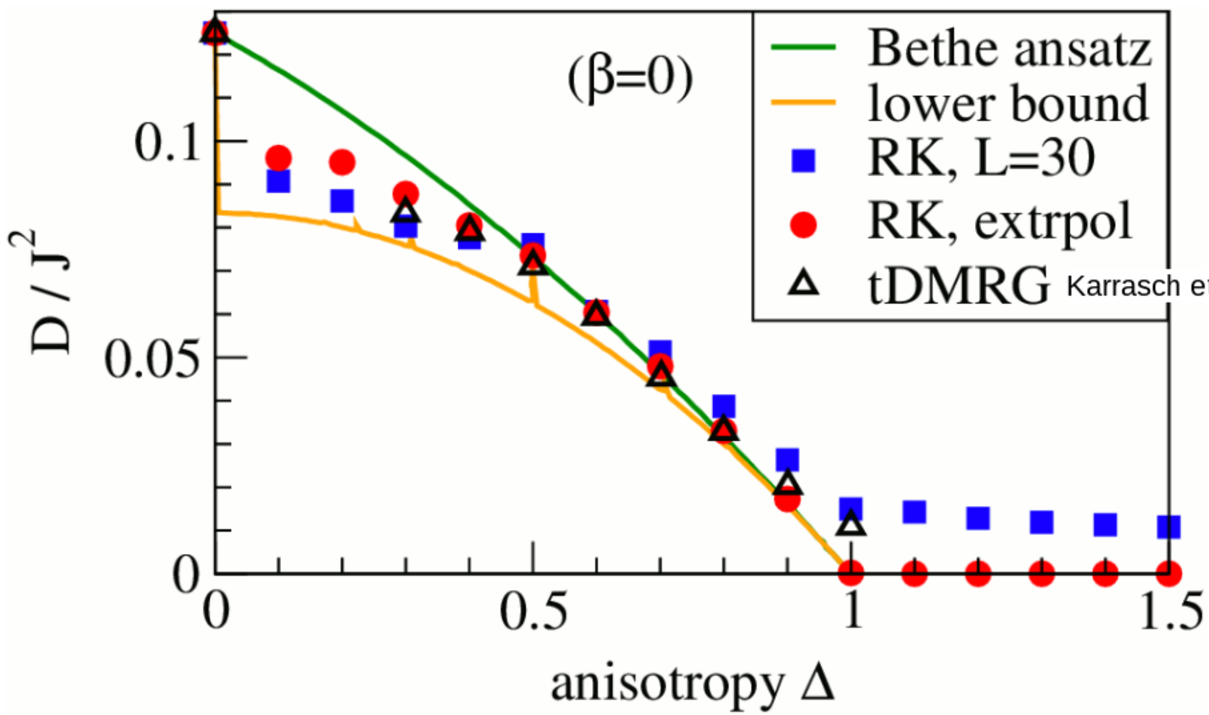
- Drude weight: finite size scaling



- D for L ≤ 20, full ρ; for L > 20 single state
- 1/L fits to 20 ≤ L ≤ 33
- Δ=1.0 the odd-site fit L ≤ 19 [4,5]
- Δ=0.5 analytic lower bound [3]

[3] Prosen, et al., PRL 106, 217206 (11)
" ibid. 111, 057203 (13)
[4] Heidrich-Meisner, WB, et al. PRB 68, 134436 (03)
[5] Karrasch, et al., PRB 87, 245128 (13)

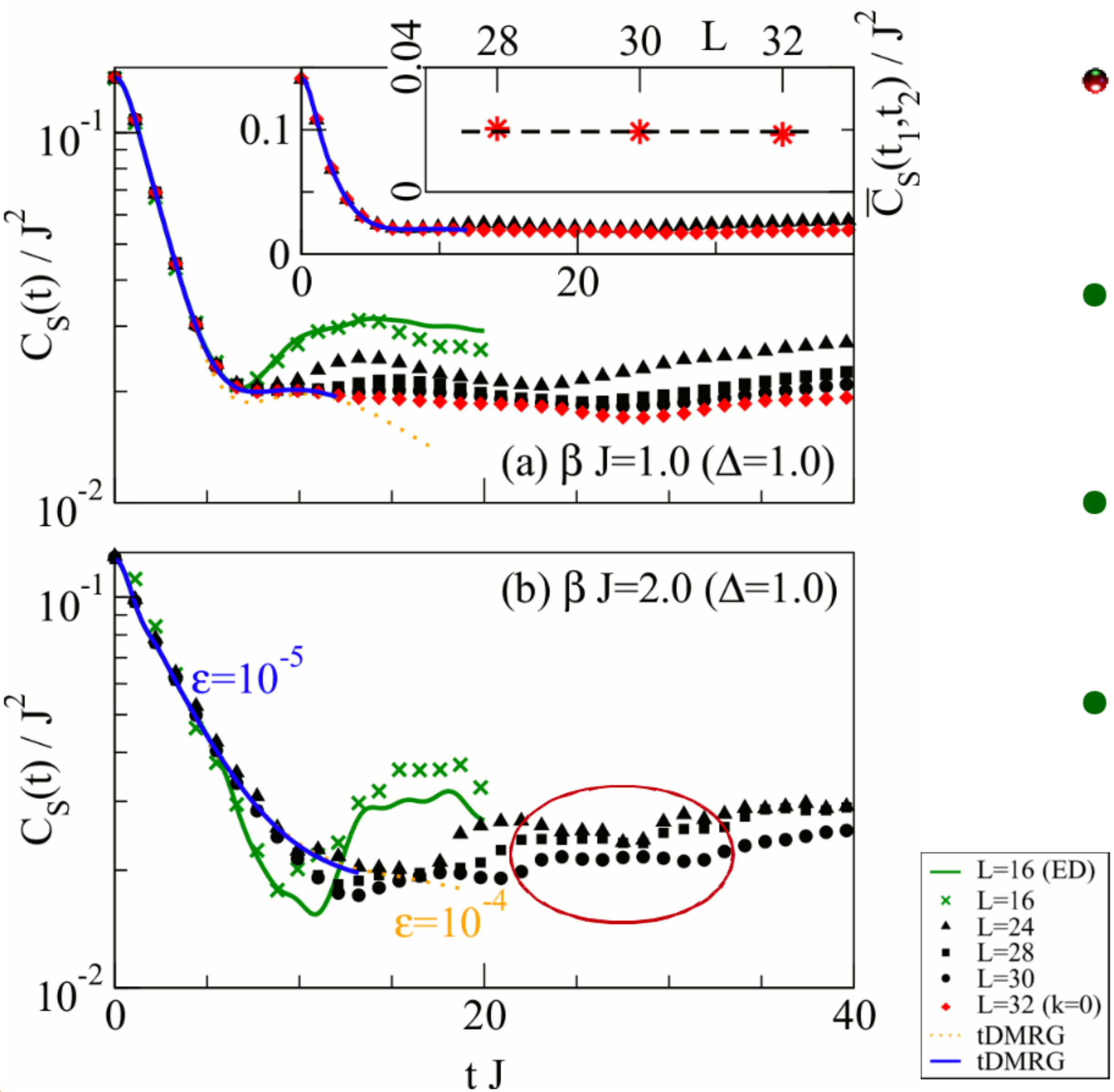
Drude Weigth vs. Anisotropy



Karrasch et al., PRL 108, 227206 (12)

- All extrapolated values above rigorous lower bound — Prosen, et al., PRL 106, 217206 (11); ibid. 111, 057203 (13)
- $0.4 \lesssim \Delta \leq 1.5$: agree with Bethe-ansatz — Zotos, PRL 82, 1764 (99)
- $\Delta \lesssim 0.4$: still above lower bound but below Bethe-ansatz
  $\leftrightarrow$ high degeneracy at small Δ

Lower Temperatures



- limiting condition:

  $1 \ll d_{eff} = e^{-\beta(H-E_0)} \propto 2^L$

- single pure state reproduces intermediate temperature tDMRG … if $T \gtrsim J$
- finite $\bar{C}_S(\beta=1)$ consistent with upper bounds from

  Carmelo, et al., arXiv:1407.0732 (14)

- Lower T potentially require pure state averaging

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- Case of energy current dissipation: study dc conductivities

$$H = J\sum_l (S_l^x S_{l+1}^x + S_l^y S_{l+1}^y + \Delta S_l^z S_{l+1}^z) + B\sum_l (-)^l S_l^z$$

$$[j_E, H] \neq 0$$

tDMRG avail.

Huang, et al., PRB 88 115126 (13)
Karrasch, et al., PRB 88 195129 (13)

- Perturbation theory DC rates: memory functions

$$T\kappa_E(z) = \frac{i\chi}{z - \underbrace{M(z)/\chi}_{=\gamma(z)}}$$

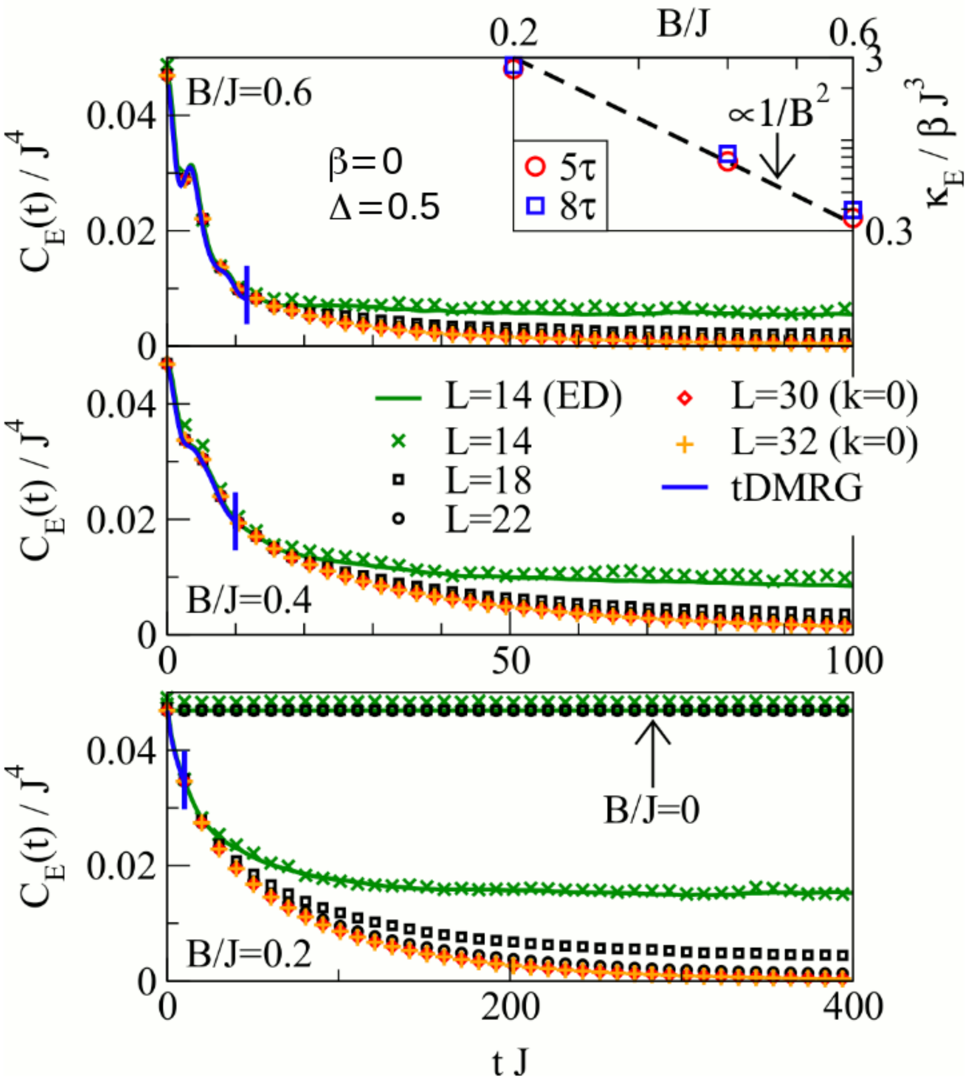
$=\gamma(z)$ relaxation rate

- $\gamma(z)$: $z \to 0$ (Markov), $B \ll 1, \Delta$, and $T \gg 1, \Delta, B$

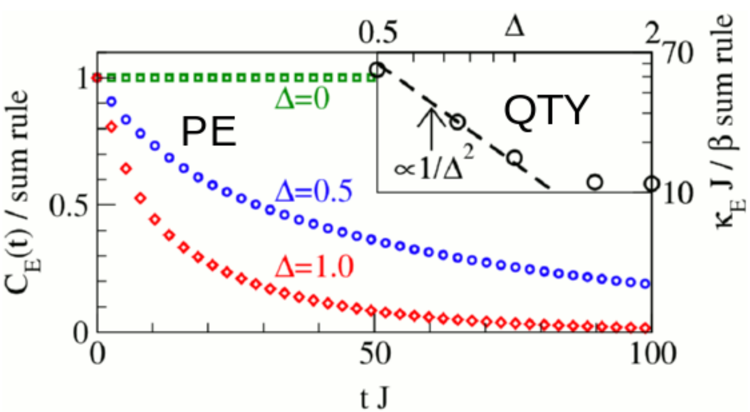
$$\gamma = \underbrace{\frac{1}{\langle j_E^2 \rangle}}_{\propto (1+2\Delta^2)} \int_0^\infty dt\, \langle \overbrace{i[j_E, H_B]}^{\propto \Delta B}(t)\, i[j_E, H_B]\rangle \quad \propto \frac{(\Delta B)^2}{1+2\Delta^2}$$

force-force correlation

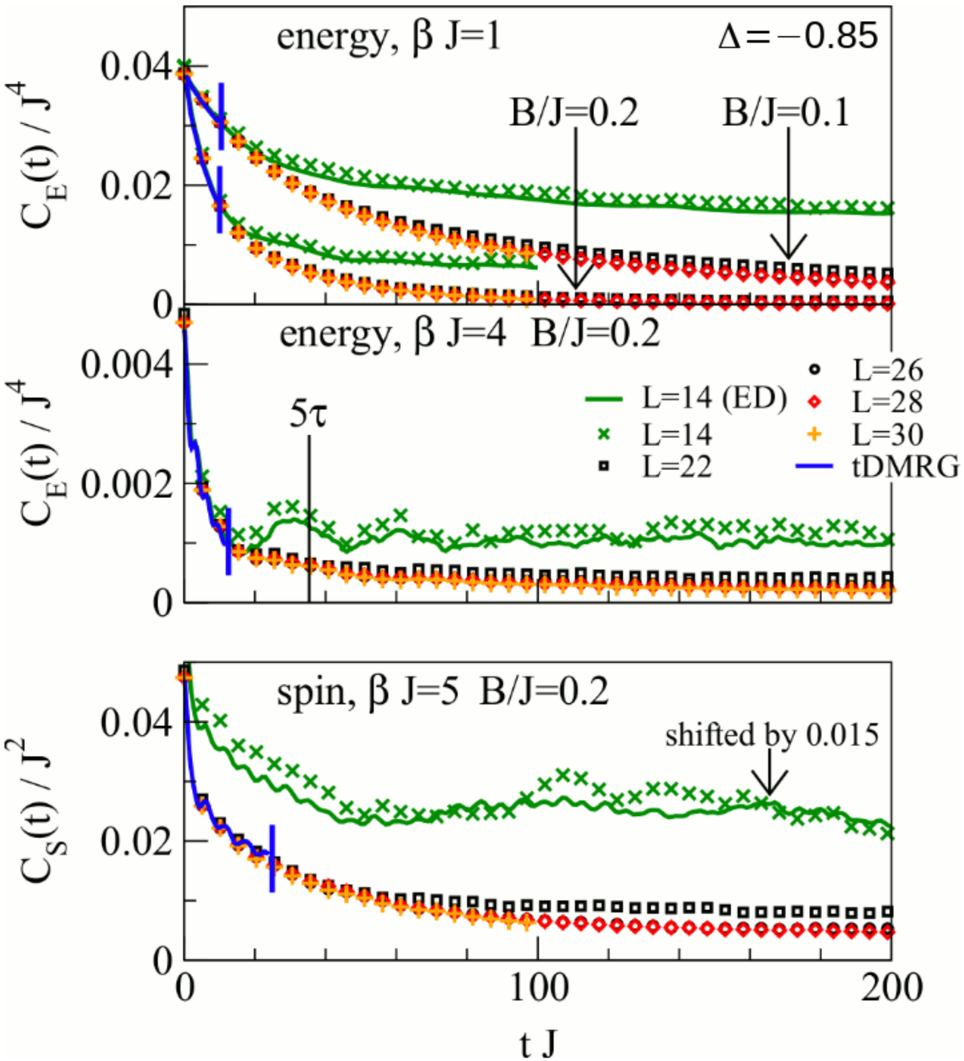
Energy Current Decay at β=0



- j_E not conserved: $[j_E, H] \sim \Delta B$
  → κ_E finite. Perturbation theory: $\kappa_E \propto (1+2\Delta^2)/(B\Delta)^2$
- ED agrees well with QTY
- QTY: ~no finite size effects N>22
  cut-off t sufficient
- tDMRG available only up to short times: agrees with ED & QTY



Spin and Energy Current Decay at finite T

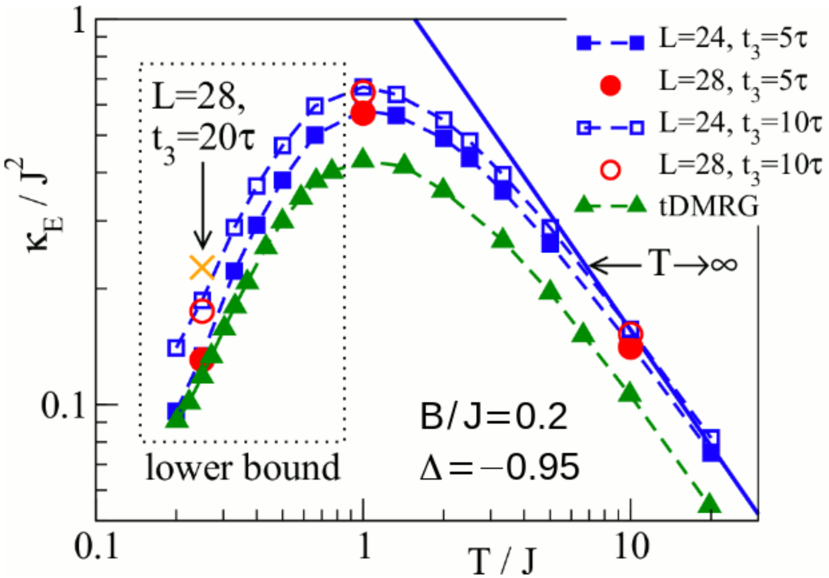


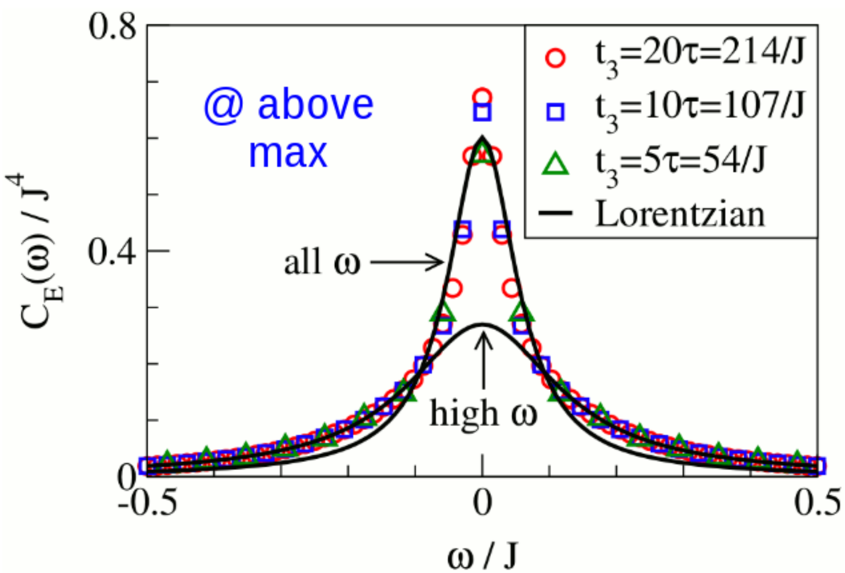
- even for rather small T, QTY for small L=14 still ~ED
- Again: ED & QTY reproduce tDMRG already for L=14 & T>0.2
- Again: QTY ~no finite size effects N>22, & cut-off t sufficient

⇓

Extract finite-T dc conductivities

T-Dependence of dc Energy Conductivity





- trivially for T≫J: $\kappa_E \sim 1/T$
- broad max at T∼J
- for T≲J: cut-off t cannot be reached
  $\kappa_{E,fig.}$ = lower bound
- at T≪J: power law?, exponent ≲1.4 ?
- tDMRG underestimate = no finite size effect: cut-off t too small

- frequency domain
  - low-ω sensitive to cut-off t
  - line shape not Lorentzian: no simple Drude behavior

tDMRG: Huang, et al., PRB 88 115126 (13)

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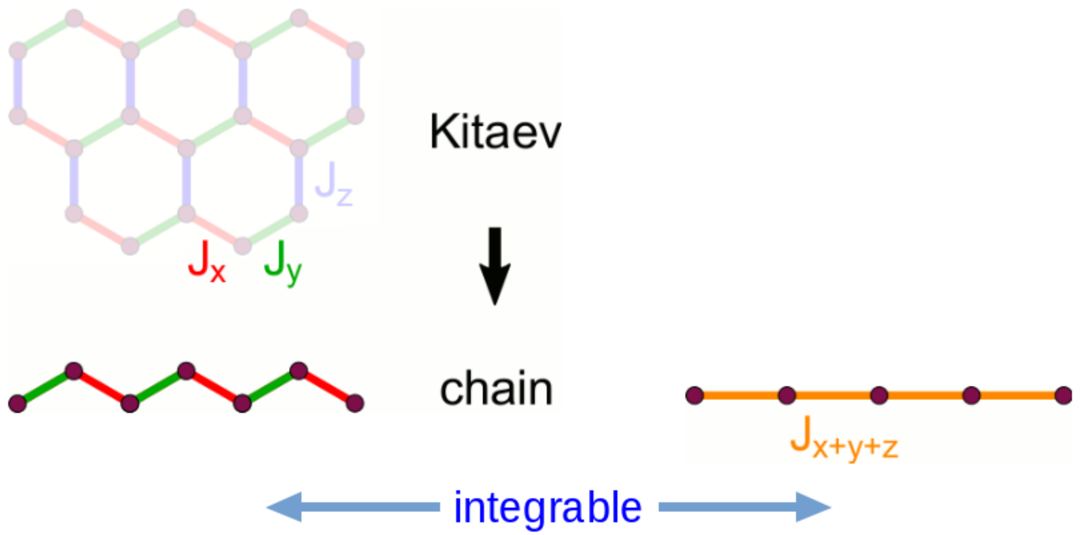


Kitaev chain

$$H=\sum_{l=1}^{L/2}\left(J_1 S^x_{2l-1} S^x_{2l} + J_2 S^y_{2l} S^y_{2l+1}\right)$$

$S^z_{2l} S^z_{2l+1}$ Z_2 invar.

Saket, ea, PRB 87, 174414 (2013)

$J_1 \neq J_2$ SOP

Feng, ea, PRL 98, 087204 (07)

- spectrum at Kitaev point: p-wave SC

$$H=\sum_{k=0}^{\pi/2}\left(\epsilon_{k,+} c_k^+ c_k + \epsilon_{k,-} d_k^+ d_k\right)$$

$$\epsilon_{k\pm}=\pm\frac{1}{2}\sqrt{J_1^2+J_2^2+2J_1 J_2 \cos 2k}$$

Kitaev chain

$$H=\sum_{l=1}^{L/2}\left(J_1 S^x_{2l-1}S^x_{2l}+J_2 S^y_{2l}S^y_{2l+1}\right)$$

$$=\sum_{l=1}^{L/2} h_l$$

two-site
energy density

energy (no spin) current

$$q\, j_q=[H,h_q]$$

- Infinite temperature energy-current autocorrelation of bare Kitaev chain

$$C_{J_1=J_2}(\omega)=\frac{J_1^4}{128}\delta(\omega)$$

Drude weight

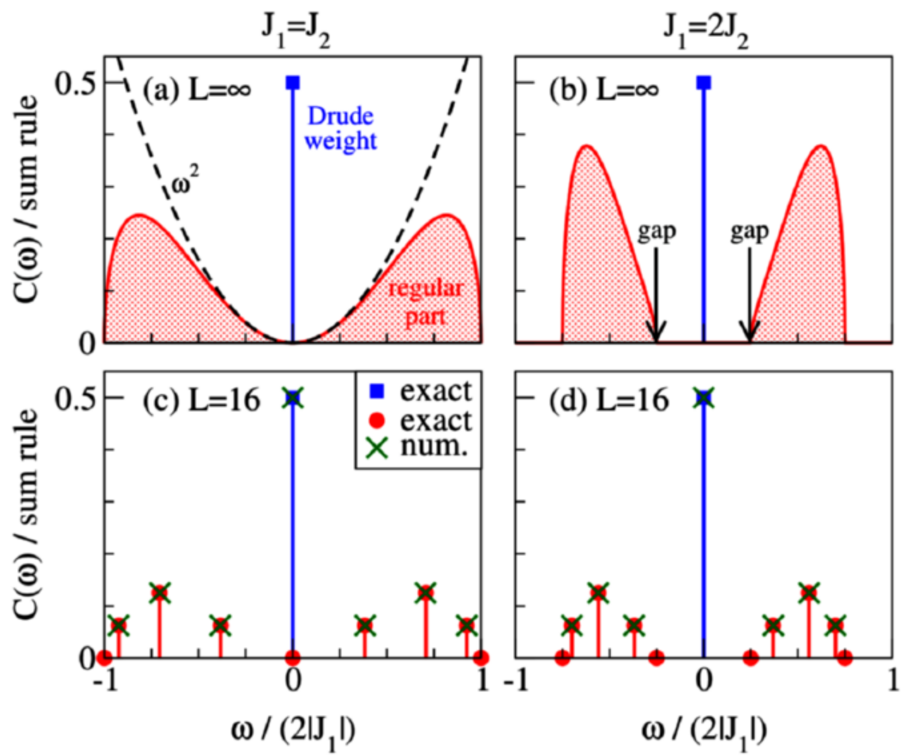
$$+\frac{J_1^3}{32\pi}\left(\frac{\omega}{2J_1}\right)^2\sqrt{1-\left(\frac{\omega}{2J_1}\right)^2}$$

regular part ~ ω^2

- spectrum at Kitaev point: p-wave SC

$$H=\sum_{k=0}^{\pi/2}\left(\epsilon_{k,+}c_k^+c_k+\epsilon_{k,-}d_k^+d_k\right)$$

$$\epsilon_{k\pm}=\pm\frac{1}{2}\sqrt{J_1^2+J_2^2+2J_1J_2\cos 2k}$$



Kitaev-Heisenberg chain

- 4 parameter model

$$H=\sum_{l=1}^{L/2}\left(J_1 S^x_{2l-1} S^x_{2l}+J_2 S^y_{2l} S^y_{2l+1}\right)$$

$$+H_{HSB(J_3,\Delta)}+B\sum_l^L S^z_l=\sum_{l=1}^{L/2} h_l$$

two-site
energy density

energy (no spin) current

$$q\, j_q=[H,h_q]$$

- Infinite temperature energy-current autocorrelation of bare Kitaev chain

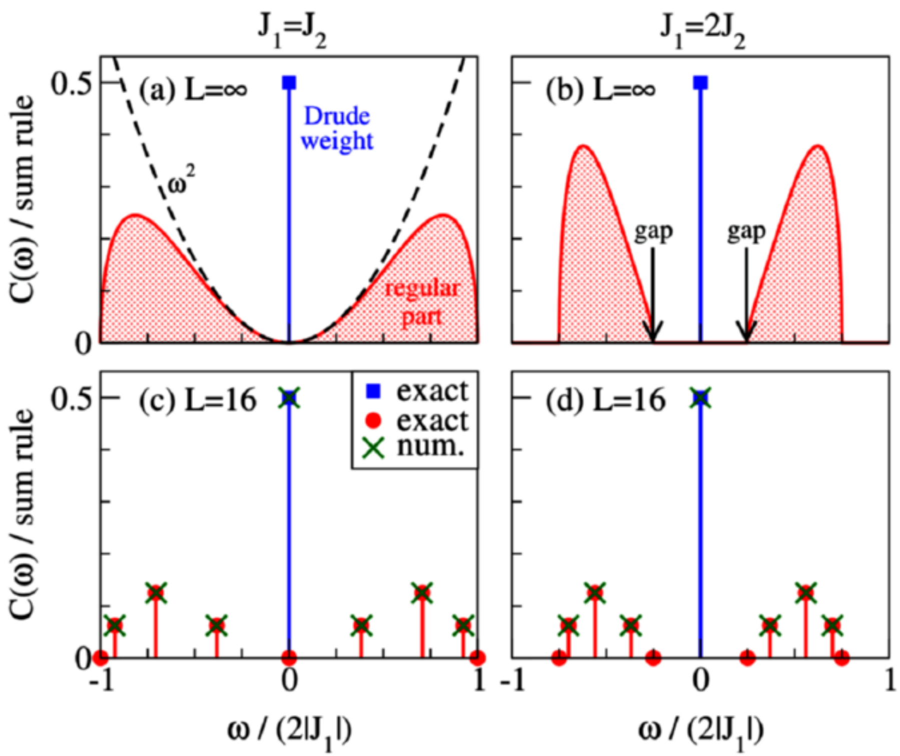
$$C_{J_1=J_2}(\omega)=\frac{J_1^4}{128}\delta(\omega)$$ Drude weight

$$+\frac{J_1^3}{32\pi}\left(\frac{\omega}{2J_1}\right)^2\sqrt{1-\left(\frac{\omega}{2J_1}\right)^2}$$ regular part $\sim \omega^2$

- spectrum at Kitaev point: p-wave SC

$$H=\sum_{k=0}^{\pi/2}\left(\epsilon_{k,+}c_k^+c_k+\epsilon_{k,-}d_k^+d_k\right)$$

$$\epsilon_{k\pm}=\pm\frac{1}{2}\sqrt{J_1^2+J_2^2+2J_1J_2\cos 2k}$$



Kitaev-Heisenberg chain

- Two addtl. integrable points

  $J_1=J_2=0, \quad J_1=J_2=-2J_3$

  Chaloupka, Jackeli, Khaliullin, PRL 105, 027204 (10)

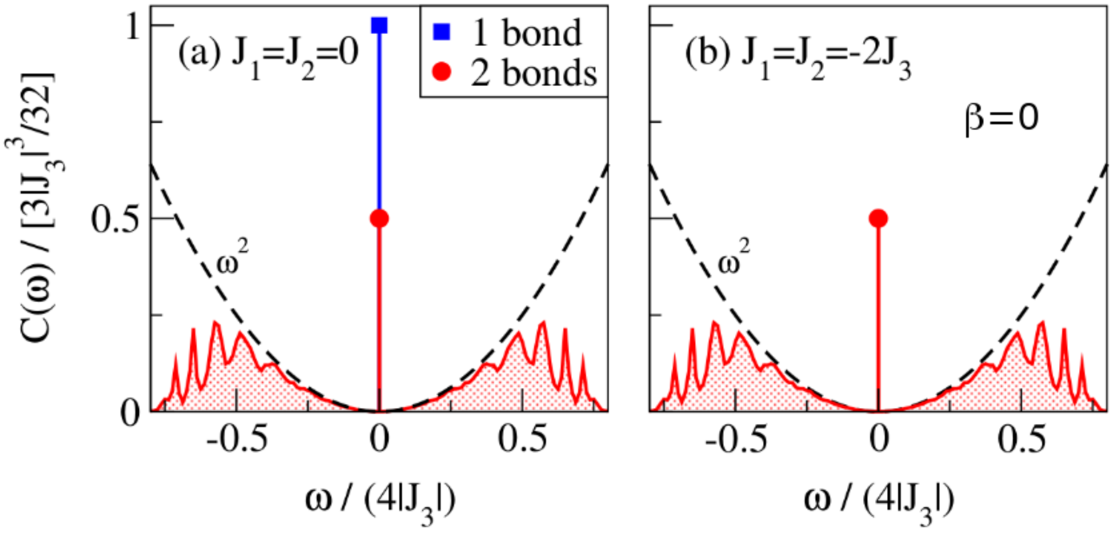
  spectra agree

- Suppression of low-ω weight at all integrable points

  $C(\omega\to 0)\sim\omega^2$

  Herbrych, et al. PRB 86, 115106 (12)

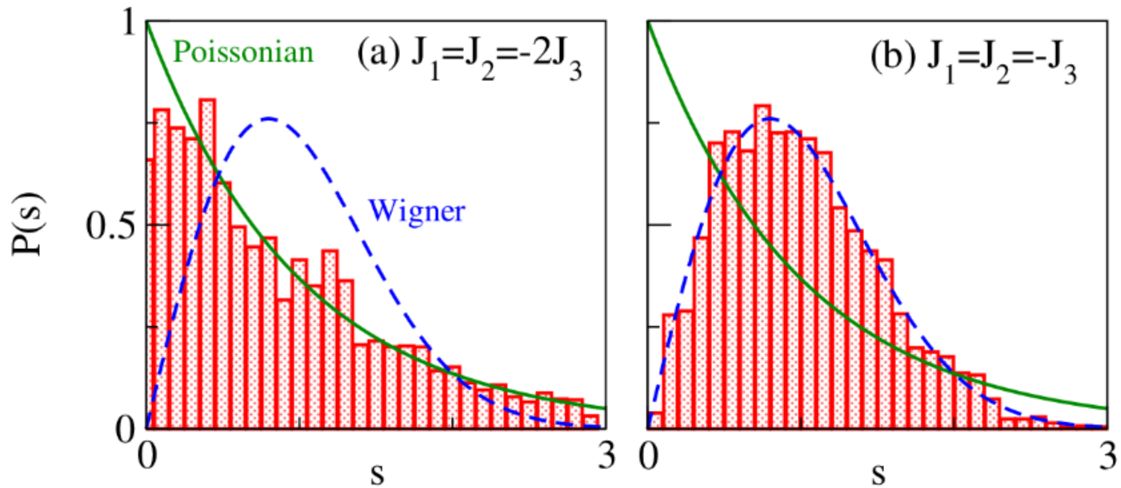
  ! 1 vs. 2 site unit cell



- Integrable points and quantum chaotic regions

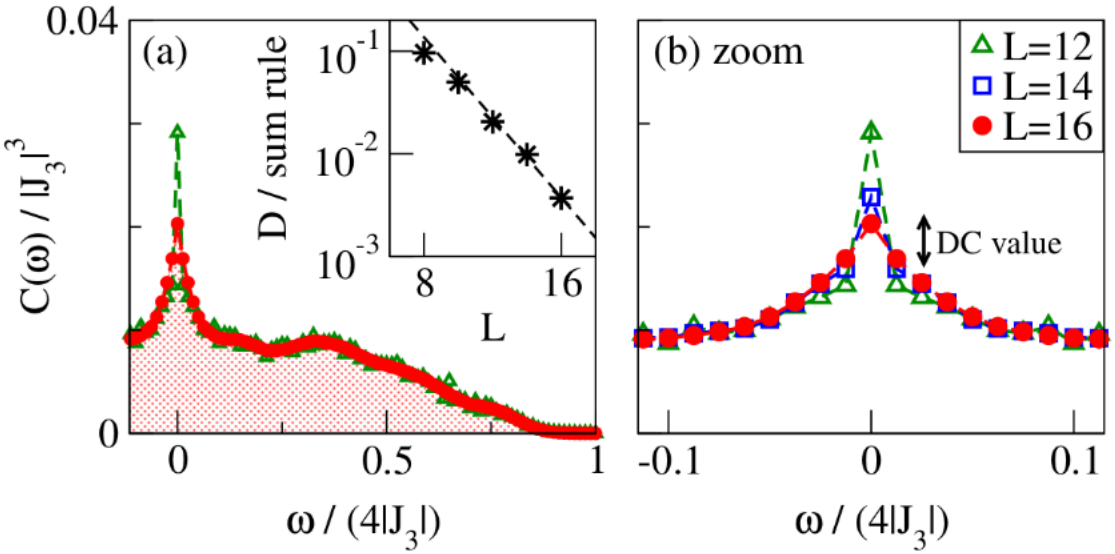
  level-spacing distribution
  Poisson @ integrable vs.
  Wigner @ non-integrable

  Rabson, ea, PRB 69, 054403 (04)
  Modak, ea, PRB 90, 075152 (14)

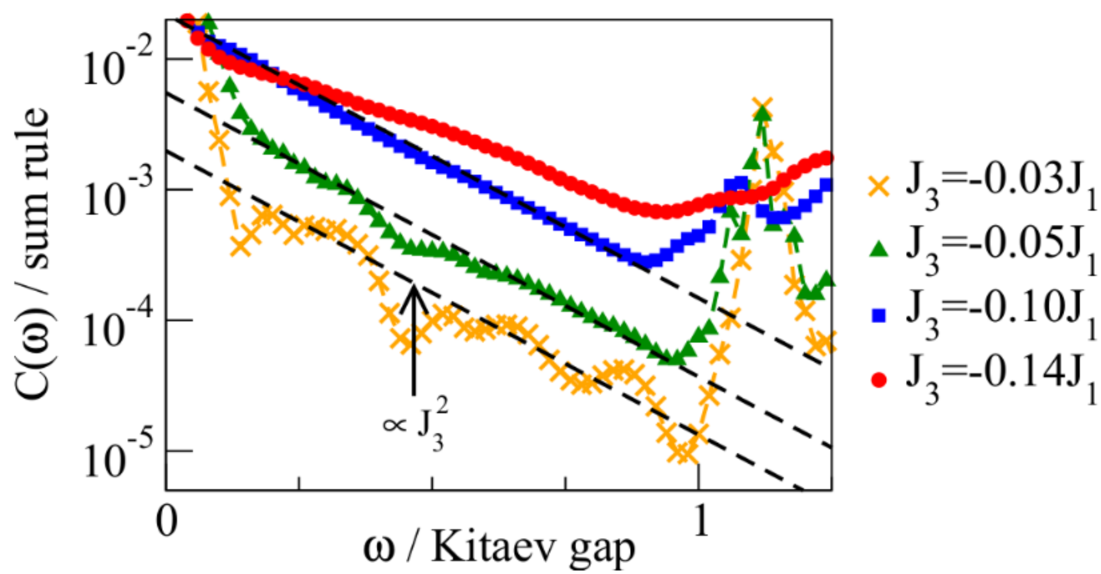


Kitaev-Heisenberg chain

- Off integrability $J_1 = J_2 = -J_3$
  - $\omega \neq 0$: $C(\omega) \neq f(L)$
  - $\omega = 0$: $D \sim e^{-L}$
  - peak at ~0: broadened Drude (width ↗ with Δ)
  - weak remnants of $\sim\omega^2$

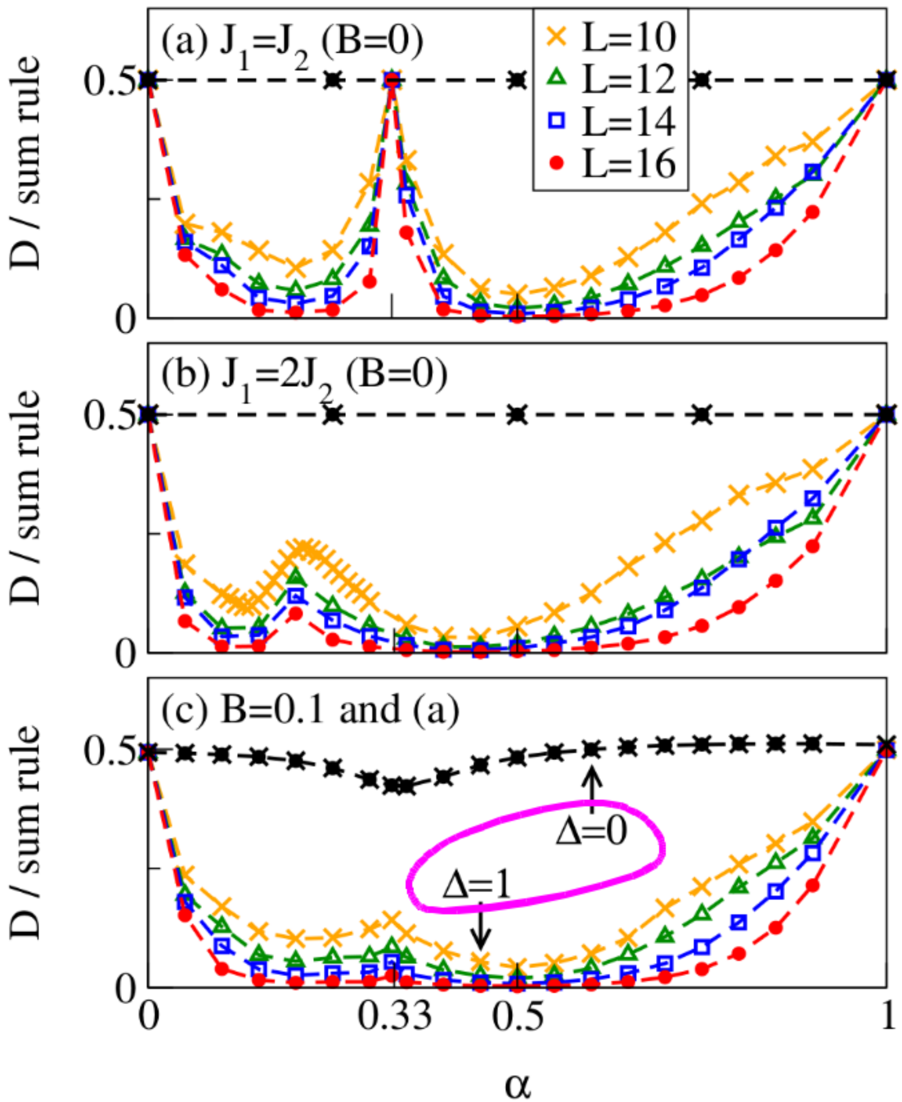


- Off integrability $J_1 = 2J_2$
  - signatures of topological gap even at $\beta = 0$
  - for $-J_3 \gtrsim 0.14\, J_1$ high-T in-gap excits. $\sim J_3^2$ ↔ perturb. theor.

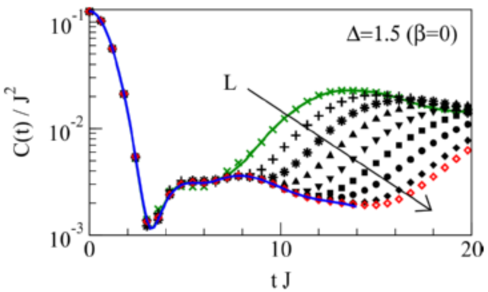


Drude weight survey

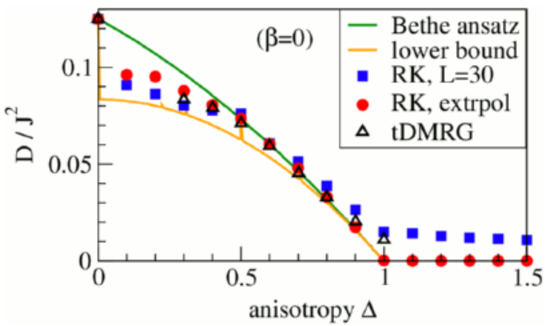
- $J_3=\alpha,\ \ J_1=\alpha-1$ and $J_2=J_1(/2)$
  - $J_2=J_1$ Kitaev $\alpha=0$
    Heisenberg $\alpha=1$
    3rd intgr. pt. $\alpha=1/3$
  - for $\Delta=0$ interpolate between free Majorana and free XY fermions
  - for $0.4\lesssim\alpha\lesssim0.7$ and $0.1\lesssim\alpha\lesssim0.2$ clearly $D\to0$ as $N\to\infty$
  - D smallest at $\alpha=1/2$
  - $\alpha=1/3$ pt. shifted at $J_1\neq J_2$
  - $\alpha=1/3$ extremely sensitive to magnetic fields



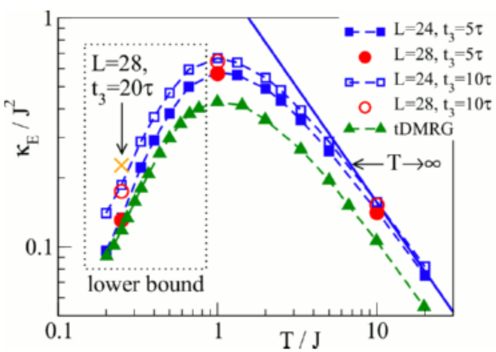
Conclusions



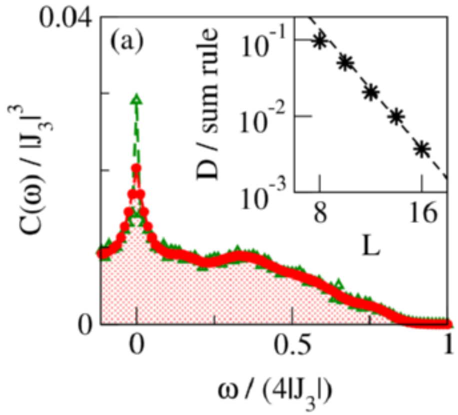
- new numerical tool: QTY



- XXZ: $D(\Delta=1,\beta=0)=0$



- low-T XXZ stagg. fields: $\kappa_E \propto T^{\sim 1.4}$



- Kitaev-XXZ: dissipative, pseudogap