Quantum mechanical probability distributions in and out of equilibrium

Fabian Essler (Oxford)

EPSRC Engineering and Physical Sciences Research Council

Osaka, September 2019

Characterizing Quantum Many-Body Systems

Complete description given by many-body state/wave-function

$$\Psi(x_1, x_2, \ldots, x_N, t) = \langle x_1, \ldots, x_N | \Psi(t) \rangle$$

In practice: typically measure particular expectation values

$$\langle \Psi | \mathcal{O}(x,t) | \Psi \rangle \qquad\qquad \langle \Psi | \mathcal{O}_1(x,t) \mathcal{O}(x',t') | \Psi \rangle$$

Averages over many measurements.

A lot more info in the **probability distribution** of a given observable $\mathcal{O}$ in a QM state $|\Psi\rangle$

$$P_{\mathcal{O}}(m) = \langle\Psi|\delta(\mathcal{O}-m)|\Psi\rangle = \sum_n |\langle n|\Psi\rangle|^2\delta(\lambda_n - m)$$

$$\mathcal{O}|n\rangle = \lambda_n|n\rangle$$ eigenstates of O

For this to be interesting $\mathcal{O}$ should have many distinct eigenvalues

Why should we care about these quantities?

Cf talks this morning by BD & JMS

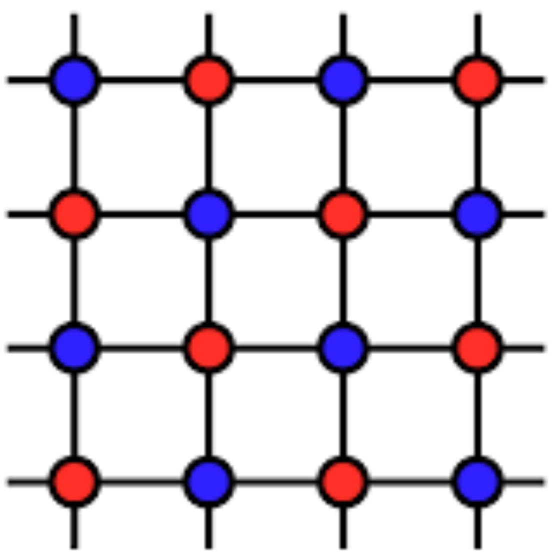
- They can be interesting and **universal**
- They are measured in cold atom experiments

Cold Atom Experiments

Probability distribution of staggered magnetization for 2D Hubbard model at finite temperature

Greiner group '17

$$H = -t \sum_{\langle j,k\rangle,\sigma=\uparrow,\downarrow} c^\dagger_{j,\sigma} c_{k,\sigma} + \text{h.c.} + U \sum_j c^\dagger_{j,\uparrow} c_{j,\uparrow} c^\dagger_{j,\downarrow} c_{j,\downarrow}$$



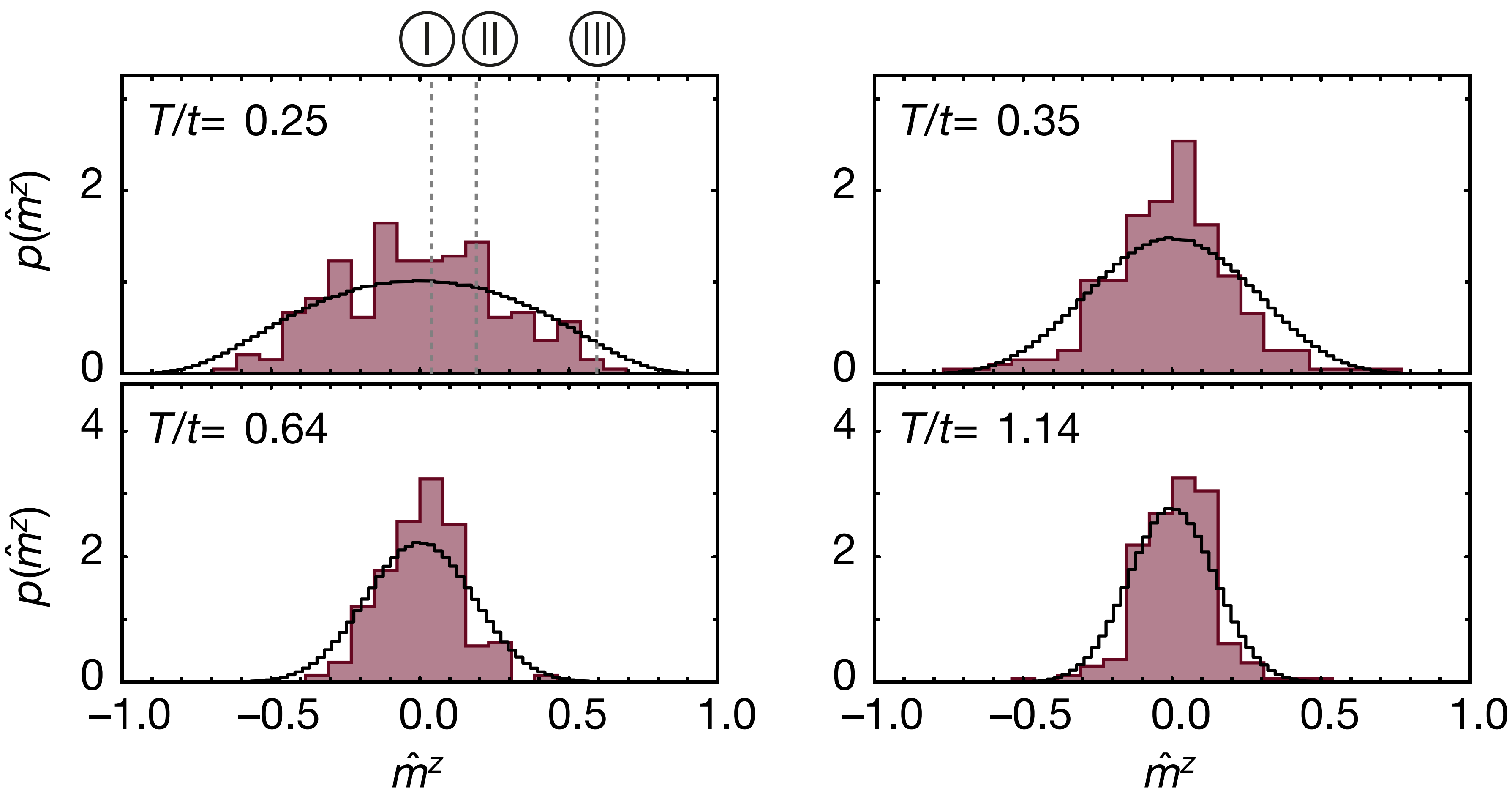
● sublattice A

● sublattice B

$$\hat{m}^z = \frac{2}{N^2}\left[\sum_{j\in A} S^z_j - \sum_{j\in B} S^z_j\right]$$

$$2S^z_j = c^\dagger_{j,\uparrow} c_{j,\uparrow} - c^\dagger_{j,\downarrow} c_{j,\downarrow}$$

- Initialize system in some initial state
- Measure m^z
- Repeat



Other examples :

Probability distribution of "relative phase" in split 1D Bose gases

Schmiedmayer group
'10–'17

Few results available in the literature for such quantities:

(homogeneous systems, no currents)

- $\int_0^\ell dx\; e^{i\Phi(x)}$ in Luttinger liquid

  Gritsev/Altman/Demler/Polkovnikov '06
  Kitagawa et al '10

- total magnetization in GS of critical Ising QFT

  Lamacraft/Fendley '08

- some numerics for GS of XXZ

  Moreno-Cardoner et al '16

- GS of Haldane-Shastry

  Stephan/Pollmann '17

- total transverse magnetisation in GS of TFIM & related free fermion problems

  Cherng & Demler '07
  Ivamov&Abanov'13
  Klich '14...

What to expect on "general grounds" ?

We consider

- lattice models;
- observables $\mathcal{O}$ (quantized eigenvalues) that act on sub-systems of linear size ℓ, e.g. sub-system magnetization;

Need ℓ to be large-ish s.t. $\mathcal{O}$ has many distinct eigenvalues

In states with finite correlation length ξ and $\xi \ll \ell$ we expect

$$P_{\mathcal{O}}(m) = \langle \Psi | \delta(\mathcal{O} - m) | \Psi \rangle = \sum_r P_w(r) \delta(m - r)$$

narrow, ≈ Gaussian

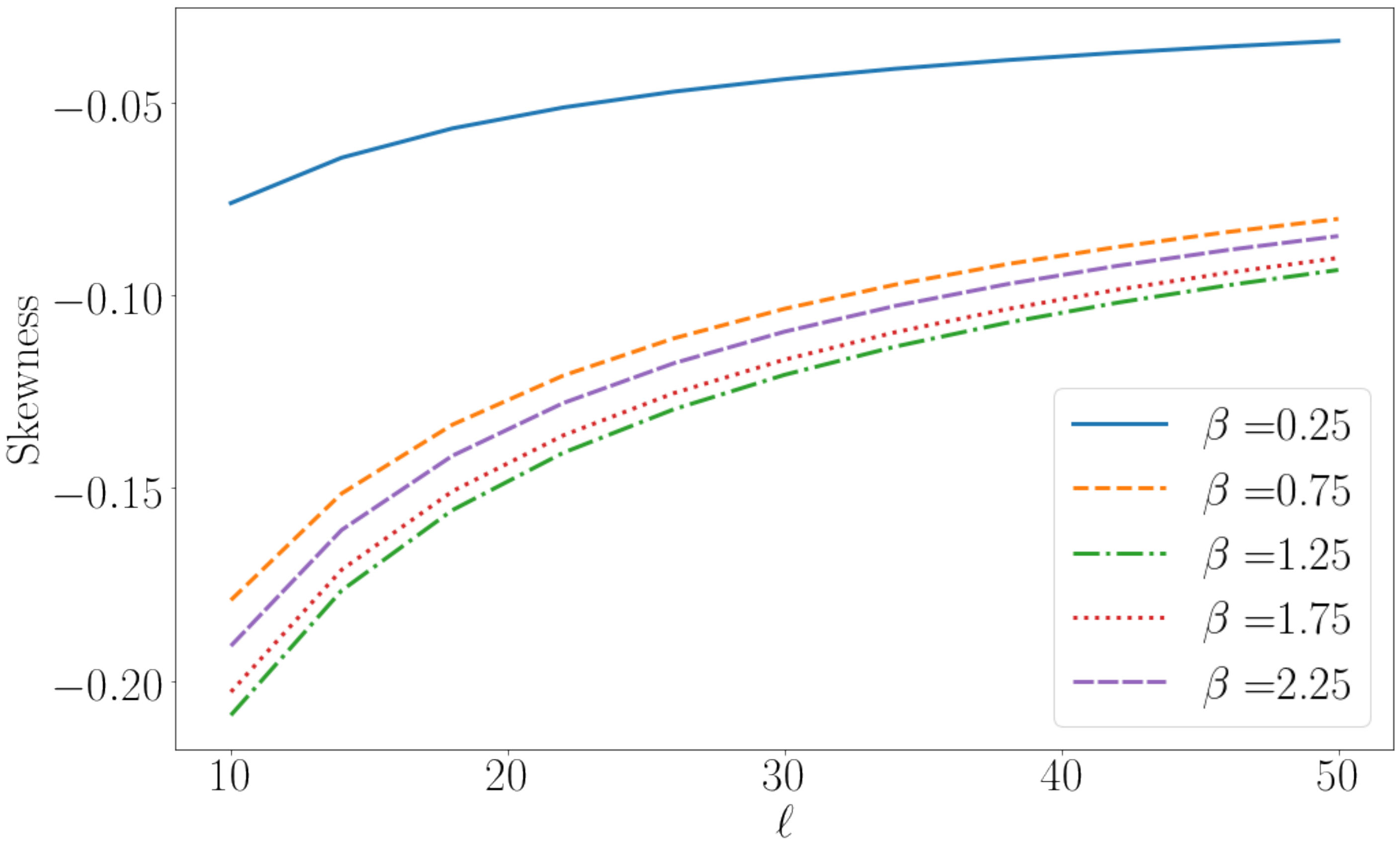
("thermodynamics")

Cases with $\xi \to \infty$ or $\xi \gtrsim \ell$ will be most interesting.

Subsystem magnetisation in the transverse field Ising chain at T>0

$$S^z_u(\ell) = \sum_{j=1}^{\ell} \sigma^z_j$$

$$P^{(u)}(m) = \mathrm{Tr}\left[\rho(\beta)\ \delta(m - S^z_u(\ell)\right] = 2\sum_{r\in\mathbb{Z}} P^{(u)}_w(r)\delta(m-2r) \qquad (\ell \text{ even})$$



$$\left\langle \left[\frac{X}{\sqrt{\langle X^2\rangle_\beta}}\right]^3 \right\rangle_\beta$$

$$X = S^z_u(\ell) - \langle S^z_u(\ell)\rangle_\beta$$

h=0.5 J

Higher cumulants behave in the same way.

Part I: FCS in equilibrium at a quantum critical point

Ground state of critical spin-1/2 XXZ chain

Collura, FHLE &Groha '17

$$H = J \sum_{j=1}^{L} S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta\, S_j^z S_{j+1}^z$$

$-1<\Delta\leq 1$

$$\Delta = -\cos(\pi\eta)$$

Quasi-long-range **AFM** order in the xy-plane

for $|n|\gg 1$

e.g. Lukyanov '97

$$\langle \mathrm{GS}|S_{j+n}^x S_j^x|\mathrm{GS}\rangle = (-1)^n \frac{A}{4n^\eta}\left(1 - \frac{B}{n^{4/\eta-4}}\right) - \frac{\tilde{A}}{4n^{\eta+1/\eta}}\left(1 + \frac{\tilde{B}}{n^{2/\eta-2}}\right) + \ldots\ ,$$

$$\langle \mathrm{GS}|S_{j+n}^z S_j^z|\mathrm{GS}\rangle = -\frac{1}{4\pi^2\eta n^2}\left(1 + \frac{\tilde{B}_z}{n^{4/\eta-4}}\frac{4-3\eta}{2-2\eta}\right) + (-1)^n \frac{A_z}{4n^{1/\eta}}\left(1 - \frac{B_z}{n^{2/\eta-2}}\right) + \ldots$$

N.B. Slowest decay close to **ferro**magnet $\Delta\approx -1$!

Subsystem Magnetization

smooth

$$S^{\alpha}(\ell) = \sum_{j=1}^{\ell} S_j^{\alpha} \,,$$

staggered

$$\boxed{N^{\alpha}(\ell) = \sum_{j=1}^{\ell} (-1)^j S_j^{\alpha}}$$

Focus on this

Probability distribution:

$$P_N^{\alpha}(m,\ell) = \langle \mathrm{GS}|\delta\big(N^{\alpha}(\ell) - m\big)|\mathrm{GS}\rangle = \int_{-\infty}^{\infty} \frac{d\theta}{2\pi} e^{-i\theta m} \boxed{\underbrace{\langle \mathrm{GS}|e^{i\theta N^{\alpha}(\ell)}|\mathrm{GS}\rangle}_{F_\ell^{\alpha}(\theta)}}$$

Characteristic function

$$P_N^{\alpha}(m,\ell) = \begin{cases} \sum_{r\in\mathbb{Z}} \widetilde{F}_\ell^{\alpha}(r)\ \delta(m-r) & \text{if } \ell \text{ is even,} \\ \sum_{r\in\mathbb{Z}} \widetilde{F}_\ell^{\alpha}(r+\frac{1}{2})\ \delta\big(m-r-\frac{1}{2}\big) & \text{if } \ell \text{ is odd.} \end{cases}$$

Universality

$$F_\ell^\alpha(\theta) = \sum_{n=0}^{\infty} \frac{(i\theta)^n}{n!} \boxed{\langle \mathrm{GS}| \big(N^\alpha(\ell)\big)^n |\mathrm{GS}\rangle}$$

moments are not universal (shown using bosonization)

But **ratios** $\dfrac{\left\langle \, (N^\alpha(\ell))^{2n} \, \right\rangle}{\left\langle \, (N^\alpha(\ell))^{2} \, \right\rangle^n}$ are!

"Rescaled" generating function is universal:

$$\boxed{\langle \mathrm{GS}| e^{i\theta' N^\alpha(\ell)} |\mathrm{GS}\rangle} \; , \qquad \theta' = \frac{\theta}{\sqrt{\langle \mathrm{GS}| \big(N^\alpha(\ell)\big)^2 |\mathrm{GS}\rangle}}$$

Have studied $F_\ell(\theta)$ by a combination of numerical (iTEBD) and analytic (exact field theory, free fermion, 2-loop RG) methods.

Field theory approach based on

Low-energy field theory

$$\mathcal{H}(\Delta) = \frac{v}{2}\int dx \left[K(\partial_x\theta)^2 + \frac{1}{K}(\partial_x\phi)^2\right]$$

Lattice spin operators

$$S_j^z \simeq -\frac{a_0}{\sqrt{\pi}}\partial_x\phi(x) + (-1)^j c_1 \sin(\sqrt{4\pi}\phi(x)) + \dots,$$

$$S_j^x \simeq b_0(-1)^j \cos\left(\sqrt{\pi}\,\theta(x)\right) + ib_1 \sin\left(\sqrt{\pi}\,\theta(x)\right)\sin\left(\sqrt{4\pi}\phi(x)\right) + \dots$$

Characteristic function

$$F_\ell^x(\theta) \approx \left\langle 0 \right| e^{-i\theta\frac{b_0}{a_0}\int_0^\ell dx\ \cos\left(\sqrt{\pi}\phi(x)\right)} \left| 0 \right\rangle$$

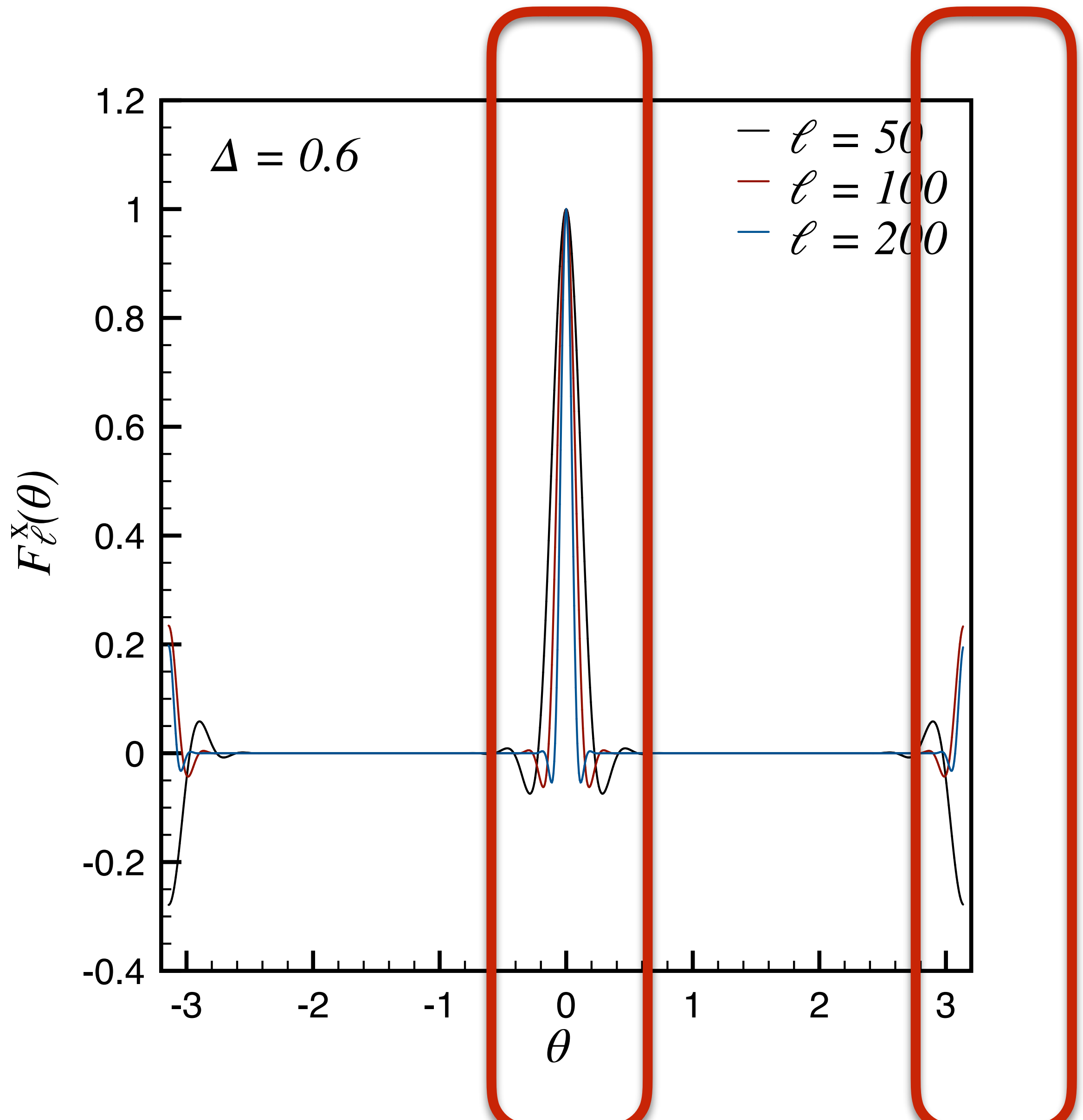
Related to partition fn of boundary-sine-Gordon model

Bazhanov, Lukyanov, Zamolodchikov '01

Results for Staggered Subsystem Magnetizations

A. Transverse component

$$F_\ell^x(\theta) = \langle \mathrm{GS} \,|\, e^{i\theta \sum_{j=1}^{\ell} (-1)^j S_j^x} \,|\, \mathrm{GS} \rangle$$

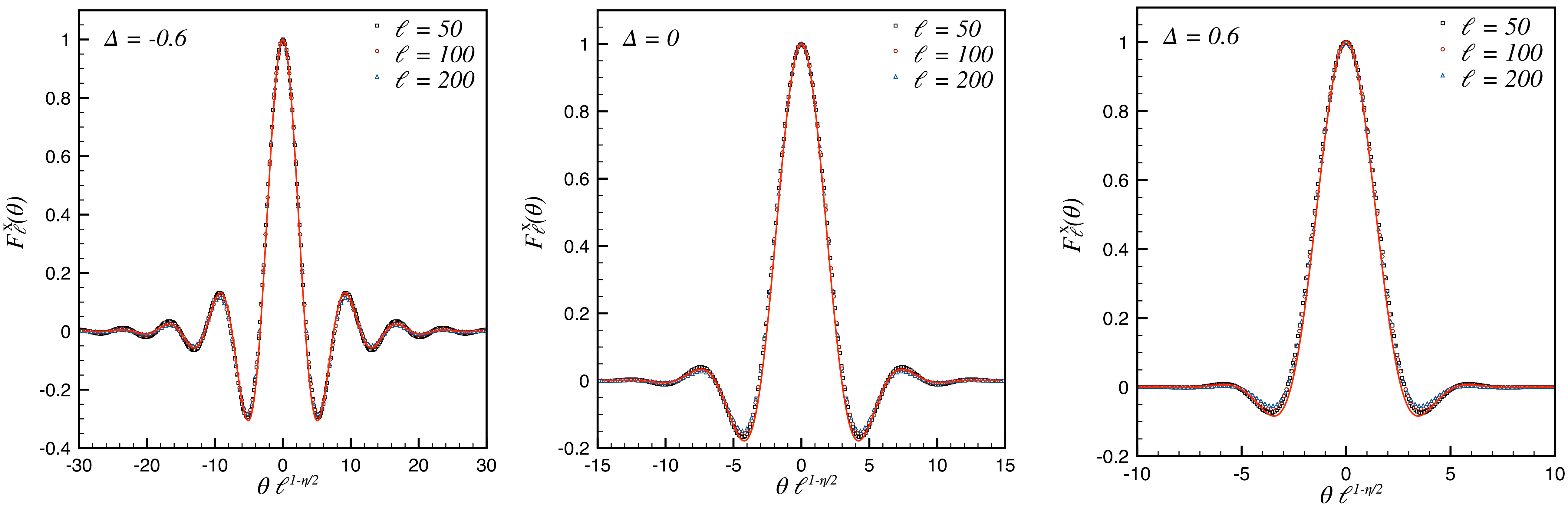


very small
except at θ≈0,π

Observe **scaling collapse** around θ=0,π:

Scaling collapse around θ≈0:

$$F^x_\ell(\theta) = F^x(\theta\ell^{1-\eta/2})$$



Red lines: exact field theory results using BSG mapping.

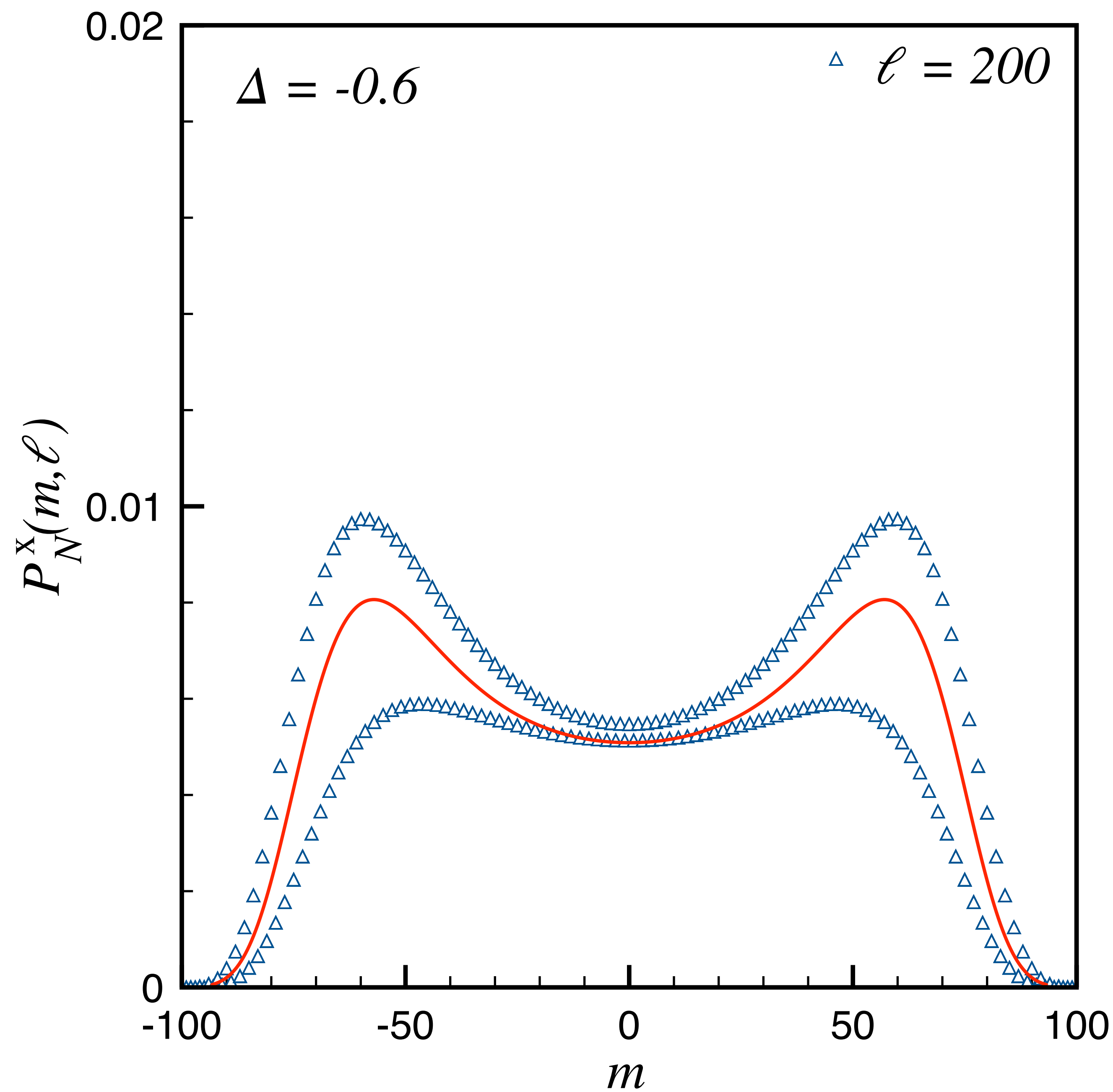
Similar scaling collapse around θ≈π (subleading contribution)

Probability distribution:

- small
- broad
- bimodal

- even/odd effect in m
- even/odd effect in ℓ

go away for large ℓ



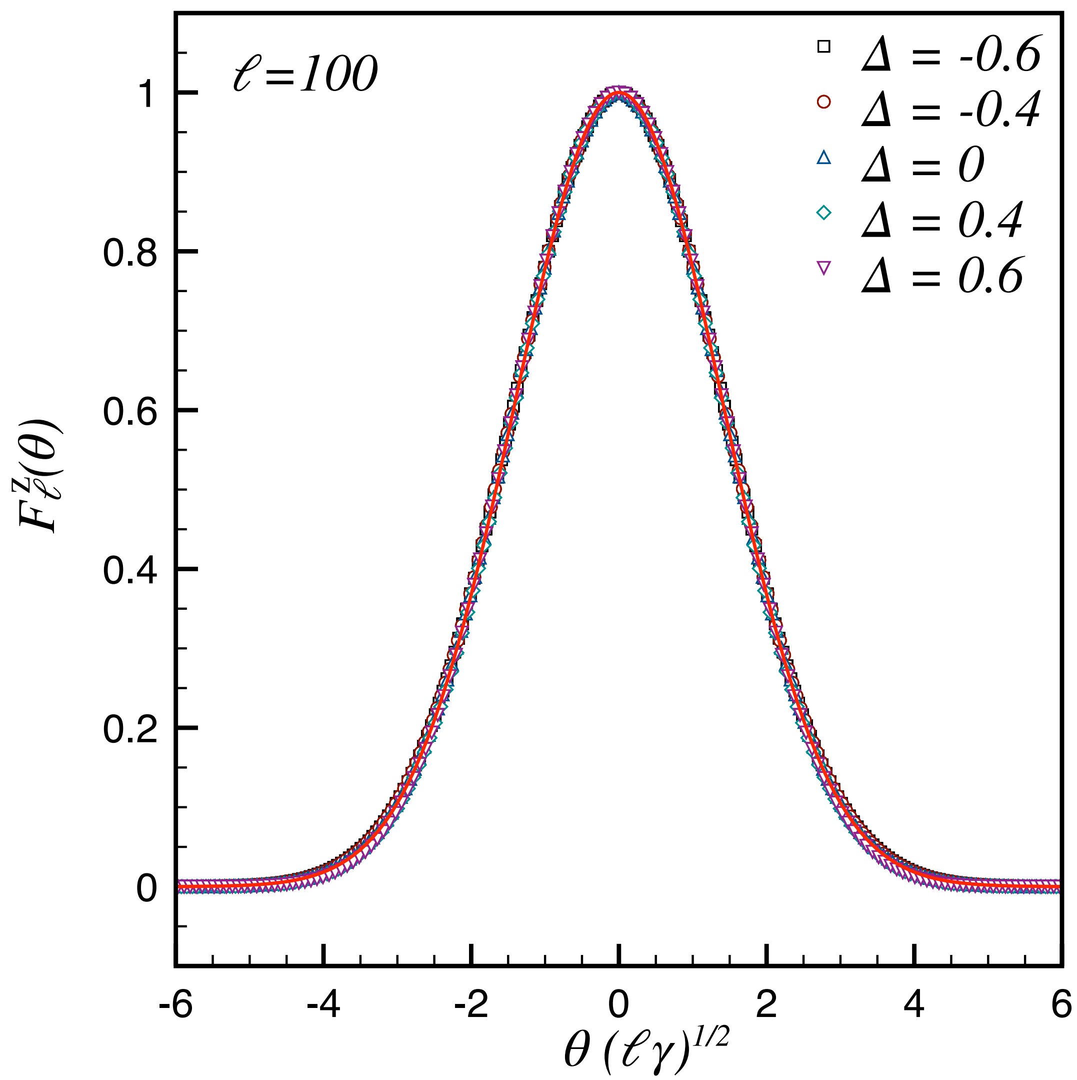
$$P_N^x(m,\ell) \simeq \underbrace{\ell^{\frac{\eta}{2}-1}\widetilde{\mathcal{F}}_0^x(m/\ell^{1-\eta/2})}_{\text{red lines, field theory results}} + \underbrace{(-1)^{\lfloor \ell/2 \rfloor + \lfloor m \rfloor}\ell^{\frac{\eta}{2}-5/4}\widetilde{\mathcal{F}}_{e/o}^x(m/\ell^{1-\eta/2})}_{\text{subleading}}$$

B. Longitudinal component

$$F_\ell^z(\theta) = \langle \mathrm{GS} \,|\, e^{i\theta \sum_{j=1}^{\ell} (-1)^j S_j^z} \,|\, \mathrm{GS} \rangle$$

Scaling collapse around θ≈0:

$$F_\ell^z(\theta \approx 0) = e^{-\gamma z^2/4}\ , \quad z = \theta \ell^{1/2}$$



simple Gaussian

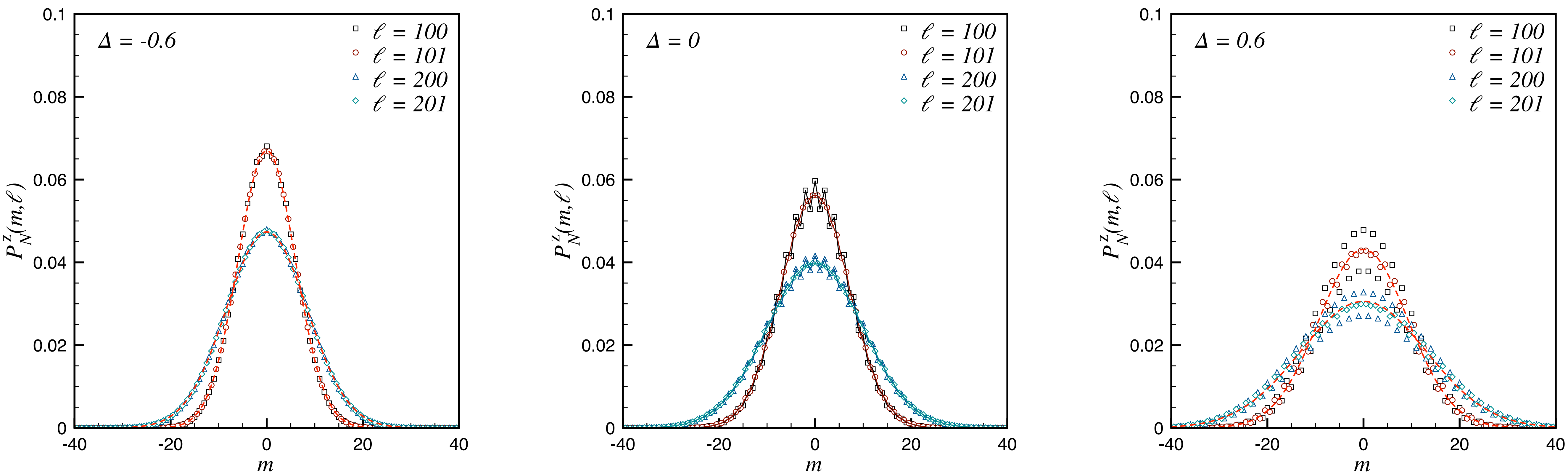
find that rescaling parameter is

$$\boxed{\gamma = \frac{1}{2 - 2\eta}}$$

red line = exact results

Similar scaling collapse around θ≈π (subleading contribution)

Probability distribution:



PD is Gaussian and much narrower than transverse analog.

Part II: FCS in isolated out-of-equilibrium systems

Melting of LRO after a "Quantum Quench"

M. Collura&FHLE '19

- Consider the spin-1/2 XXZ chain

$$H = J \sum_{j=1}^{L} S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta\, S_j^z S_{j+1}^z$$

- Prepare the system at time t=0 in a classical Néel state

$$|\Psi(0)\rangle = |\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\ldots\rangle$$

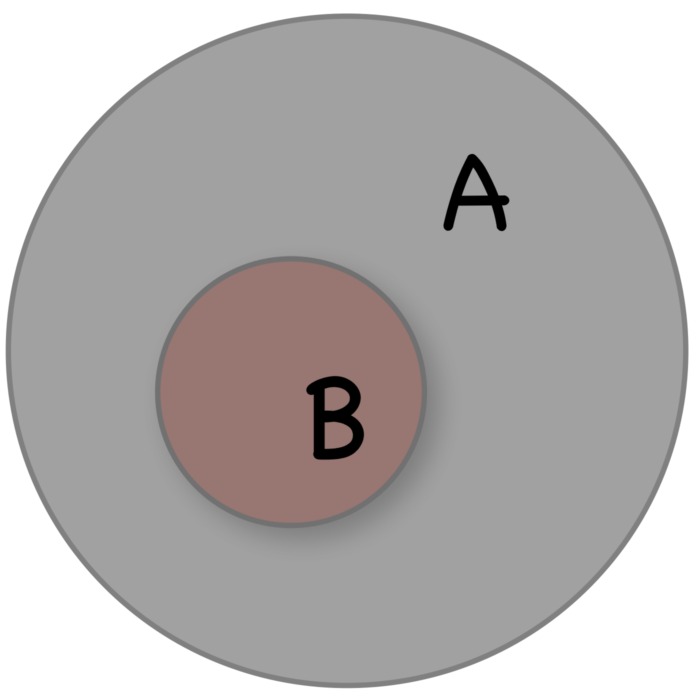
  - AFM Long-range order $\quad \langle\Psi(0)|\sum_j (-1)^j S_j^z|\Psi(0)\rangle \neq 0$
  - not an eigenstate of H

- time-evolve with H $\quad |\Psi(t)\rangle = e^{-iHt}|\Psi(0)\rangle$

We are interested in the prob. dist. of $\quad N_\ell^z = \sum_{j=1}^{\ell} (-1)^j S_j^z$

→ require $\quad \langle \Psi(t) | e^{i\theta N_\ell^z} | \Psi(t) \rangle$

This will initially depend on time, but eventually **relax** to a stationary value (“**local relaxation**”).



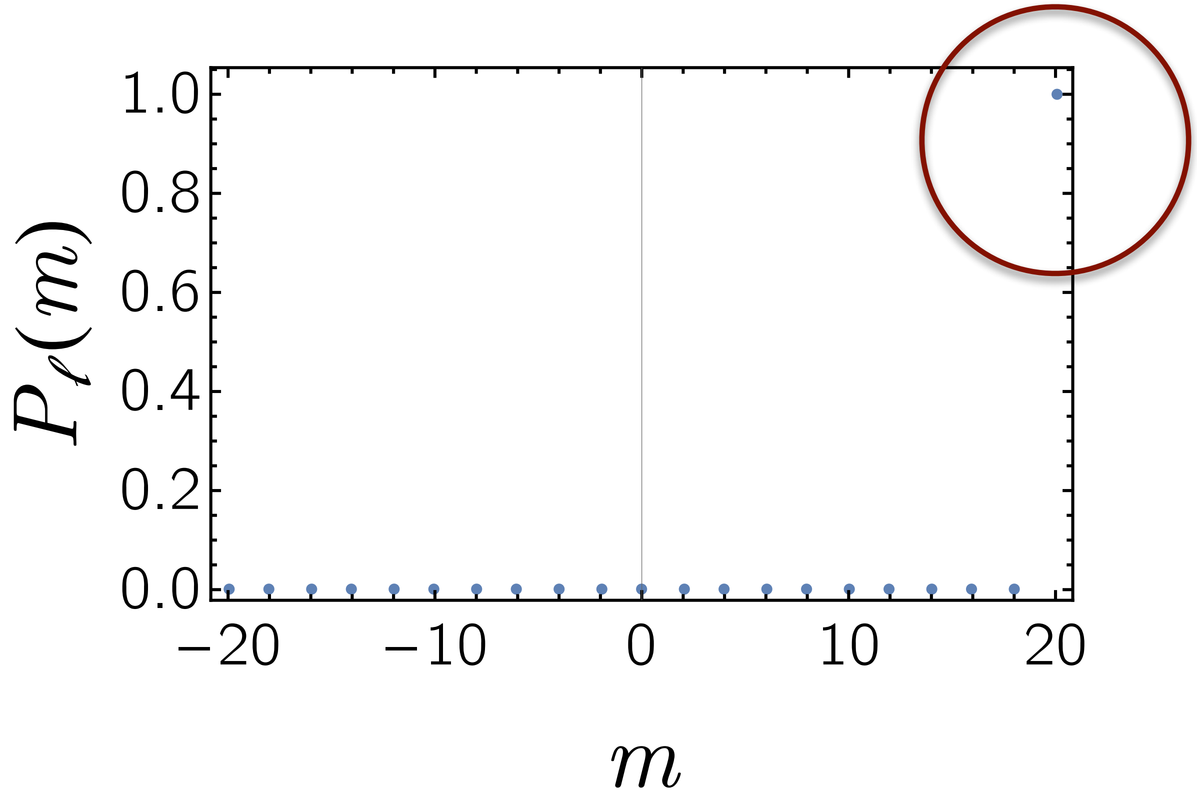
- Entire System: A∪B
- Take A infinite, B finite
- Ask questions only about B:

$$\boxed{\lim_{t\to\infty} \lim_{L\to\infty} \langle \Psi(t) | \mathcal{O}_B | \Psi(t) \rangle = \mathrm{Tr}\left[\rho_{SS}\mathcal{O}_B\right]}$$

ρ_{SS} = steady state density matrix

Physical Picture: A acts like a bath for B.

Probability distribution in **initial state (t=0)**:



→ delta-function at m=ℓ/2

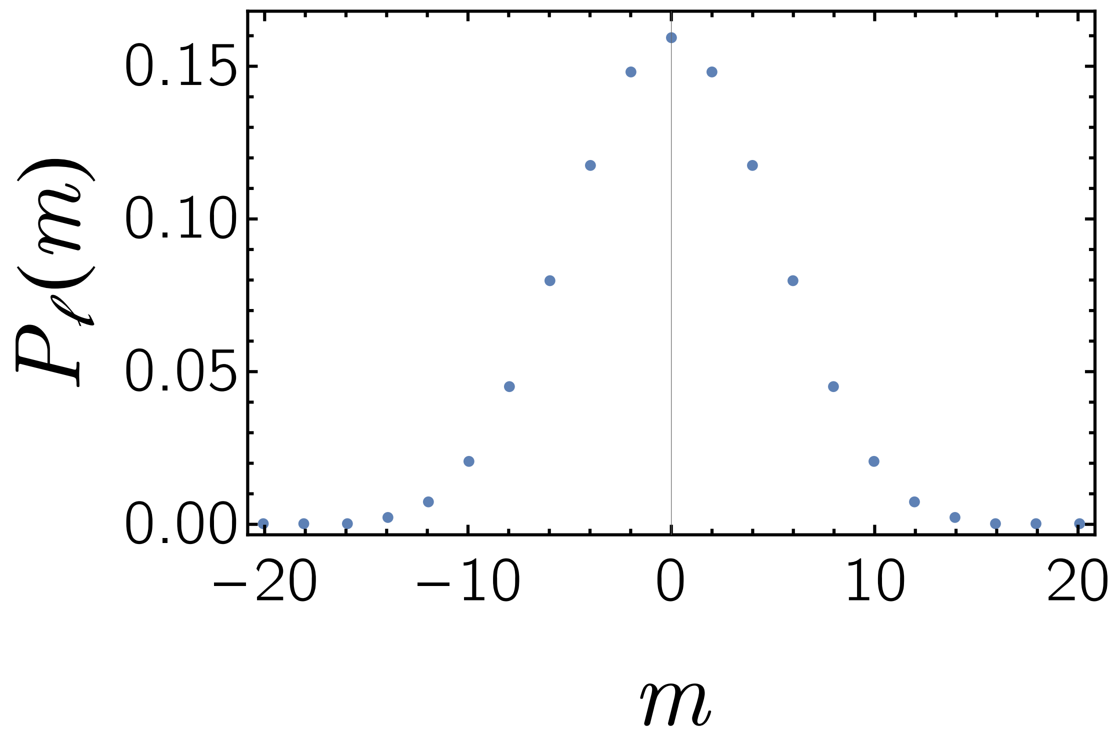
What do we expect in the stationary state?

Stationary State:

Finite correlation length ξ

$\xi < \ell$

SRO has melted



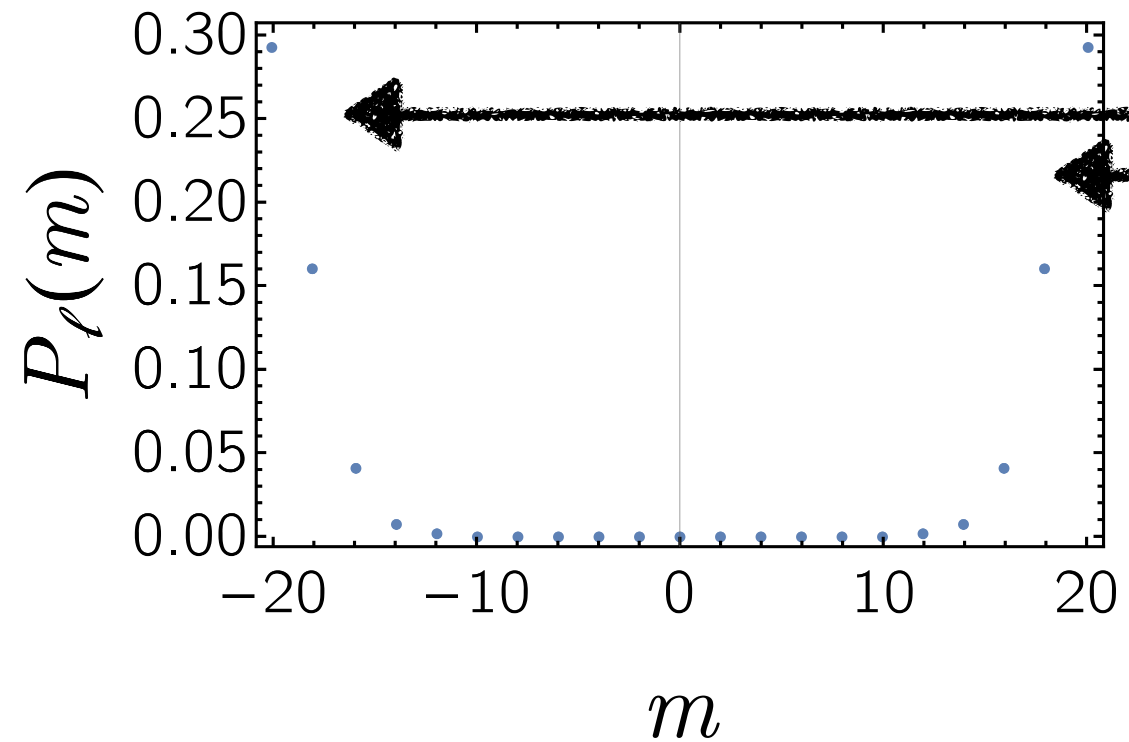
part. relevant for "large quenches"

Approximately Gaussian

Stationary State: **Finite** correlation length ξ

$\xi > \ell$

SRO remains, but spin-flip symmetry should be restored.

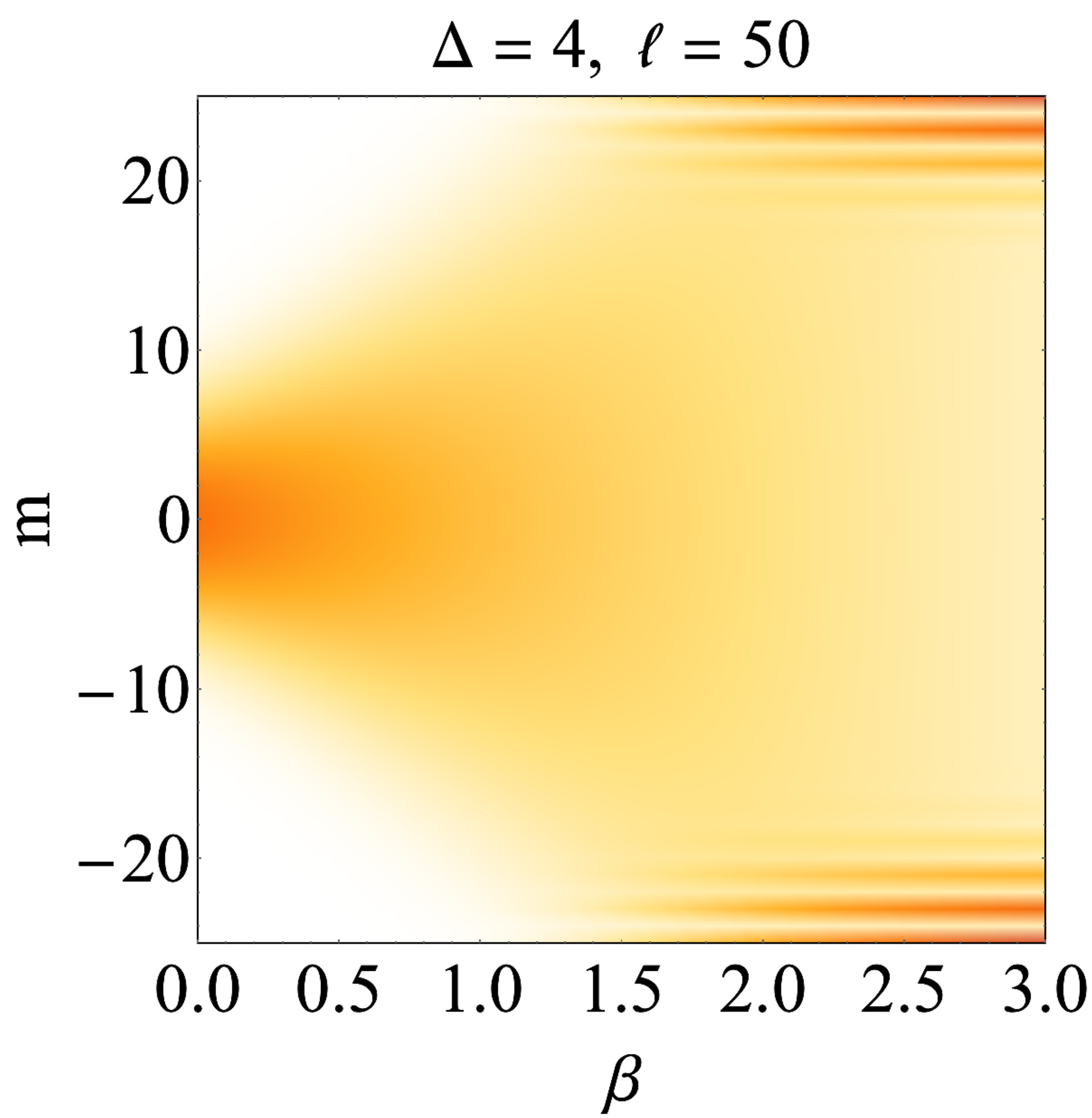


short-ranged order

part. relevant for "small quenches"

Analytic understanding for large Δ.

cf finite temperature equilibrium states

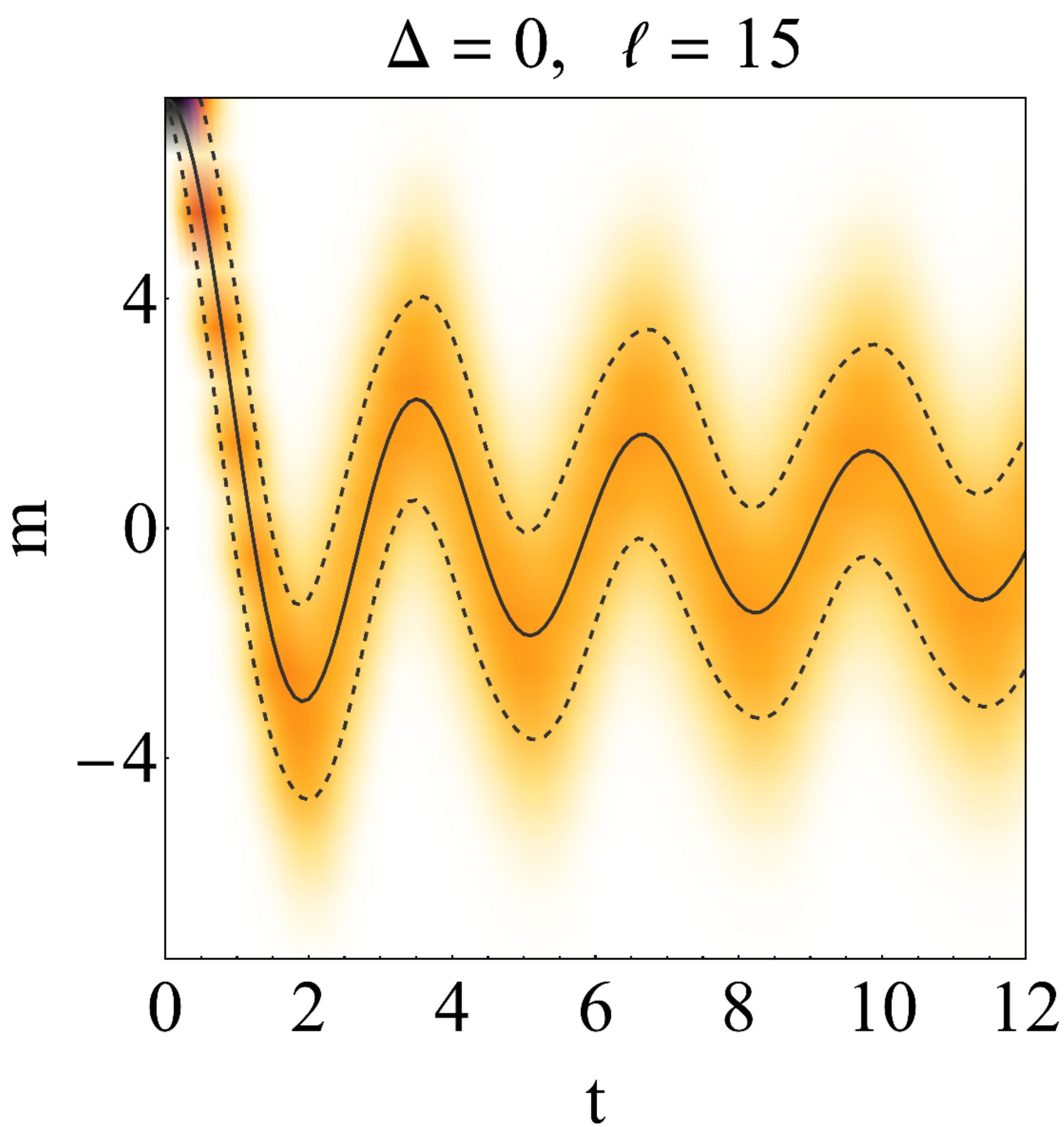


$\xi(T)<\ell$

$\xi(T)>\ell$

Time evolution for a “large quench”

(obtained from iTEBD)



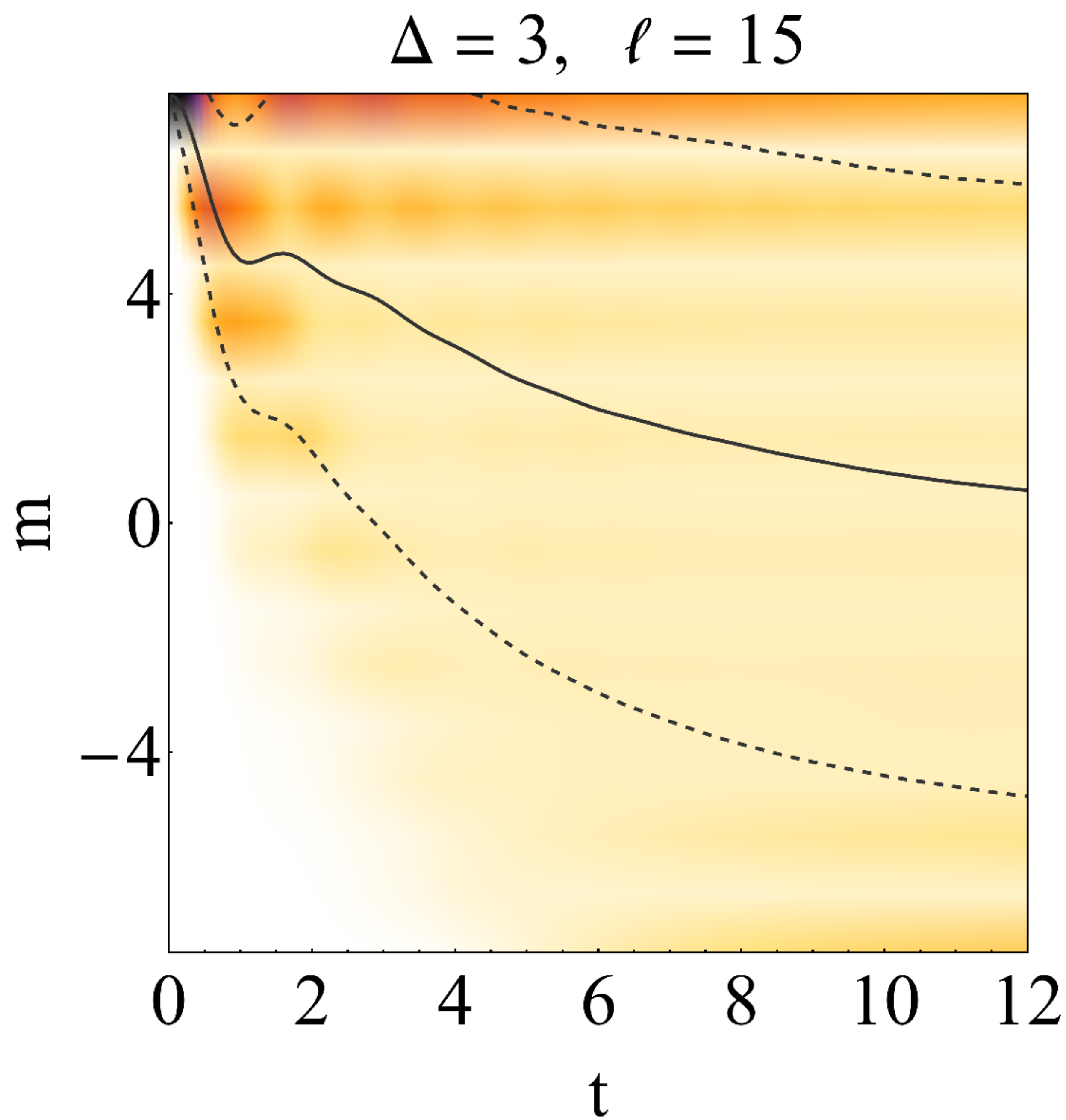
Prob. dist. = narrow Gaussian

average

Here the prob. dist. does not give a lot of extra info (except at short times)...

Time evolution for a "small quench"

(obtained from iTEBD)



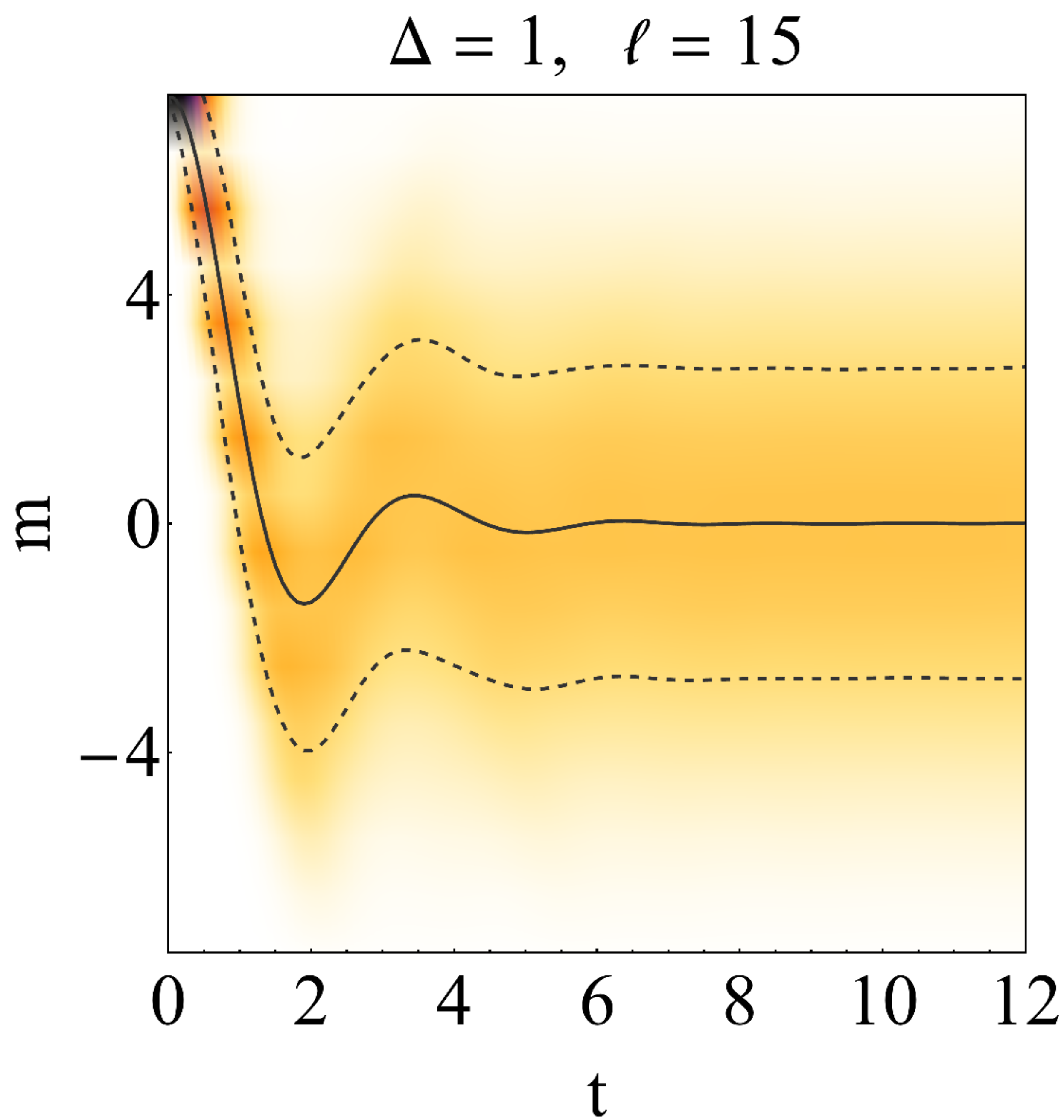
peak at $m=\ell/2$ remains

average

peak at $m=-\ell/2$ develops

Prob. dist. reveals a lot of physics beyond the average!

Time evolution for an "intermediate quench"



Broad prob. dist.

average

For XXZ we understand the "small-Δ" and short time regimes by a self-consistent time-dependent mean-field approximation in the fermionic representation; no analytic results.

To make analytic progress consider TFIM.

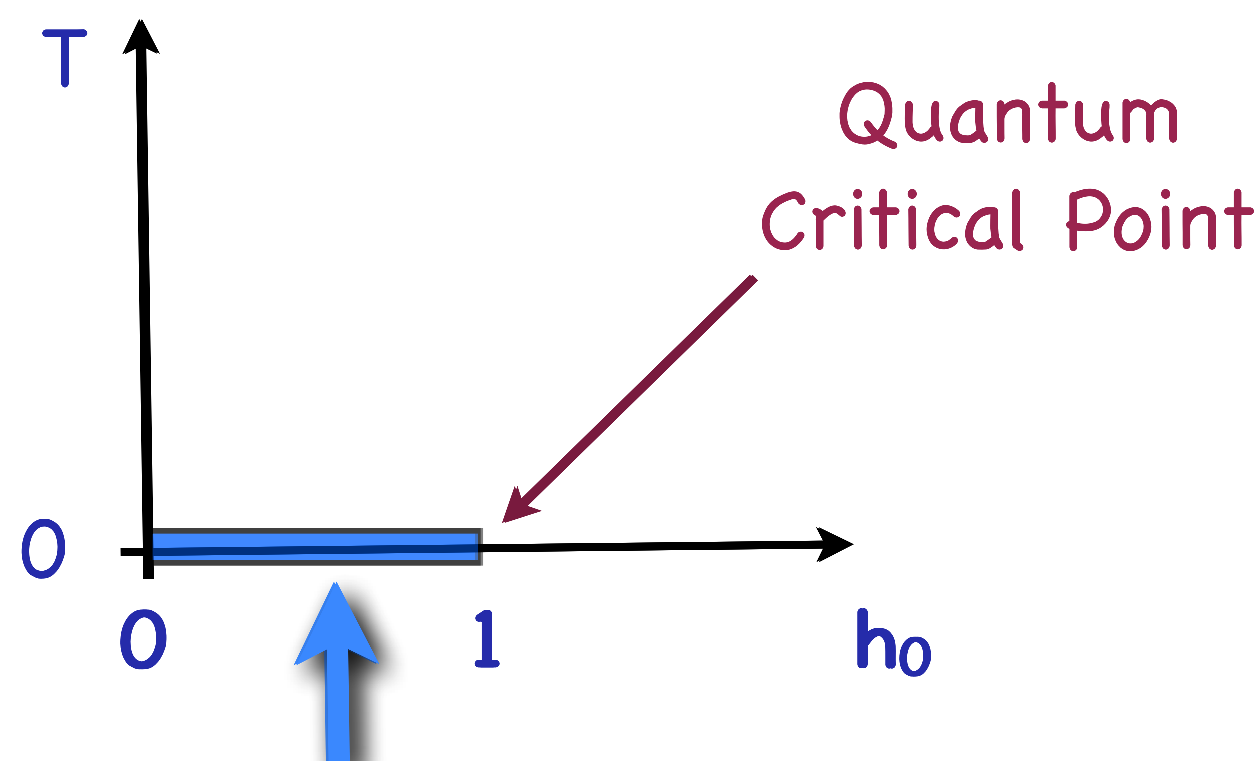
Analytic results: Transverse-Field Ising Chain

S. Groha, FHLE & P. Calabrese '18

$$H(h) = -\sum_{j=-\infty}^{\infty} \left[\sigma_j^x \sigma_{j+1}^x + h\sigma_j^z\right].$$

$\mathbb{Z}_2$ symmetry: rotations around z-axis by π $\qquad \sigma_j^x \to -\sigma_j^x$

Phase Diagram:



$\langle \sigma_j^x \rangle \neq 0$

T>0: order melts

TFIM can be mapped to free fermions by JW trafo:

$$\sigma_j^z = 1 - 2c_j^\dagger c_j \ , \qquad \sigma_j^x = \prod_{l=-\infty}^{j-1} (1 - 2c_l^\dagger c_l)(c_j + c_j^\dagger)$$

$$H(h) = -J \sum_{j=-\infty}^{\infty} (c_j^\dagger - c_j)(c_{j+1} + c_{j+1}^\dagger) - Jh(c_j c_j^\dagger - c_j^\dagger c_j).$$

Consider QQs e.g. from **ground states** of $H(h_0)$ and determine PD of transverse subsystem magnetisation:

$$S_u^z(\ell) = \sum_{j=1}^{\ell} \sigma_j^z = \sum_{j=1}^{\ell} 1 - 2c_j^\dagger c_j$$

local in fermions

$$P_{S_u^z(\ell),|\Psi(t)\rangle}(\mu) = \langle \Psi(t) \,|\, \delta\big(S_u^z(\ell) - \mu\big) \,|\, \Psi(t) \rangle = \int_{-\infty}^{\infty} d\lambda \ e^{-i\mu\lambda} \underbrace{\langle \Psi(t) \,|\, e^{i\lambda S_u^z(\ell)} \,|\, \Psi(t) \rangle}_{\boxed{\chi_u(\lambda,\ell)}}$$

$$= 2 \sum_{r\in\mathbb{Z}} P_w^{(u)}(r,t)\ \delta(m - 2r) \quad (\ell \text{ even})$$

How to obtain analytic results after QQ:

Step 1: exact determinant representation for generating function

$$\chi^{(u)}(\lambda,\ell) = (2\cos\lambda)^{\ell}\sqrt{\det\left(\frac{1-\tan(\lambda)\Gamma'}{2}\right)},$$

known 2ℓx2ℓ matrix

Step 2: multiple integral representation

$$\ln\chi^{(u)}(\lambda,\ell,t) = \ell\ln(\cos\lambda) - \frac{1}{2}\sum_{n=1}^{\infty}\frac{\big(\tan(\lambda)\big)^n}{n}\,\mathrm{Tr}\big[(\Gamma')^n\big]$$

$$\mathrm{Tr}\big[(\Gamma')^n\big] = \left(\frac{\ell}{2}\right)^n\int_{-\pi}^{\pi}\frac{dk_1\ldots dk_n}{(2\pi)^n}\int_{-1}^{1}d\zeta_1\ldots d\zeta_{n-1}\;\mu(\vec{\zeta})\;C(\vec{k})\;F(\vec{k})\;\exp\left(-i\ell\sum_{j=1}^{n-1}\frac{\zeta_j}{2}(k_j-k_0)\right)$$

Step 3: asymptotics from multi-dim stationary phase approx and summing result over all n

difficult.

Result:

$$\boxed{\ln\chi(\lambda,\ell,t)\approx \ell\log(\cos\lambda)+\frac{\ell}{2}\sum_{n=0}^{\infty}\int_0^{2\pi}\frac{dk_0}{2\pi}\Theta(\ell-2n|v_k|t)\left[1-\frac{2n|v_k|t}{\ell}\right]\sum_{m=0}^{n+1}\cos\left(2m\varepsilon(k_0)t\right)f_{n,m}(\lambda,k_0)+\mathcal{C}}$$

$$\begin{aligned}
f_{0,0}(\lambda,k_0) &= 2\ln\left(1+i\cos\Delta_{k_0}\tan\lambda e^{i\theta_{k_0}}\right)\ ,\\
f_{1,0}(\lambda,k_0) &= \ln\left[1-\frac{\sin^2\Delta_{k_0}\tan^2\lambda(\cos\theta_{k_0}+i\cos\Delta_{k_0}\tan\lambda)^2}{(\sin^2\theta_{k_0}+(\cos\theta_{k_0}+i\cos\Delta_{k_0}\tan\lambda)^2)^2}\right]\ ,\\
f_{2,0}(\lambda,k_0) &= \ln\left[1+\frac{\sin^4\Delta_{k_0}\tan^4\lambda\sin^2\theta_{k_0}(\cos\theta_{k_0}+i\cos\Delta_{k_0}\tan\lambda)^2}{((\sin^2\theta_{k_0}+(\cos\theta_{k_0}+i\cos\Delta_{k_0}\tan\lambda)^2)^2-\sin^2\Delta_{k_0}\tan^2\lambda(\cos\theta_{k_0}+i\cos\Delta_{k_0}\tan\lambda)^2)^2}\right]
\end{aligned}$$

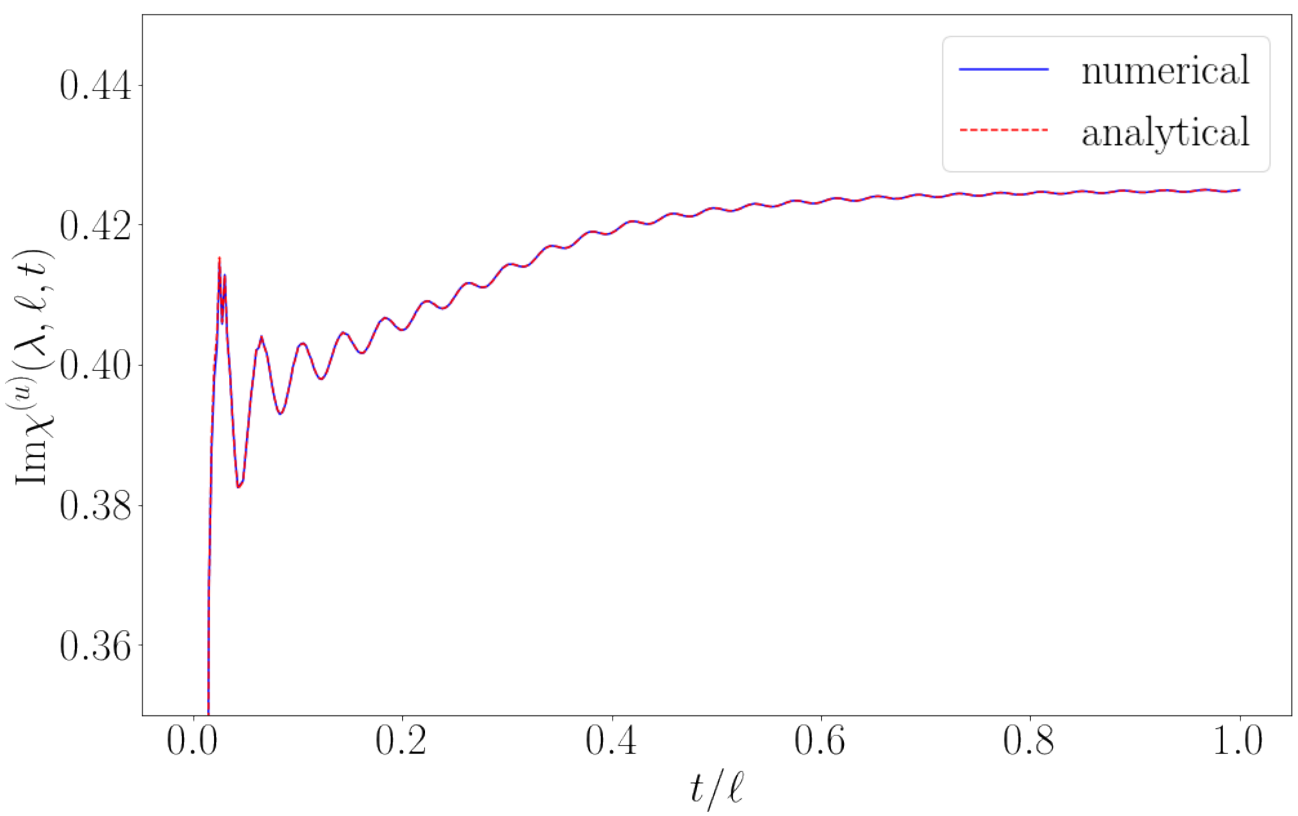
$$\begin{aligned}
f_{0,1} &= -i\tan\Delta_{k_0}\ln\left[\frac{1+ie^{i\theta_{k_0}}\cos\Delta_{k_0}\tan\lambda}{1+ie^{-i\theta_{k_0}}\cos\Delta_{k_0}\tan\lambda}\right]\ ,\\
f_{1,1} &= \tan\Delta_{k_0}\left(i\log\left[\frac{1+ie^{i\theta_{k_0}}\cos\Delta_{k_0}\tan\lambda}{1+ie^{-i\theta_{k_0}}\cos\Delta_{k_0}\tan\lambda}\right]-\frac{4\cos\Delta_{k_0}\tan\lambda\sin\theta_{k_0}}{\sin^2\theta_{k_0}+(\cos\theta_{k_0}+i\cos\Delta_{k_0}\tan\lambda)^2}\right)+\mathcal{O}\left(\sin^3(\Delta_{k_0})\right)
\end{aligned}$$

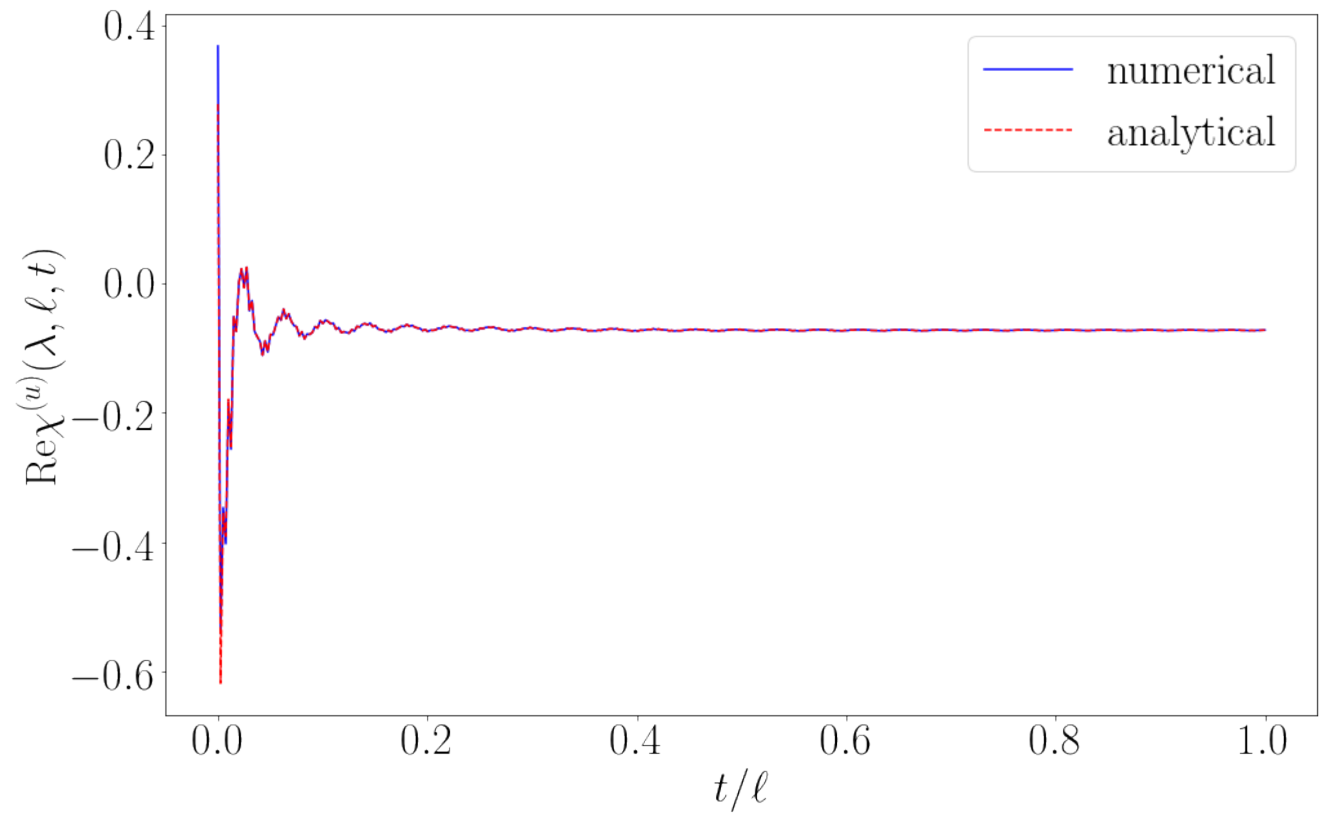
$$e^{i\theta_k}=\frac{h-e^{ik}}{\sqrt{1+h^2-2h\cos k}}\qquad \varepsilon(k)=2J\sqrt{1+h^2-2h\cos(k)}.\qquad v_k=\frac{d\epsilon(k)}{dk}$$

$$\cos\Delta_k=4\frac{hh_0-(h+h_0)\cos k+1}{\varepsilon_h(k)\varepsilon_{h_0}(k)}$$

How well does this work?

→ Compare to numerically exact results.





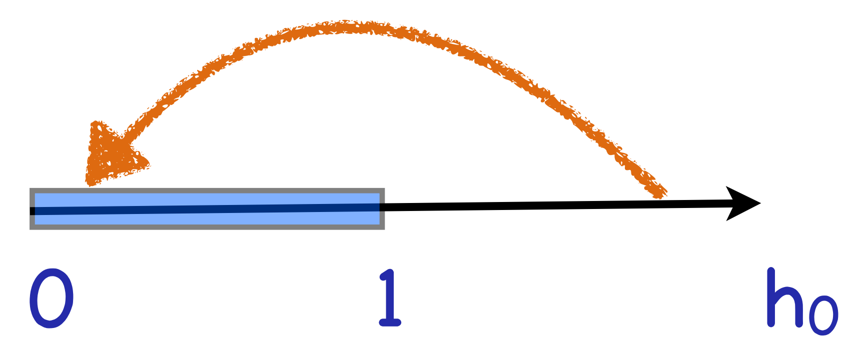
λ=0.1, ℓ=200, h_0=0, h=0.2

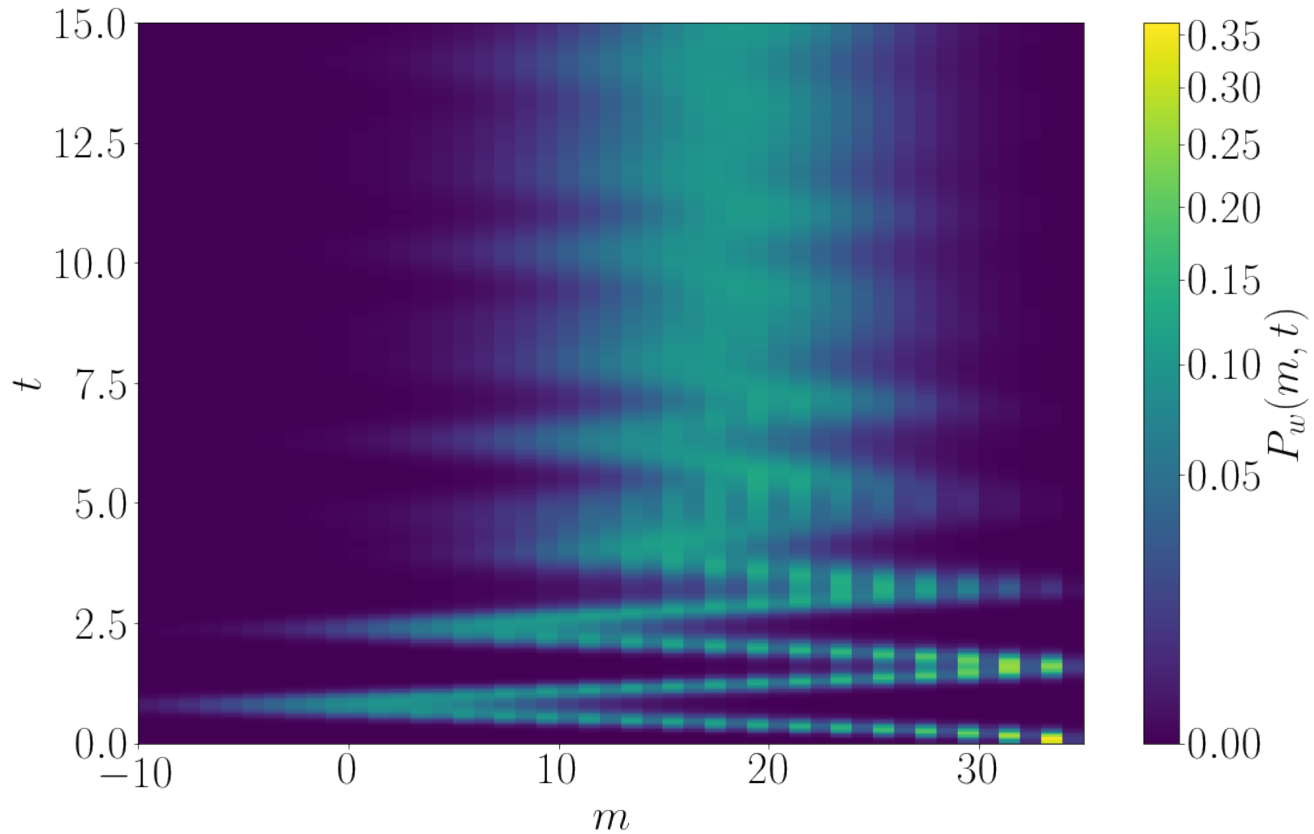
Not bad.

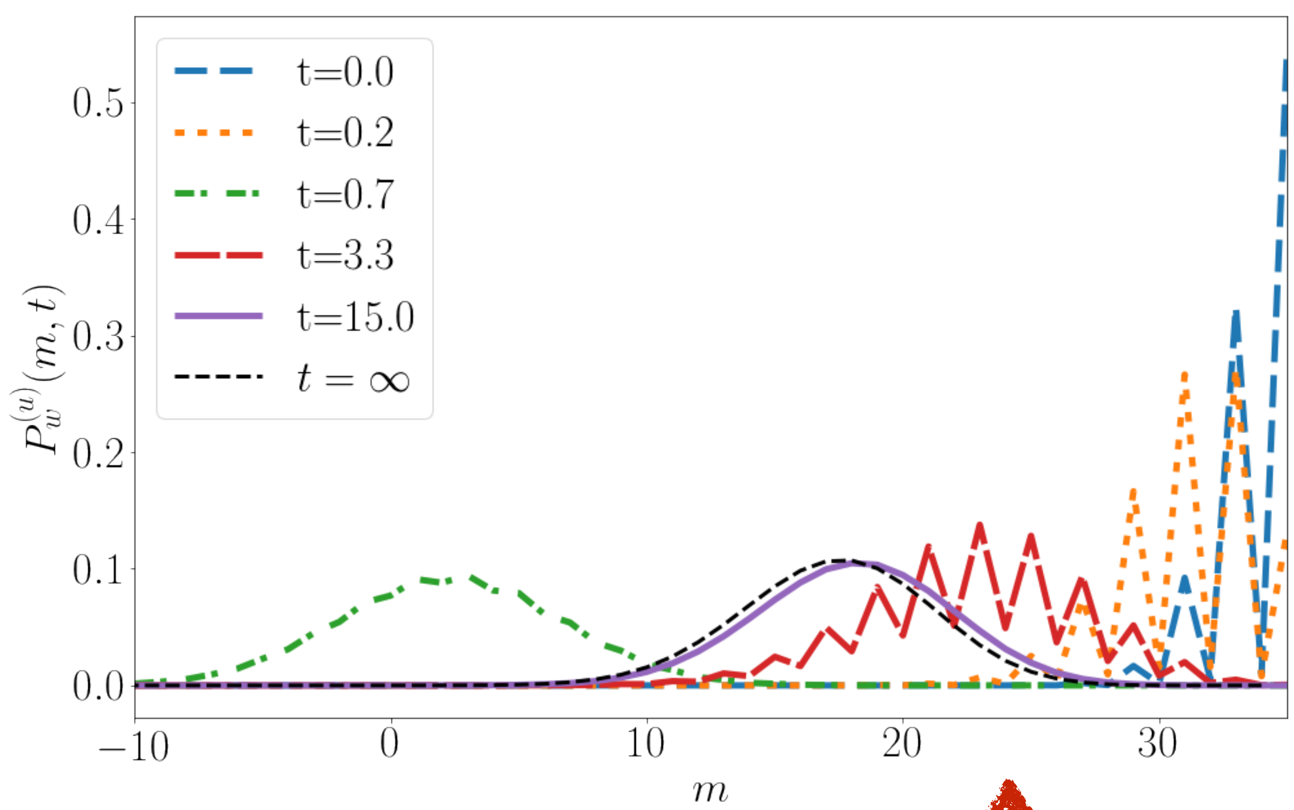
Slight caveat: when $\chi^{(u)}(\lambda, \ell, t)$ becomes very small as a fn of λ our approximation becomes poor. Not a problem for getting the PD.

"Transverse field quench": prepare system in GS of $H(h_0)$, time evolve with $H(h)$

$h_0=3$, $h=0.2$







even/odd structure that washes out over time

Summary

1. Full counting statistics for subsystems can be interesting; can be **universal** at critical points.
2. FCS is not easy to calculate analytically.
3. FCS in ground state of quantum critical XXZ chain
4. FCS of transverse magnetisation in TFIM in equilibrium & after quantum quenches
5. FCS after Neel quench in XXZ: melting of LRO

Many open questions:

- Subleading scaling functions in ground state of XXZ?
- Order-parameter PDF for TFIM in equilibrium/after QQs?
- How to get PDF's from Bethe Ansatz?
- ...