# Numerics for an XXZ spin-1/2 chain out of equilibrium

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Phys. Rev. B 88, 245114 (2013)

ICFO, Barcelona, March 2014

# Quantum quenches

- Prepare the (quantum) system in the ground state $|\psi_0\rangle$ of $H_0$

- Evolve with $H \neq H_0$ $$|\psi(t)\rangle = \exp(-itH)\,|\psi_0\rangle$$

$$\langle n|\psi(t)\rangle = e^{iE_n t}\langle n|\psi_0\rangle$$

- Questions :

  Steady state ?

  Equilibrium ? Thermalization ? (if yes, what about conserved quantities ?)

  Experiments ? Cold atoms systems ?

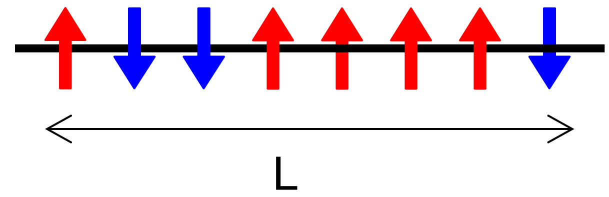
Review: "*Nonequilibrium dynamics of closed interacting quantum systems*"
A. Polkovnikov *et al*., Rev. Mod Phys. 83, 863 (2011)

# Outline

- Model: XXZ spin chain & Antal’s “density” quench
- Free fermion case – semiclassical approximation
- Some numerical (TEBD) results in the interacting case
  - steady state region
  - fronts

# Ising-Heisenberg Hamiltonian – XXZ spin chain

- Hamiltonian

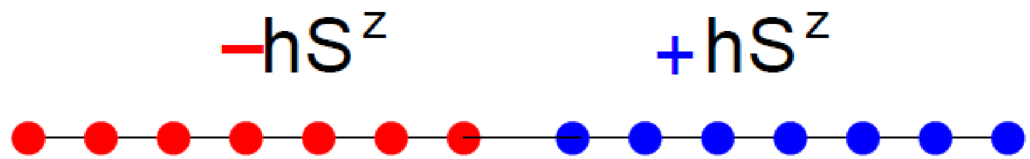



$$H_{XXZ} = -\sum_{i=-L/2}^{L/2-2}\left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z\right)$$

$$= -\sum_{i=-L/2}^{L/2-2}\frac{1}{2}\left(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+\right) + \Delta S_i^z S_{i+1}^z$$

- Initial state: add an external magnetic field to $H_{XXZ}$

$$H_0 = H_{XXZ} + h\left[\left(\sum_{i=-L/2}^{-1} S_i^z\right) - \left(\sum_{i=1}^{L/2} S_i^z\right)\right]$$

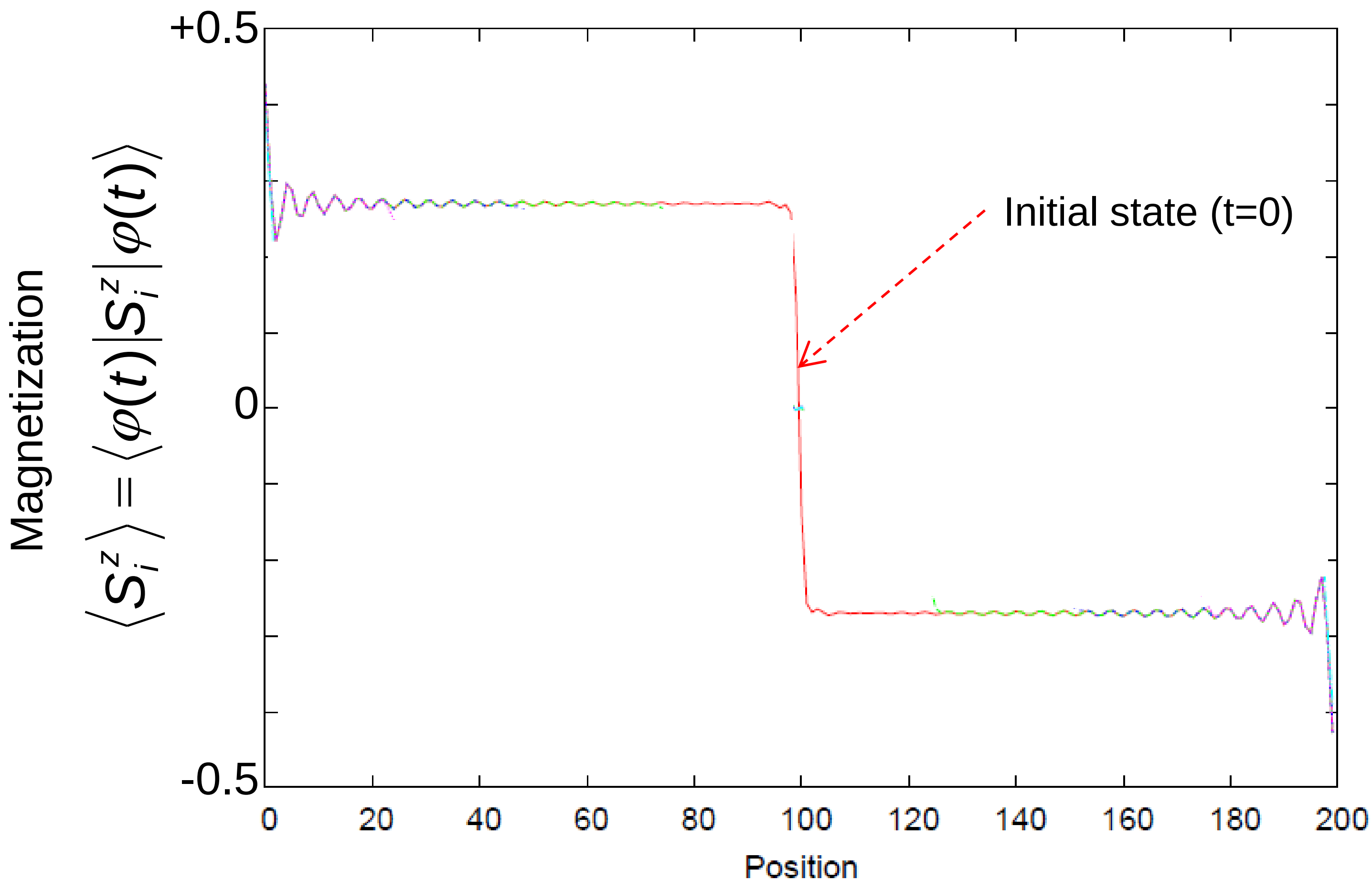



- t>0: switch "off" the magnetic field ($h\rightarrow 0$) and evolve with $H_{XXZ}$

"*Transport in the XX chain at zero temperature: Emergence of flat magnetization profiles*" Antal *et al.* Phys. Rev. E **59**, 4912 (1999)

# Δ =0 – Initial magnetization profile

$$H_{XX} = -\sum_{i=-L/2}^{L/2-2} \left( S_i^x S_{i+1}^x + S_i^y S_{i+1}^y \right)$$



# Δ =0 – « Free fermion »

- Jordan-Wigner transformation: Spin-1/2 ↔ fermions creation/annihilation operators

$$c_m^+ = S_m^+ \exp\left( i\pi \sum_{n<m} S_n^z \right) \quad , \quad c_m^+ c_m = S_m^z + \frac{1}{2}$$

Spinless fermion creation operator

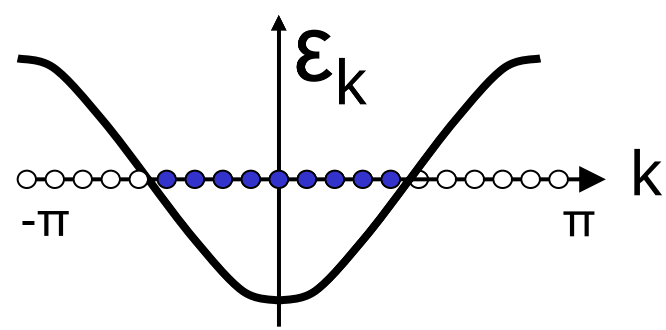
Spin up = one fermion
Spin down = empty site

- XY Hamiltonian ↔ *free* fermions

$$H_{XX} = -\sum_{i=-L/2}^{L/2-2} \left( S_i^x S_{i+1}^x + S_i^y S_{i+1}^y \right)$$

$$= -\frac{1}{2} \sum_{i=-L/2}^{L/2-2} \left( c_i^+ c_{i+1} + c_i c_{i+1}^+ \right) = -\sum_{k=-\pi\cdots\pi} \cos(k)\, c_k^+ c_k$$

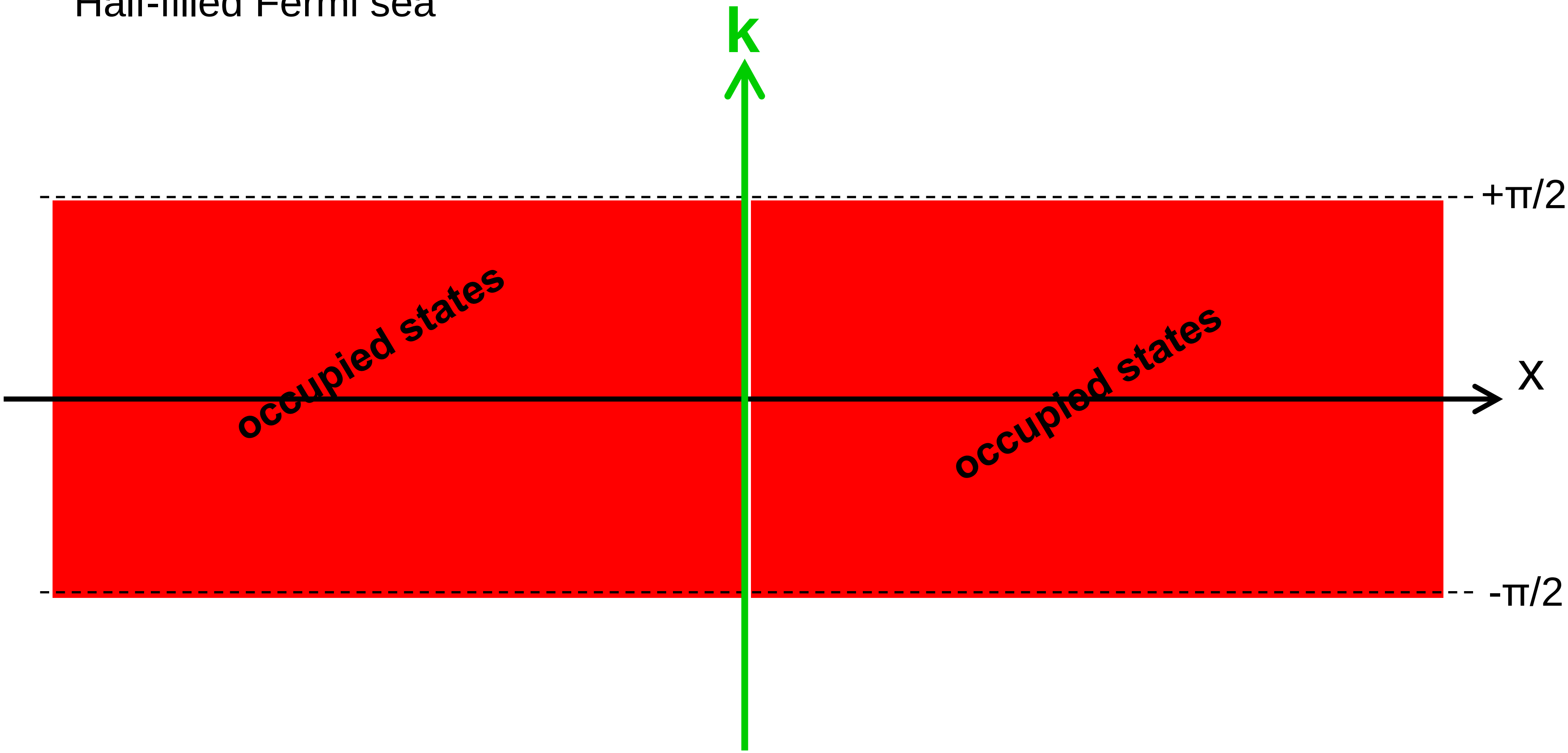
- Ground state : (half filled) Fermi sea



# Shape of the front

Hunyadi *et al.*, PRE 2004
Antal *et al.* PRE 2008

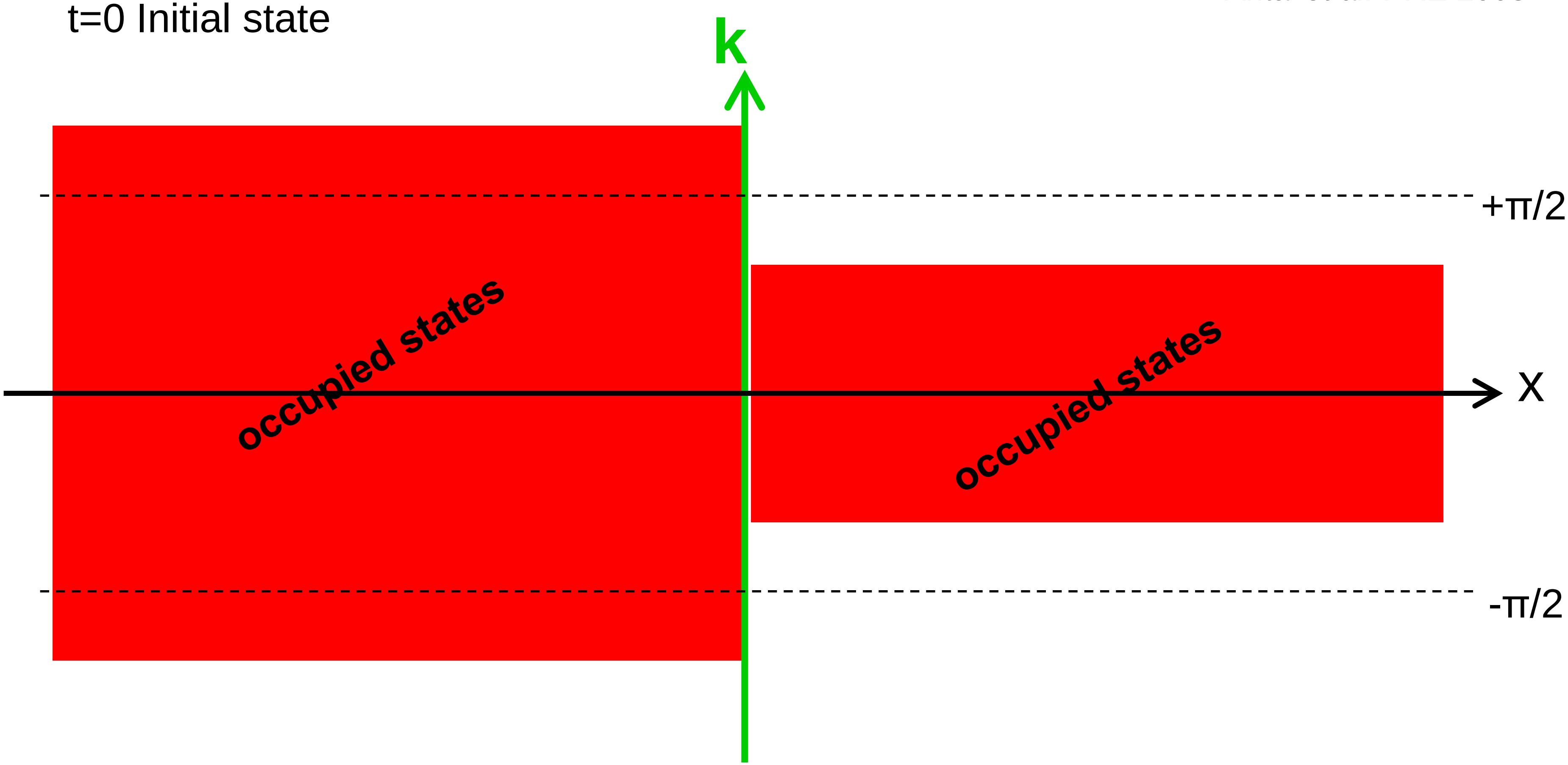
Half-filled Fermi sea



# Shape of the front

Hunyadi *et al.*, PRE 2004
Antal *et al.* PRE 2008

t=0 Initial state



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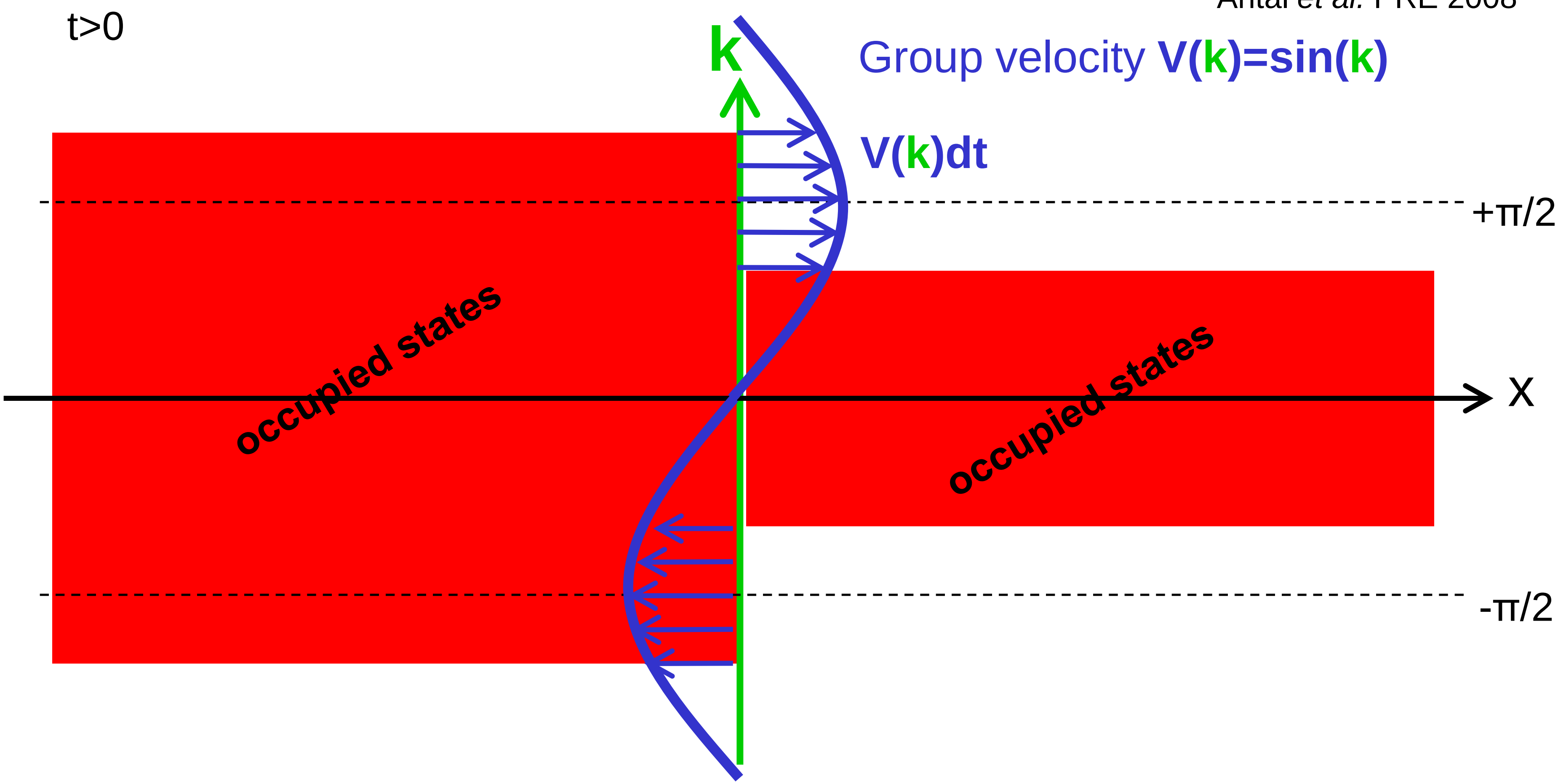

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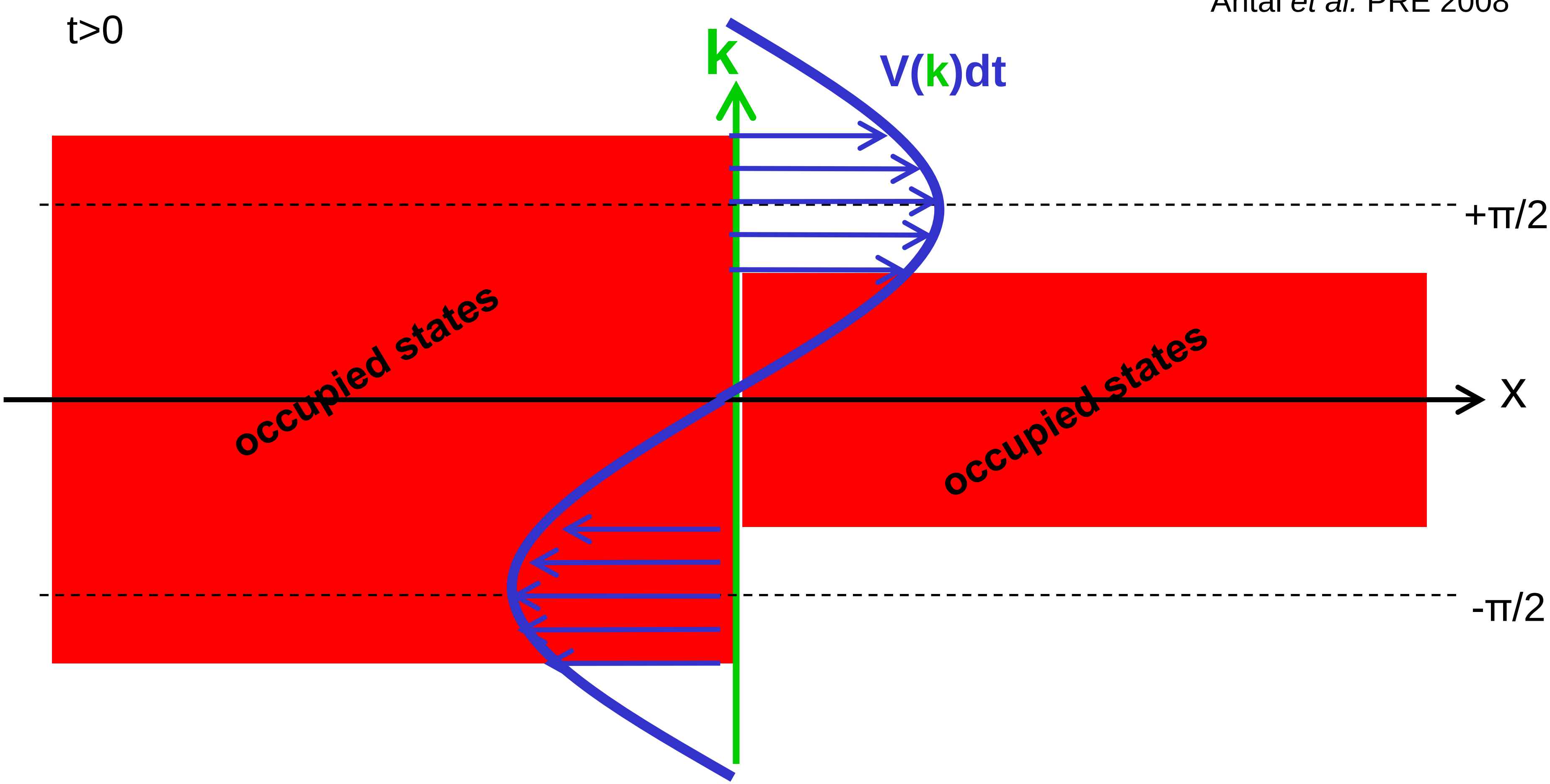

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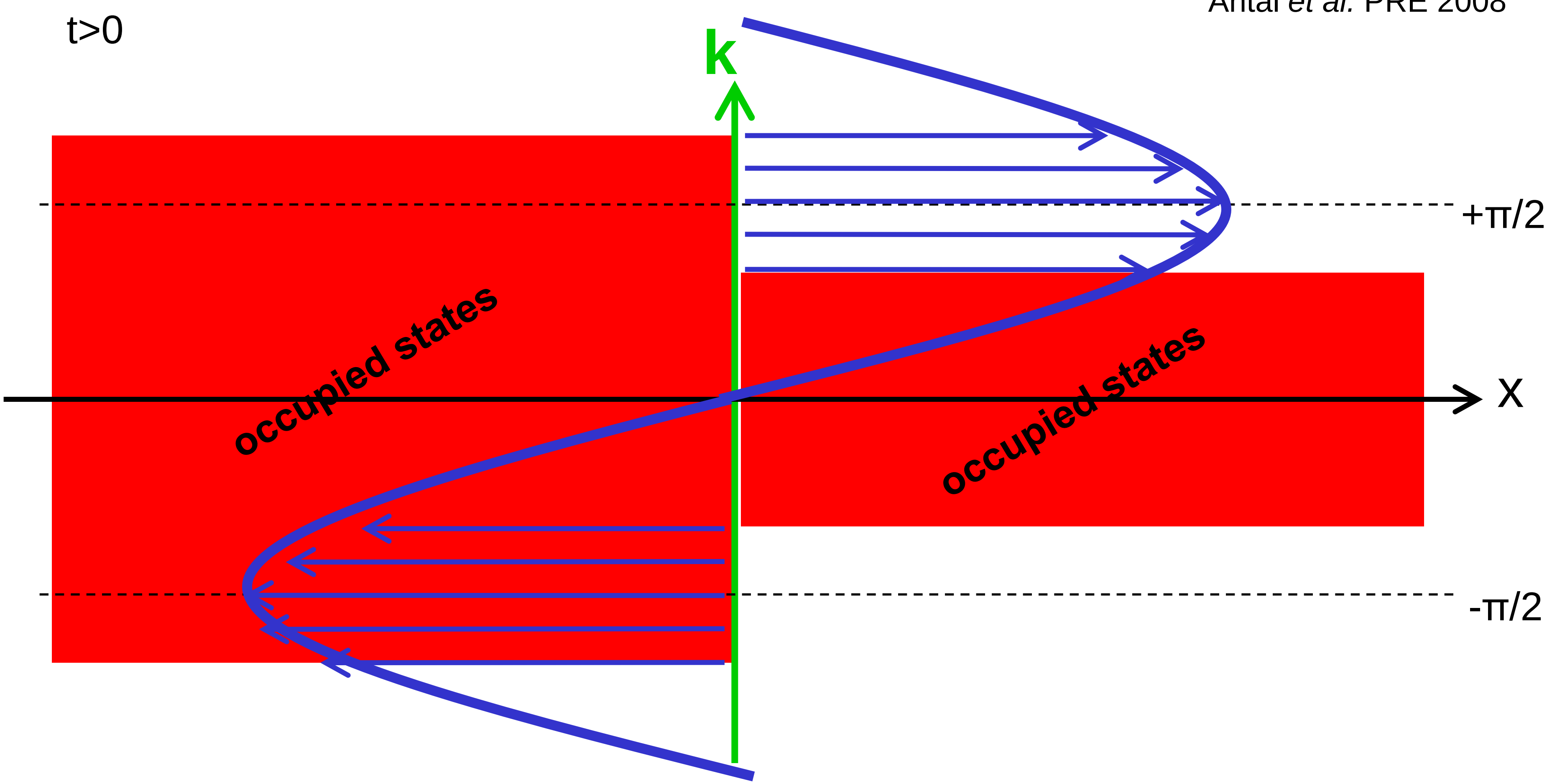

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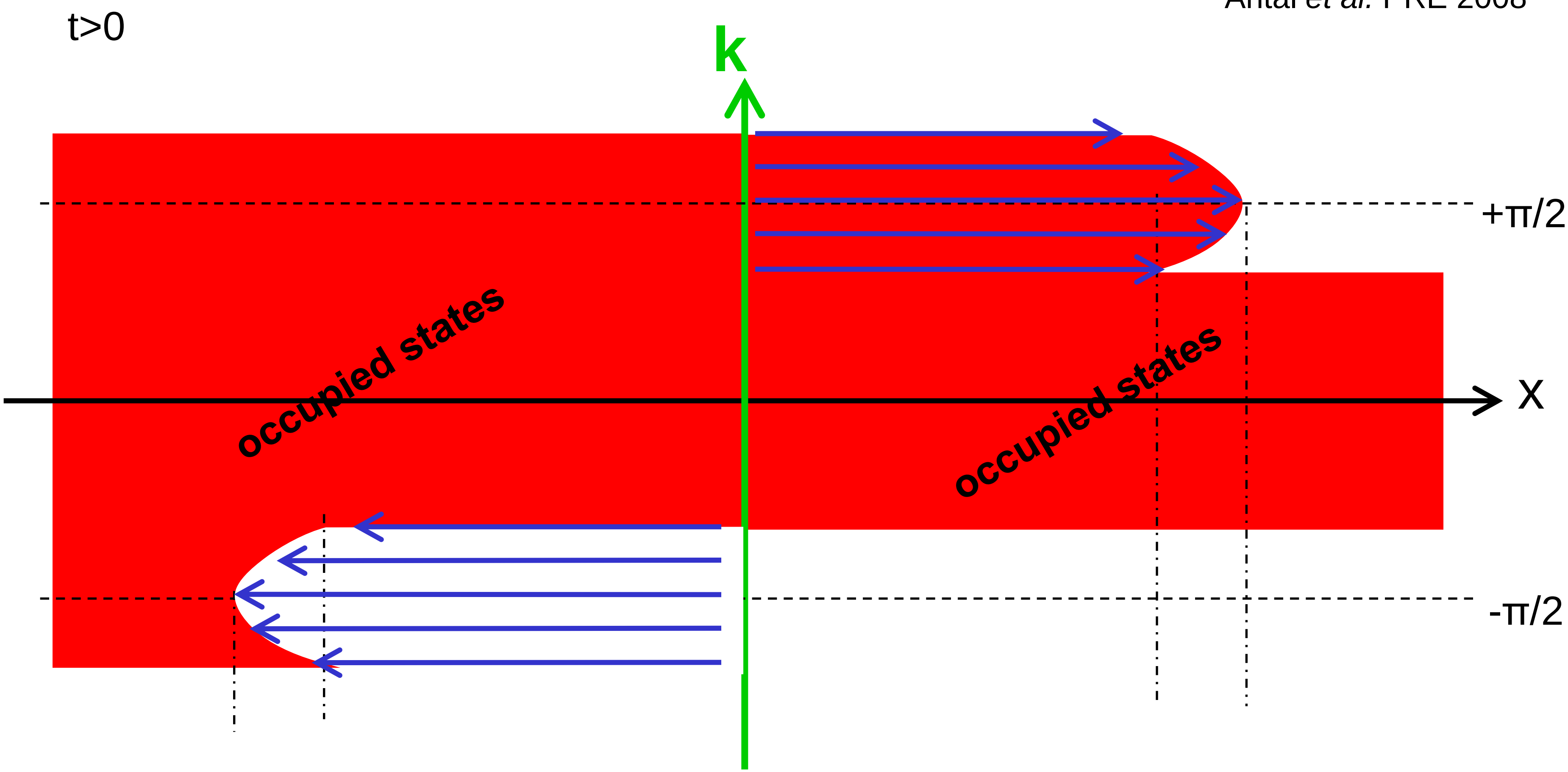

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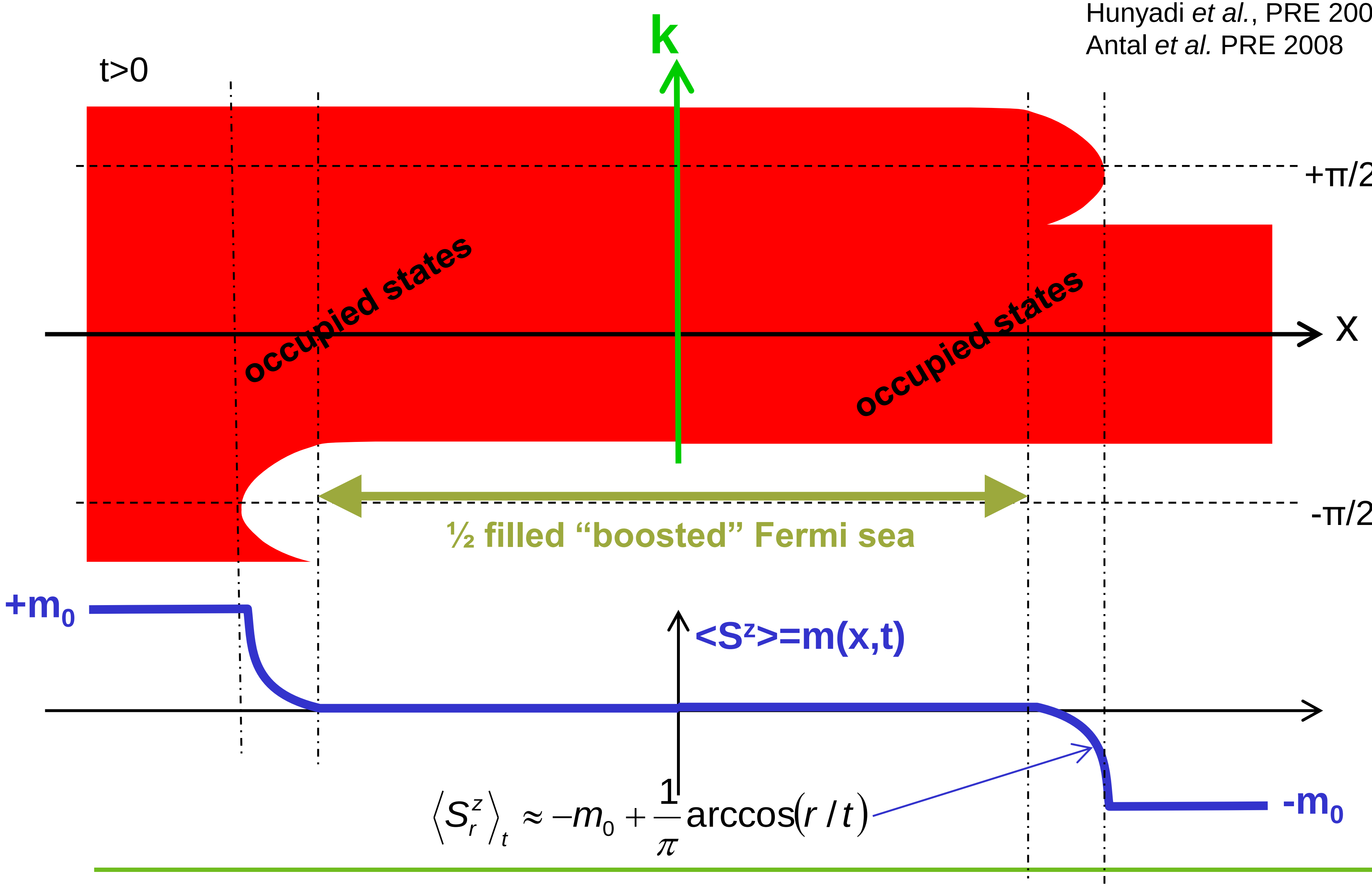
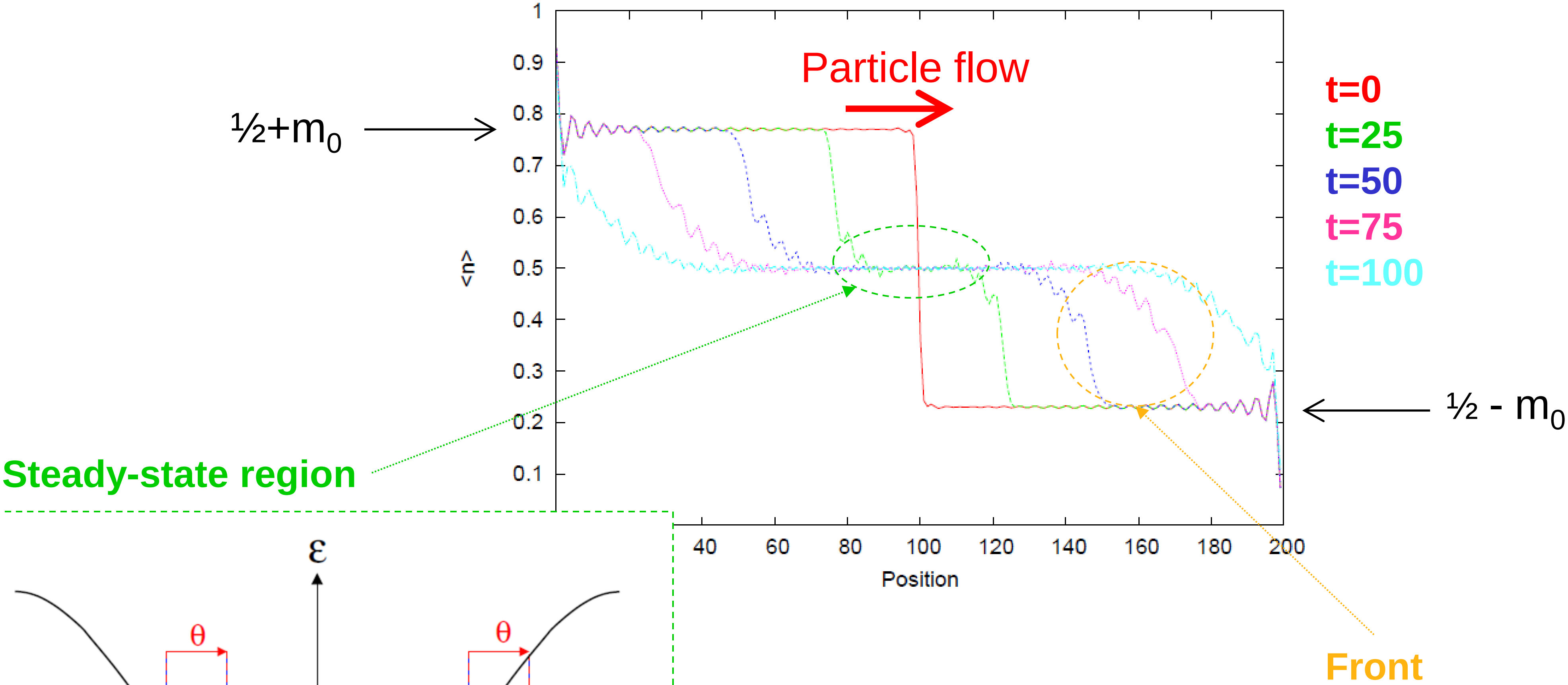
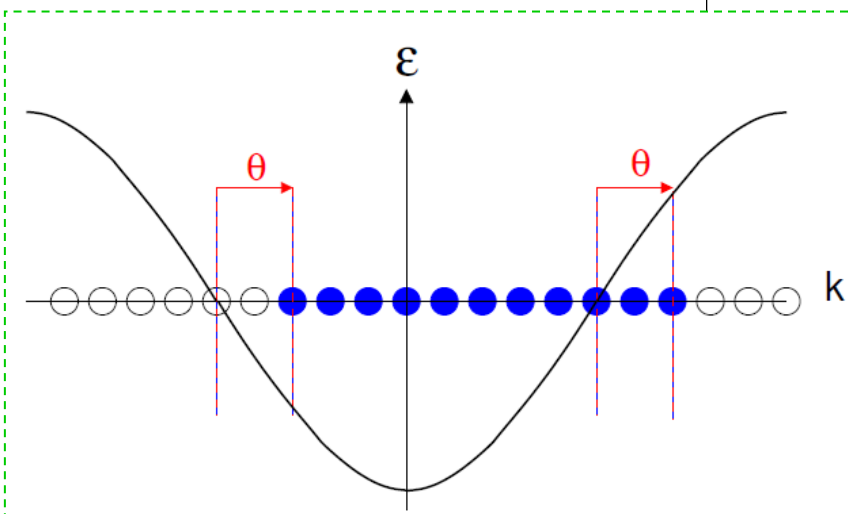


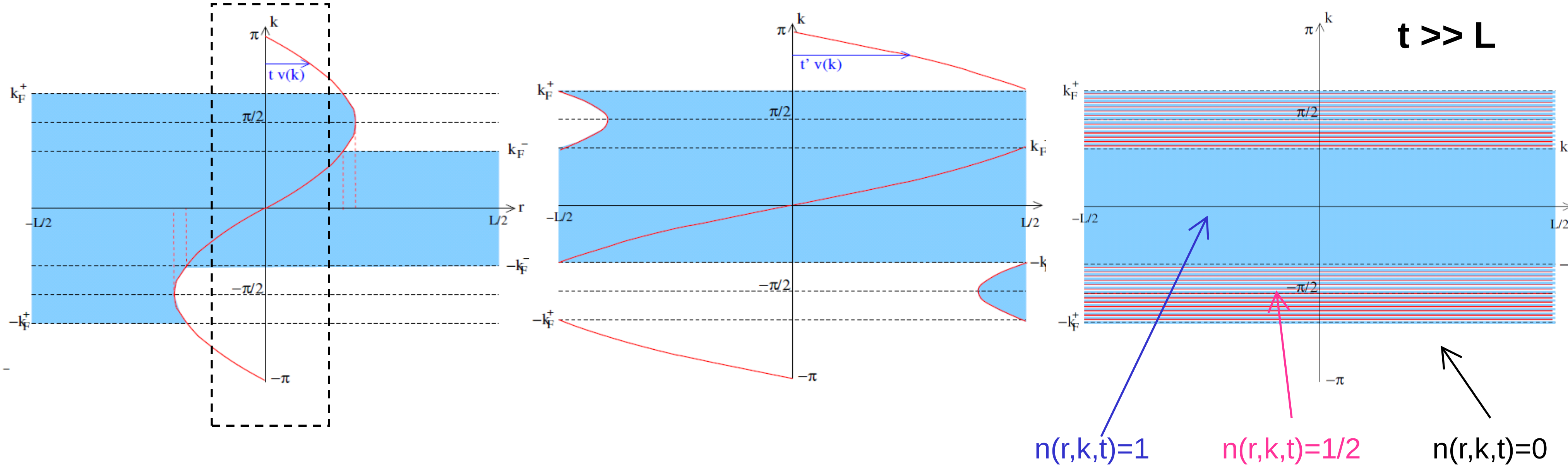

$$\langle S_r^z \rangle_t \approx -m_0 + \frac{1}{\pi}\arccos(r/t)$$

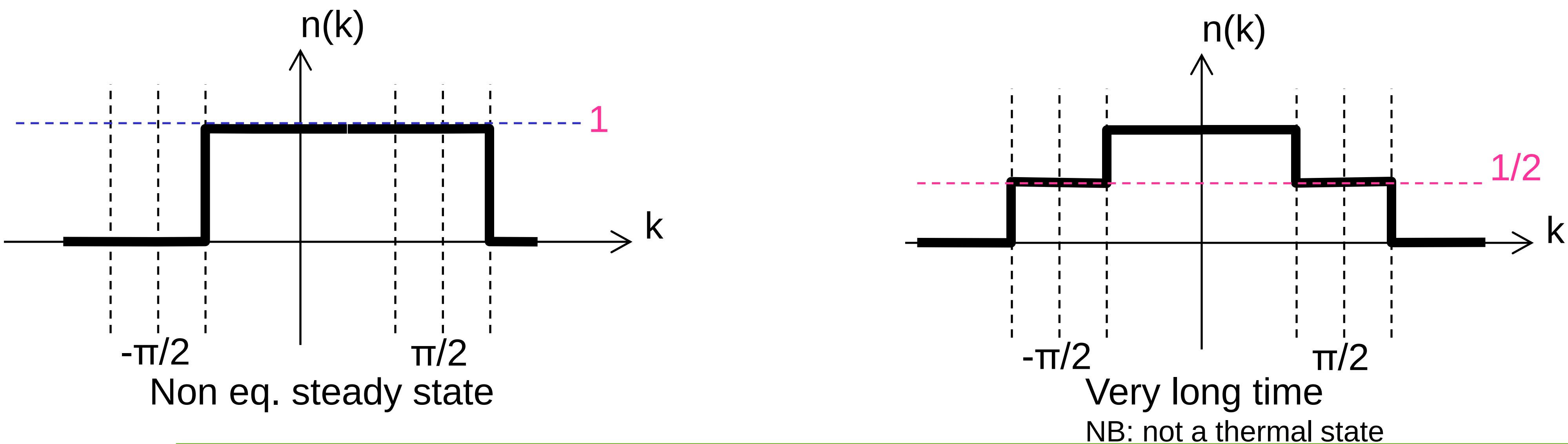
# Δ =0 – Evolution of the magnetization profile



# After many bounces (t>>L)



# Interacting case, $\Delta \neq 0$

# $\Delta \neq 0$: interacting case

$$H_{XXZ} = -\sum_{i=-L/2}^{L/2-2}\left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z\right)$$

$\Delta$=1: Heisenberg model
$\Delta=\pm\infty$: classical Ising model
$\Delta$=0: XX chain – free fermions

- Integrable system (Bethe Ansatz)
  → wave functions of the eigenstates
  → correlation functions
  → thermodynamics

- What about real-time dynamics following a "quench" ?
  This work: numerical simulations

- We focus here on $|\Delta|<1$, corresponding to gapless systems
  Luttinger liquid phase, algebraic correlation
  Linear dispersion relation of the magnetic ("spinon") excitations

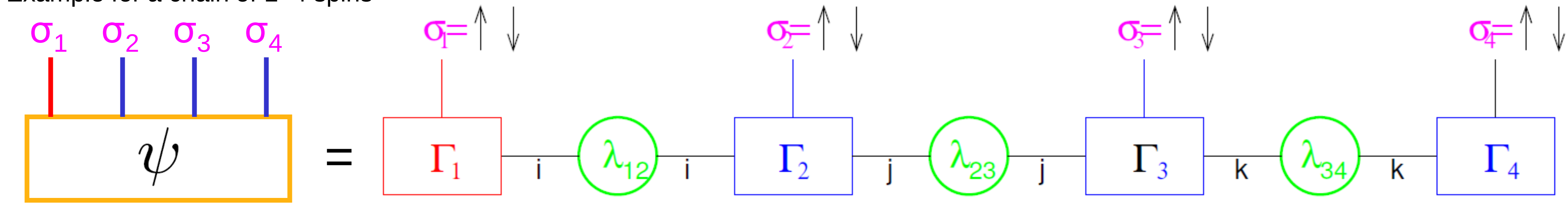
# Time Evolving Block Decimation (TEBD)

G. Vidal, PRL 2004

- **Matrix-product** representation of the wave-function

  Closely related to DMRG & tDMRG

Example for a chain of L=4 spins




$$\psi(\sigma_1,\sigma_2,\sigma_3,\sigma_4) = \sum_{i,j,k=1..n} \Gamma_1^{\sigma_1}(i)\lambda_{12}(i)\Gamma_2^{\sigma_2}(i,j)\lambda_{23}(j)\Gamma_3^{\sigma_3}(j,k)\lambda_3(k)\Gamma_4^{\sigma_4}(k)$$

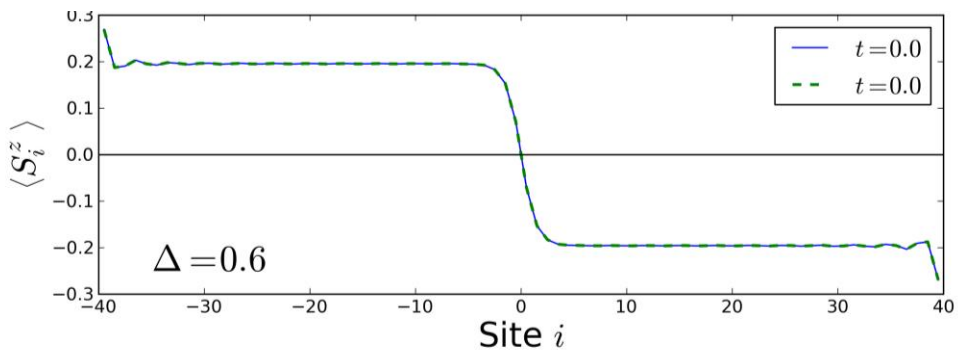
- This ansatz can encode any |Ψ> if the **internal dimension n** is equal to the total Hilbert space dimension n=2^L (… but really not useful in such a case !)

- One can limit ourselves to “small” **n** if |Ψ> has a « small » amount of **quantum entanglement**. If entanglement entropy S~log(L) then n~$L^\alpha$ is ok !

Review by U. Schollwöck, Annals of Phys. **326**, 96 (2011)

# Magnetization and entanglement entropy dynamics

TEBD simulation
L=80
Δ=0.6
M=80 Schmidt values



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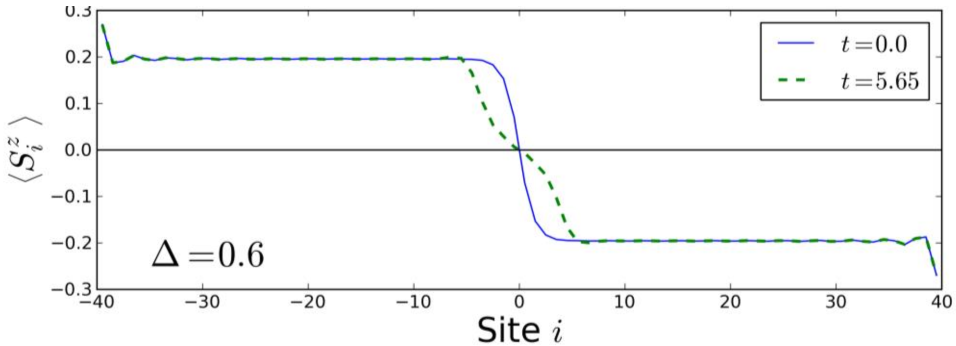

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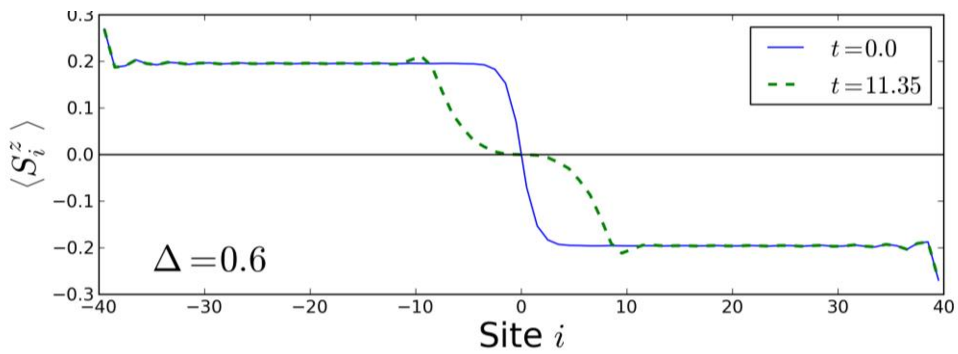

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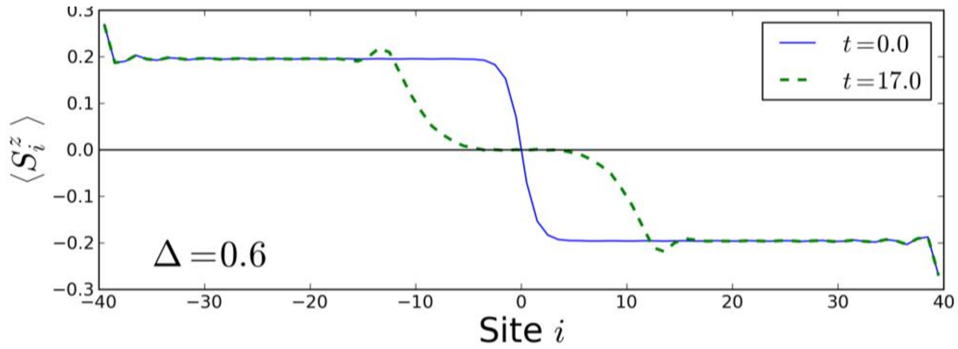

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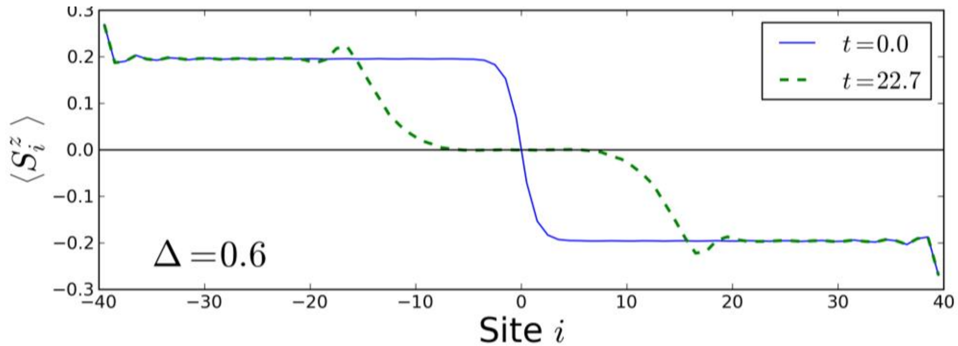

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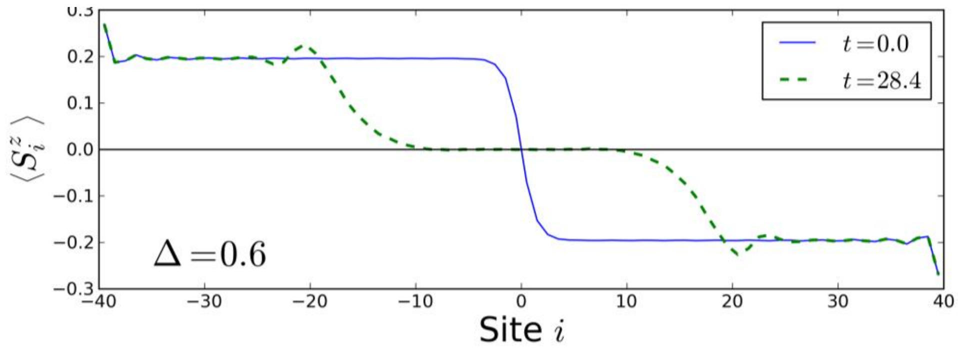

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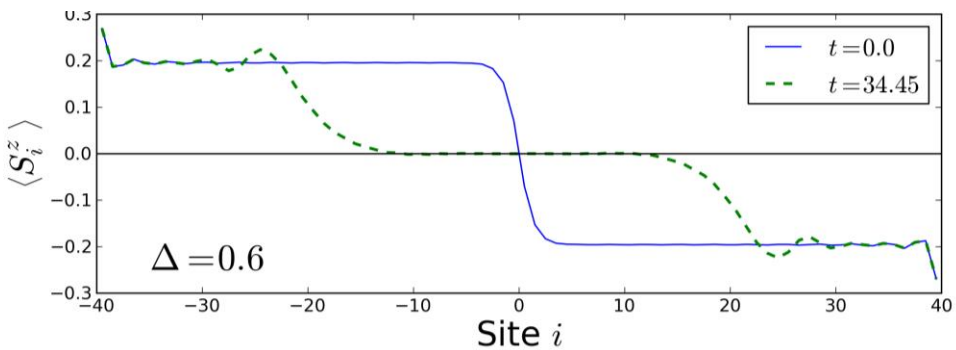

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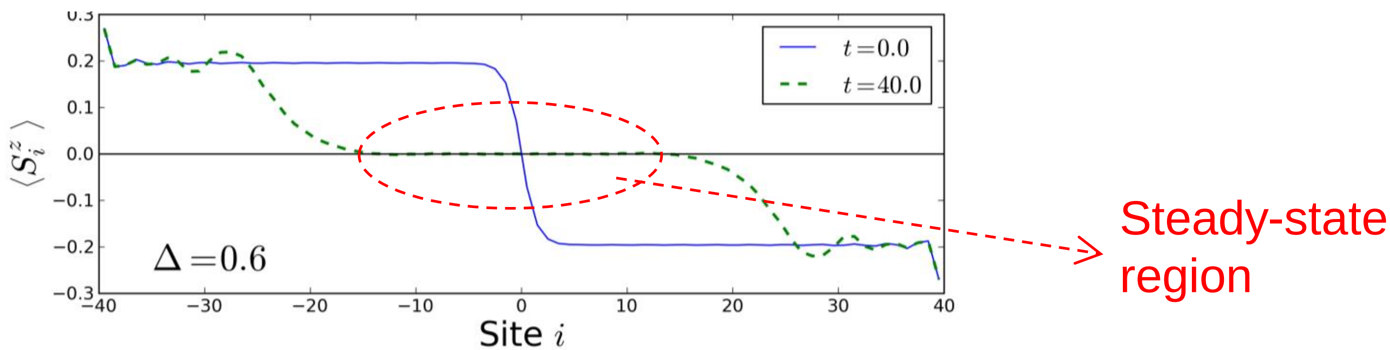
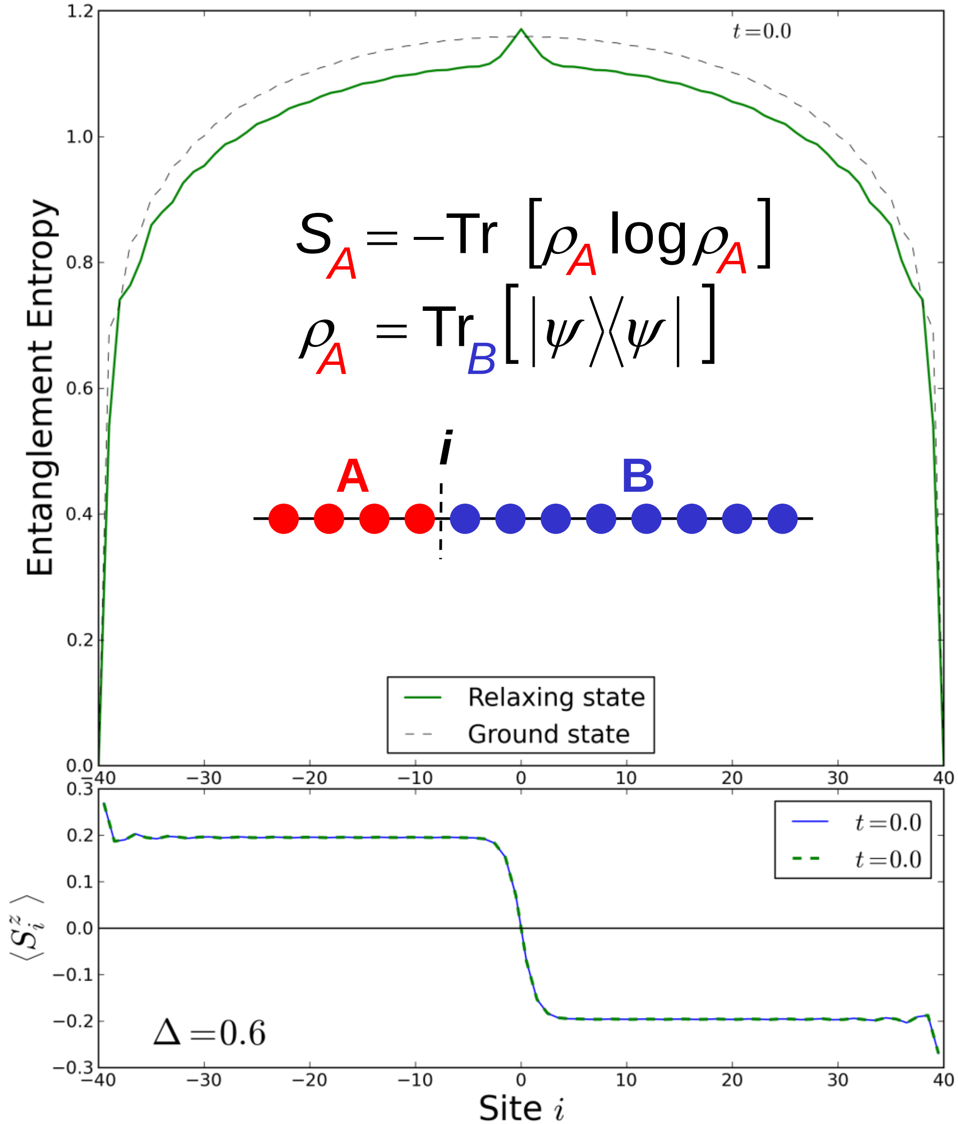



- Front propagation and flat magnetization region, qualitatively similar to the Δ=0 case.

# Magnetization and entanglement entropy dynamics

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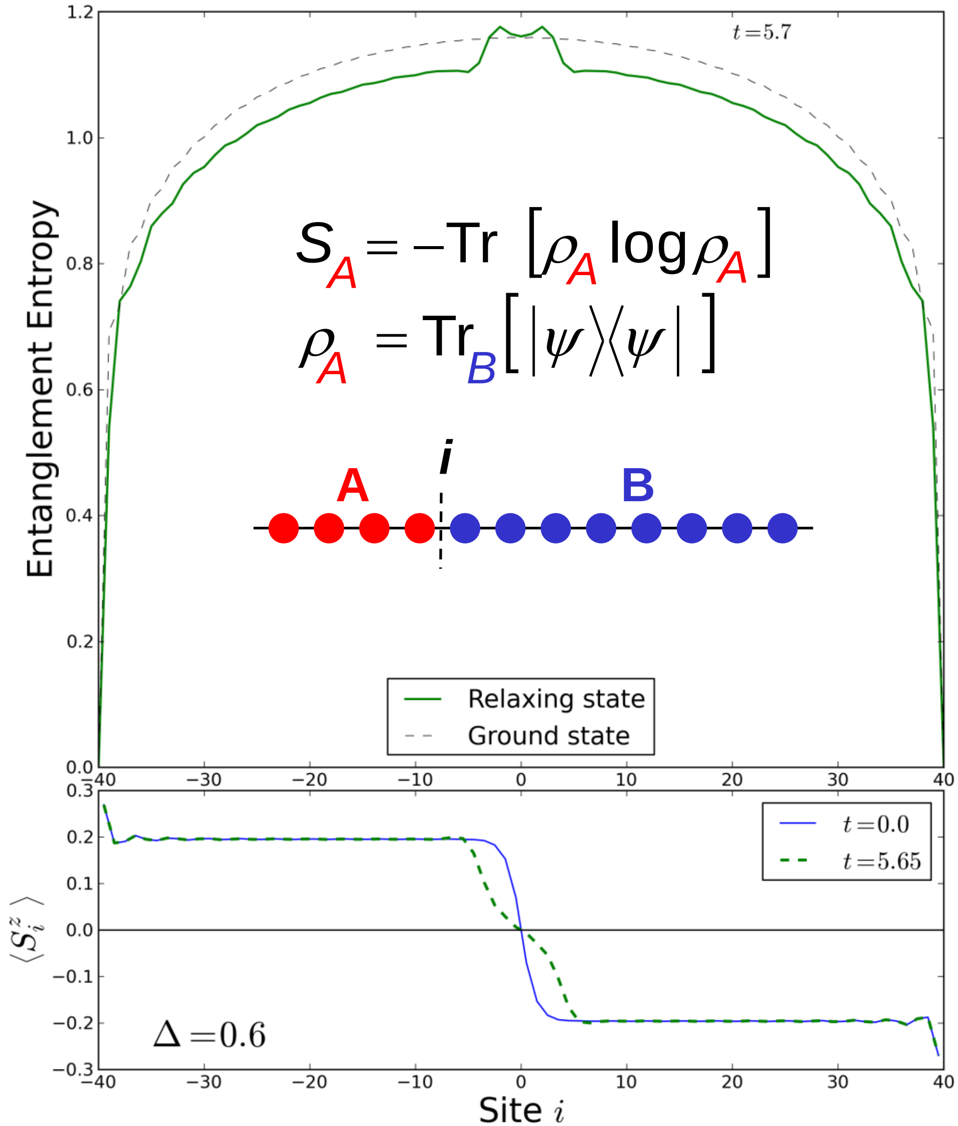


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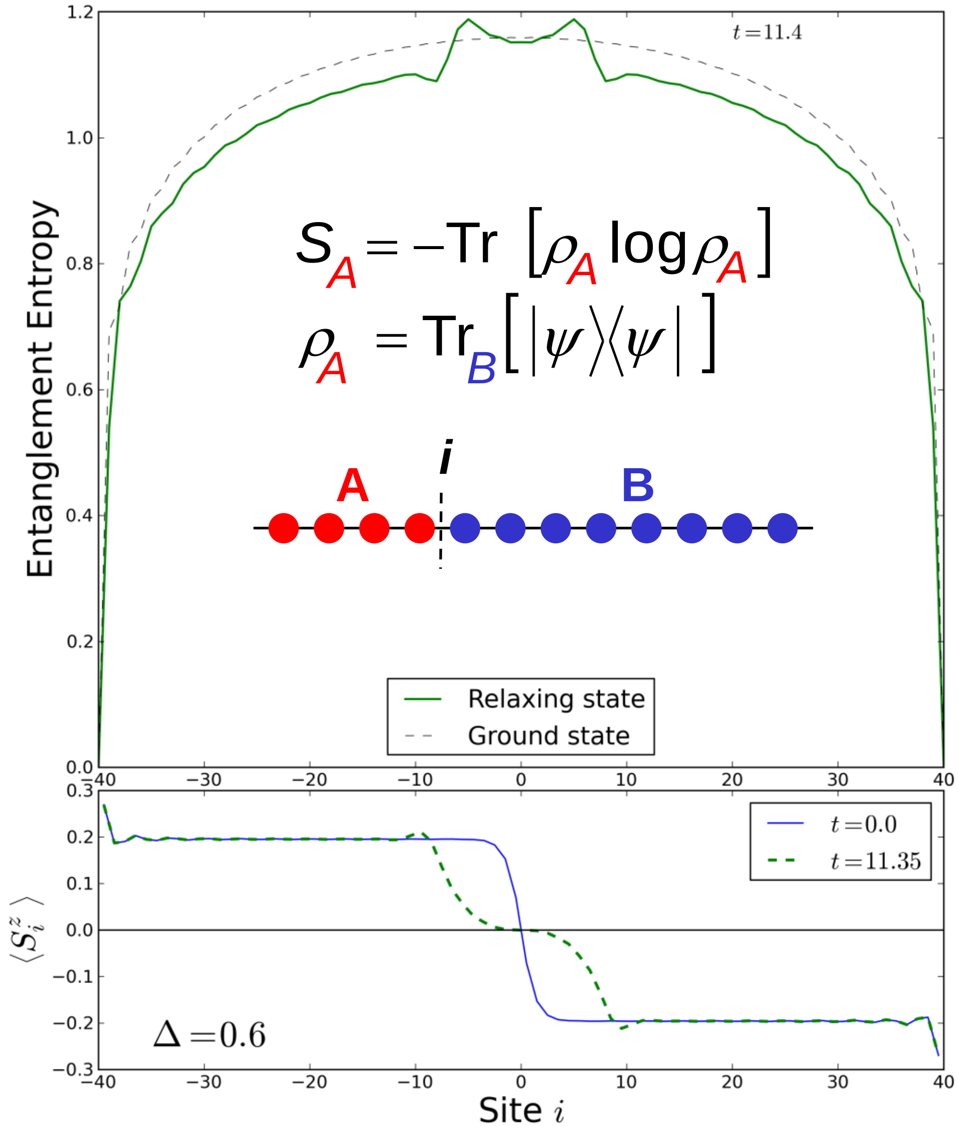


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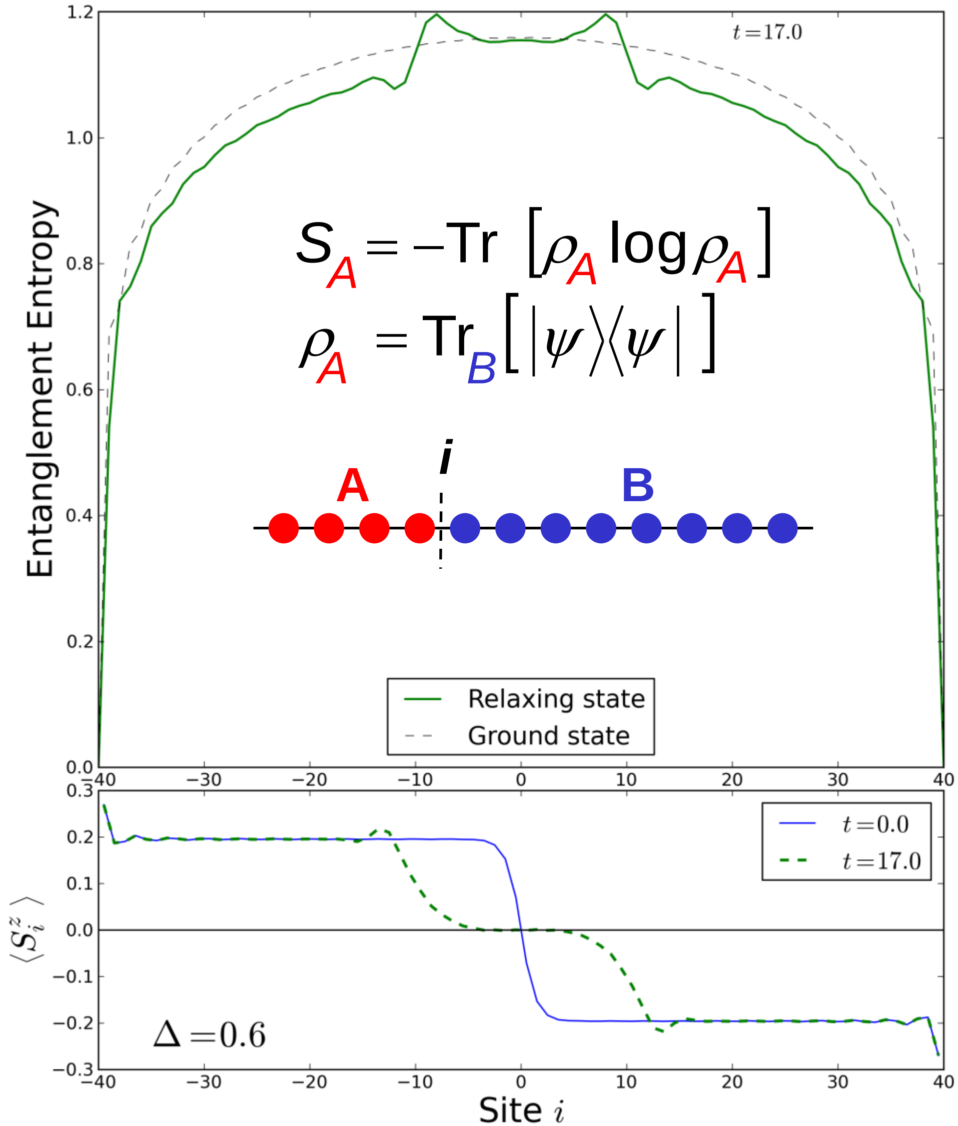


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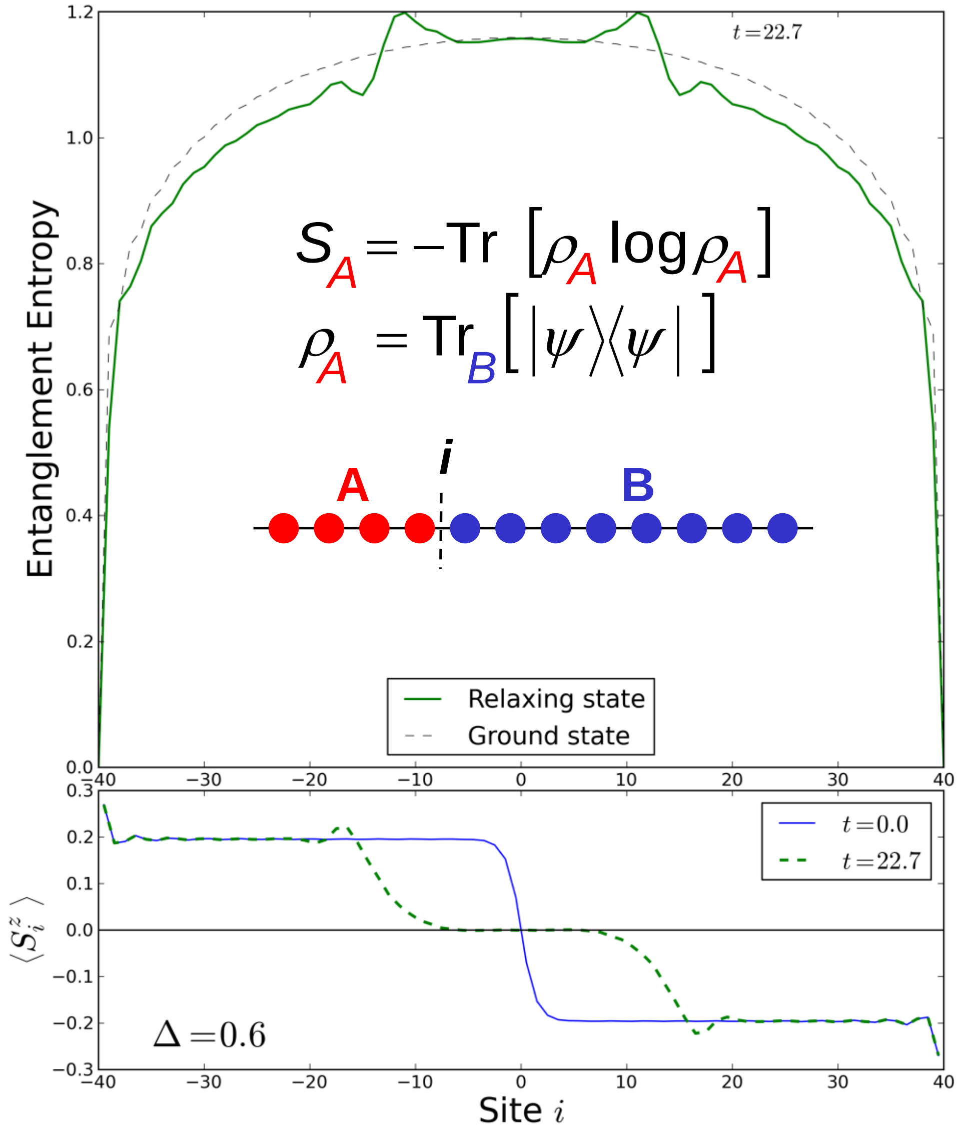


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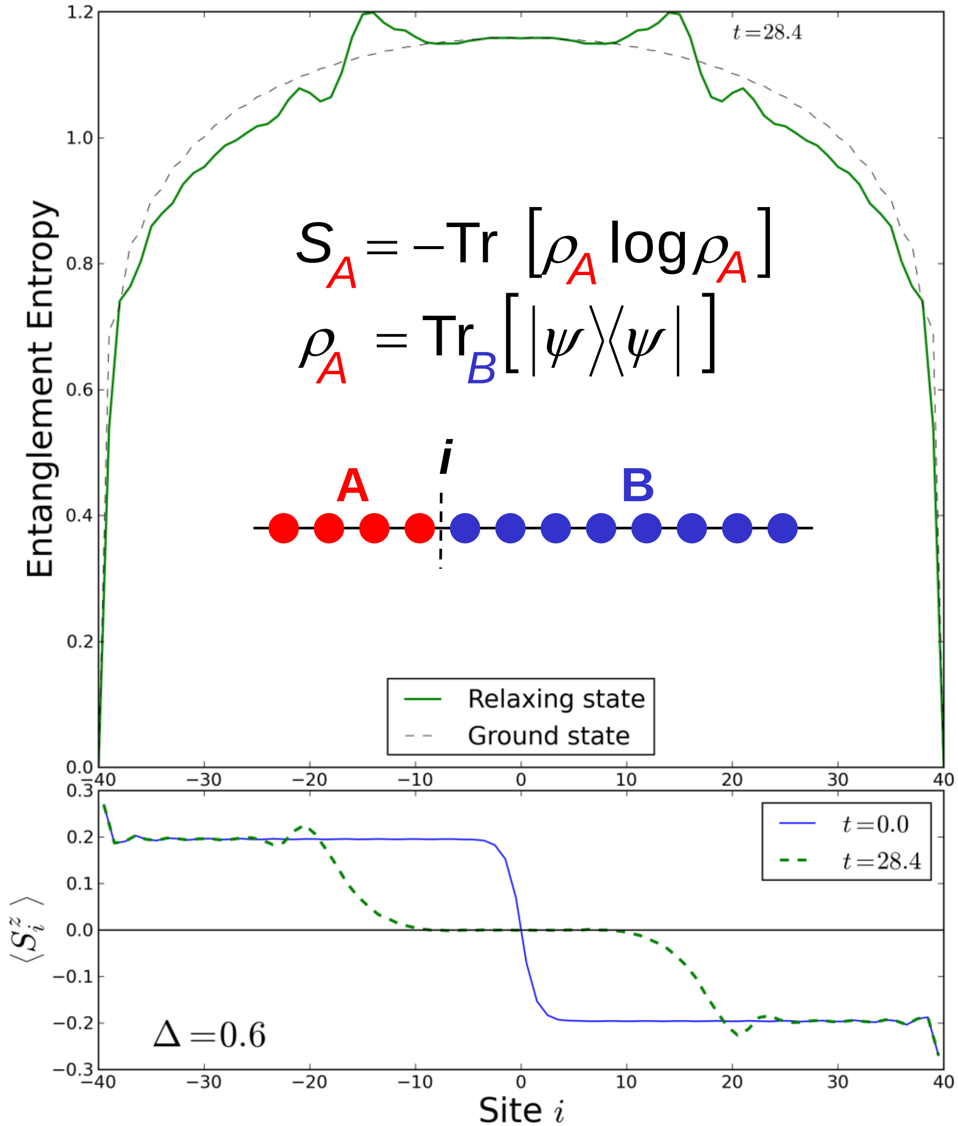


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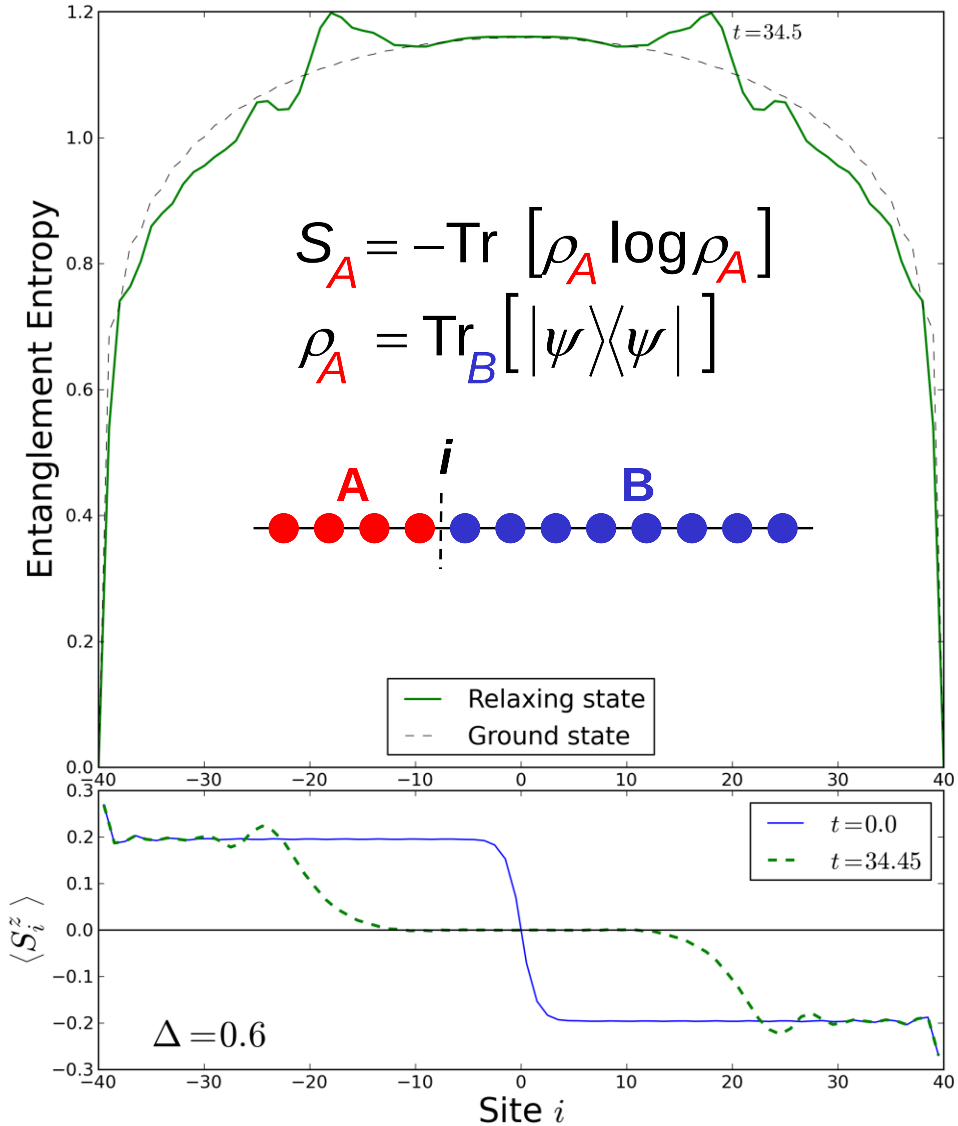


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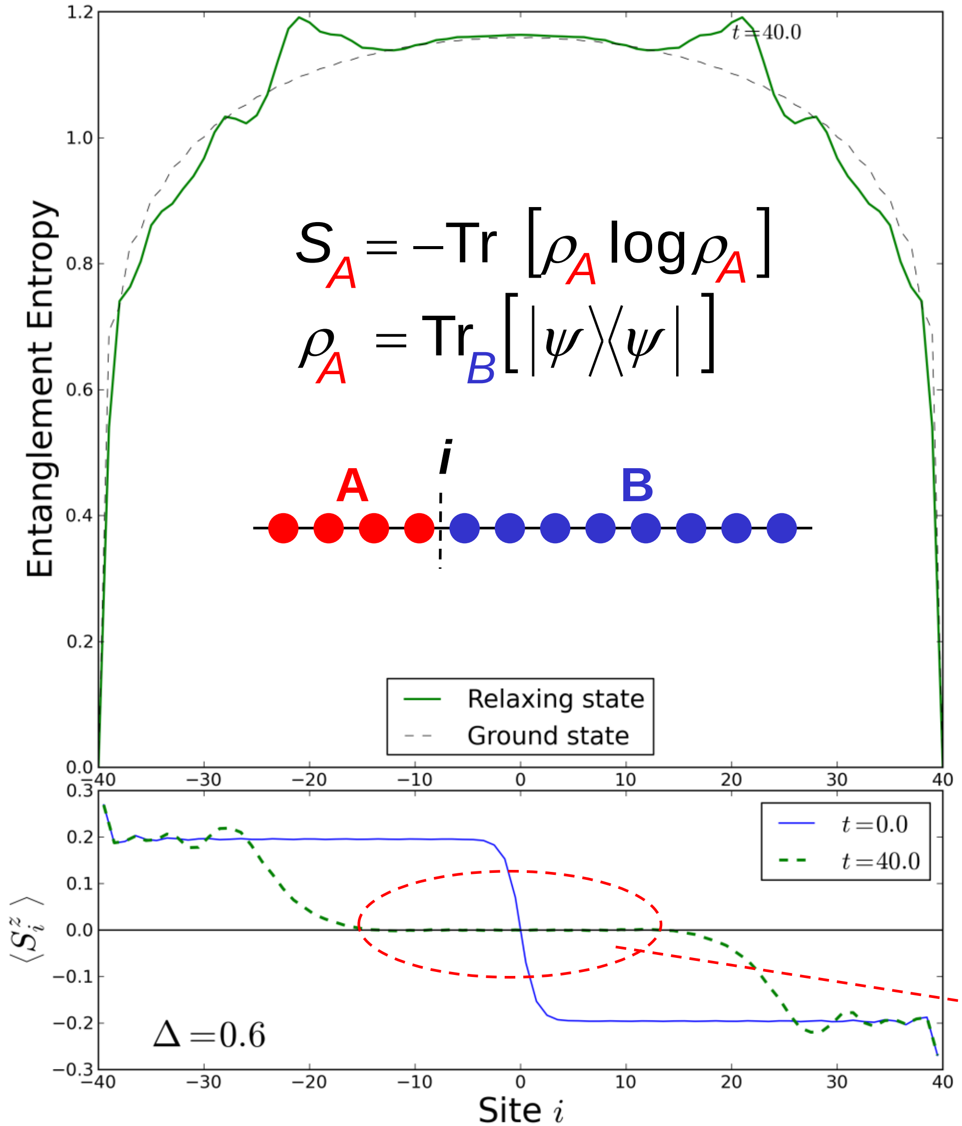



TEBD simulation
L=80
Δ=0.6
M=80 Schmidt values

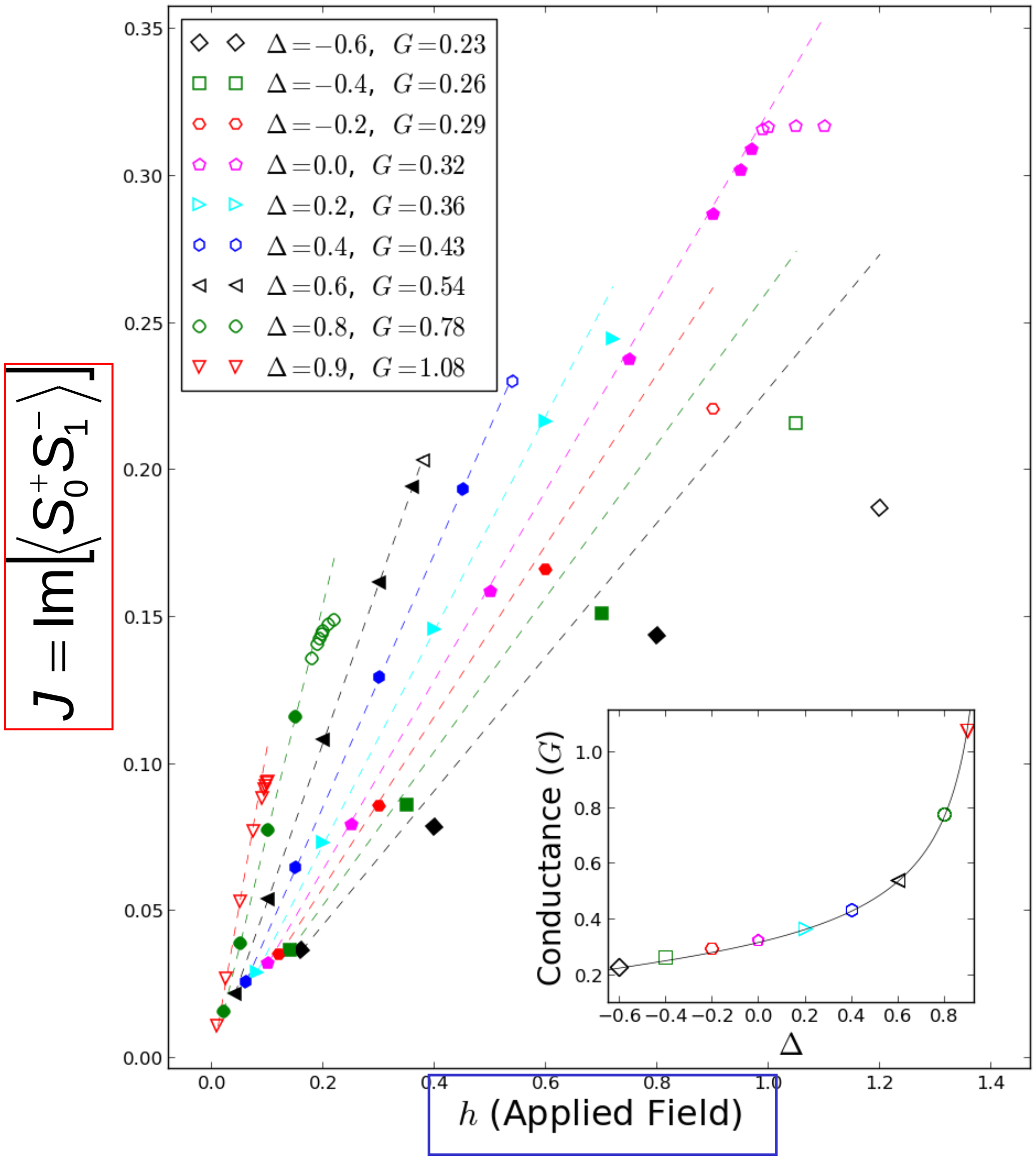
- Entanglement entropy stays small

Steady-state region

# Steady state

## = central region of the chain

# Current and conductance




Measure the current **J** in the center of the chain as a function of the magnetic field **h** applied in the initial state.

Compare with the prediction of the Tomonaga-Luttinger theory :

Conductance

$$J = G \cdot h$$

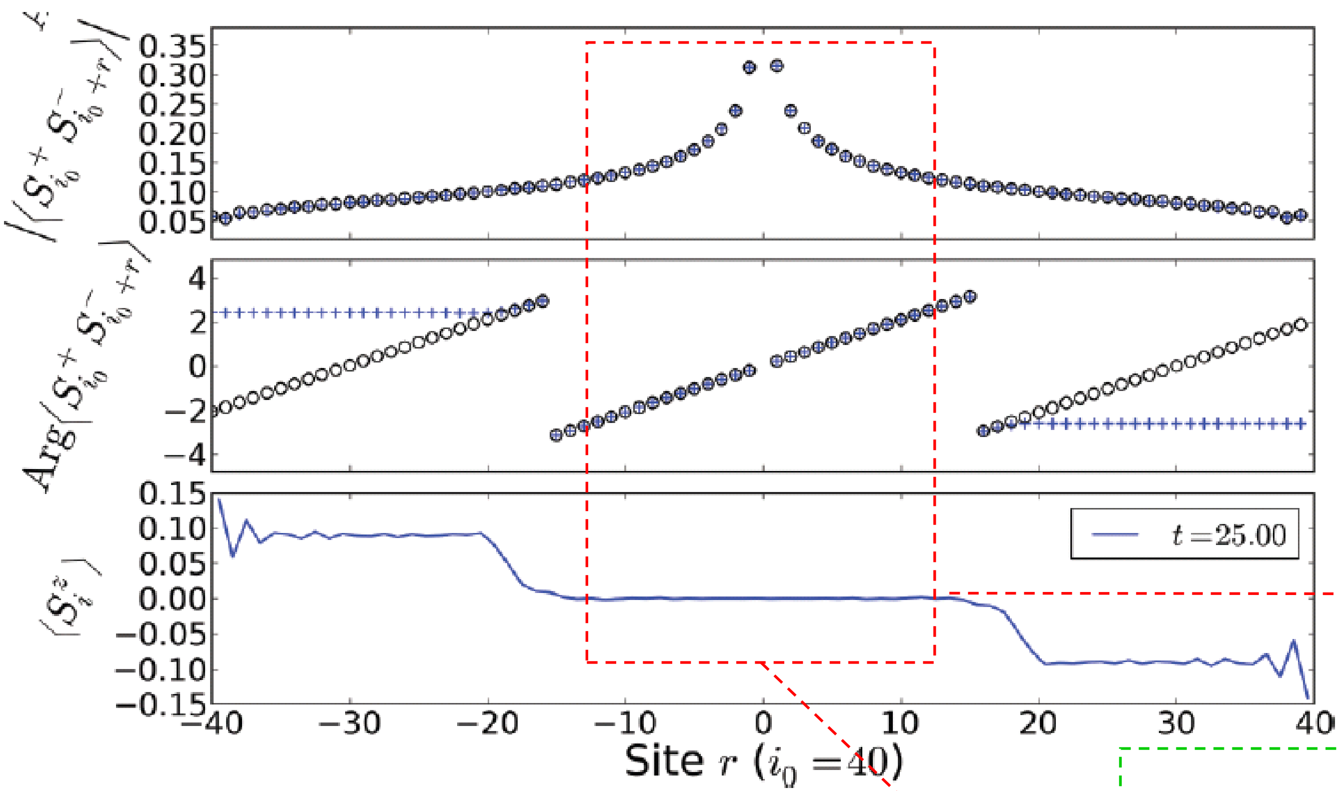
Luttinger parameter

$$G = \frac{K(\Delta)}{\pi}$$

$$K(\Delta) = \frac{\pi}{2\arccos(\Delta)}$$

Two closely related numerical studies:
Gobert et al., PRE 2005
Einhellinger,et al, PRB 2012.

# Correlations in the steady-state region




$$\Delta = 0.4$$

$$h / h_{\mathrm{sat}} = 0.25$$

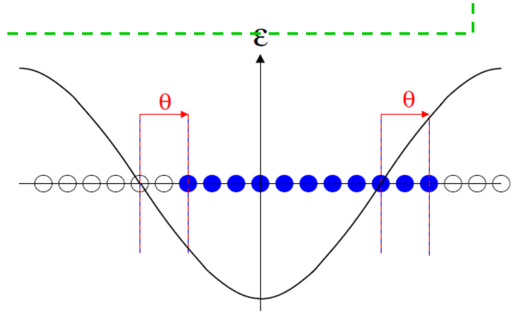
✚ $\langle S^+_{i0} S^-_{i0+r} \rangle_{\text{dynamics}}$

○ $\langle S^+_{i0} S^-_{i0+r} \rangle_{\text{ground st.}} \times \exp(i\theta r)$

Steady-state region

**Weak current regime :**

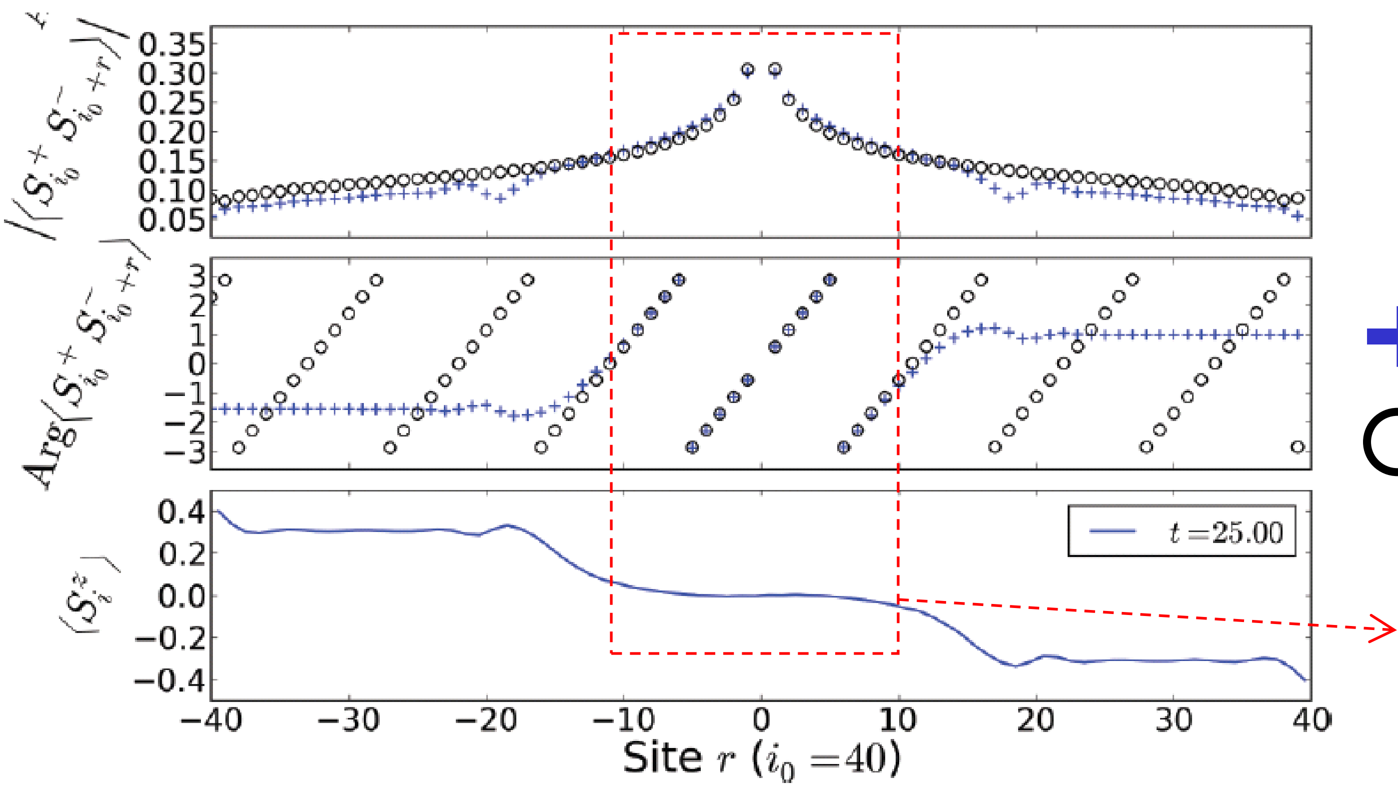
$$\frac{\langle S^+_i S^-_{i+r} \rangle_{\text{steady st.}}}{\langle S^+_i S^-_{i+r} \rangle_{\text{ground st.}}} \approx \exp(i\theta r)$$




Correlations in the steady state are simply related to the ground state correlations !

Boost in momentum space
↔ phase factor in real space

# Correlations in the steady-state region




$\Delta = 0.6$

$h / h_{\text{sat}} = 0.75$

+ $\langle S^+_{i0} S^-_{i0+r} \rangle_{\text{dynamics}}$

○ $\langle S^+_{i0} S^-_{i0+r} \rangle_{\text{ground st.}} \times \exp(i\theta r)$

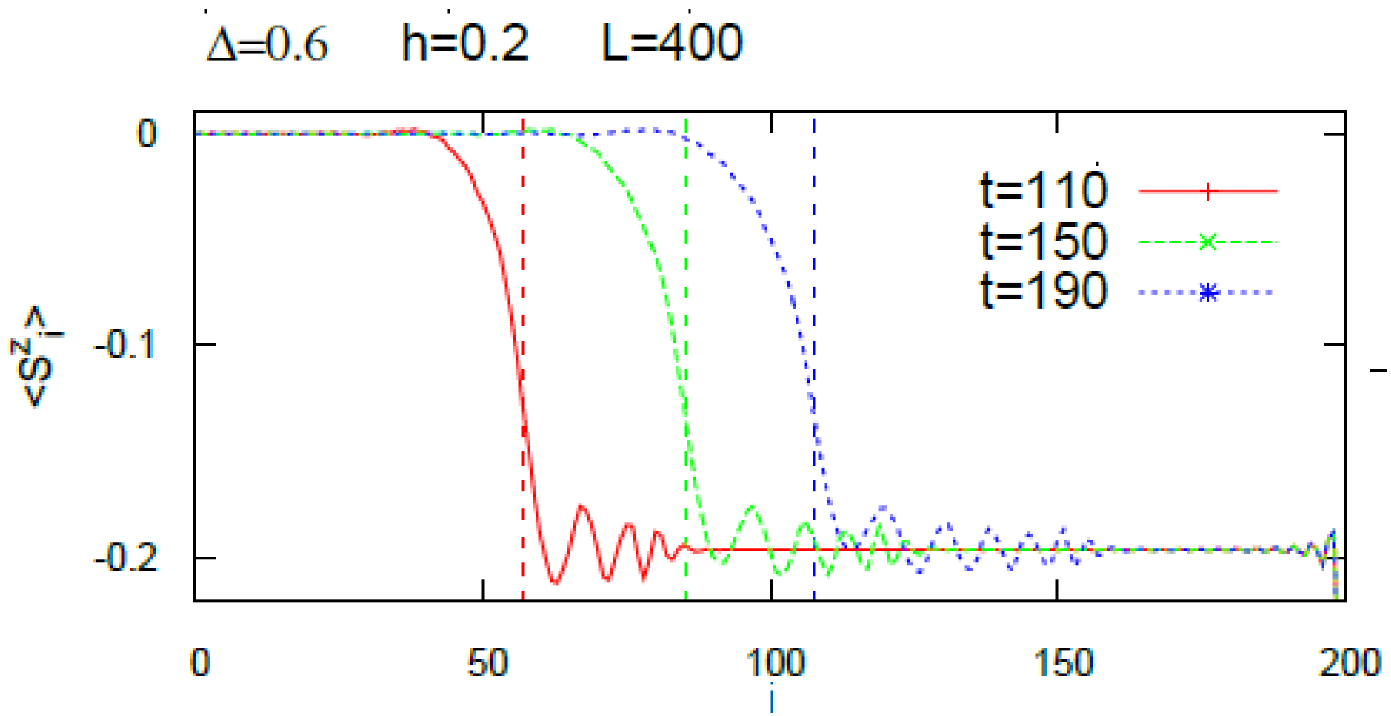
**Intermediate current regime :** $\dfrac{\langle S^+_i S^-_{i+r} \rangle_{\text{steady st.}}}{\langle S^+_i S^-_{i+r} \rangle_{\text{ground st.}}} \approx \exp(i\theta r)$

Still a **very good approximation. Why ?**

See also: bosonization approach by Lancaster and Mitra, Phys. Rev. E **81**, 061134 (2010).

# Front propagation

# Front propagation

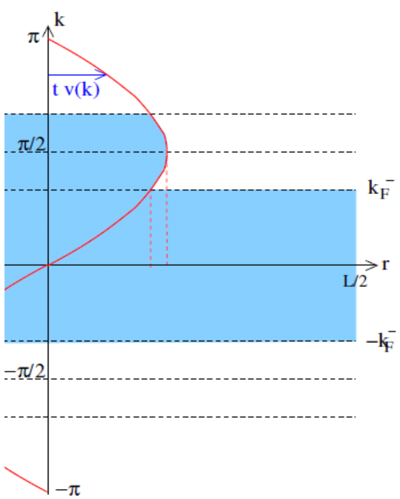


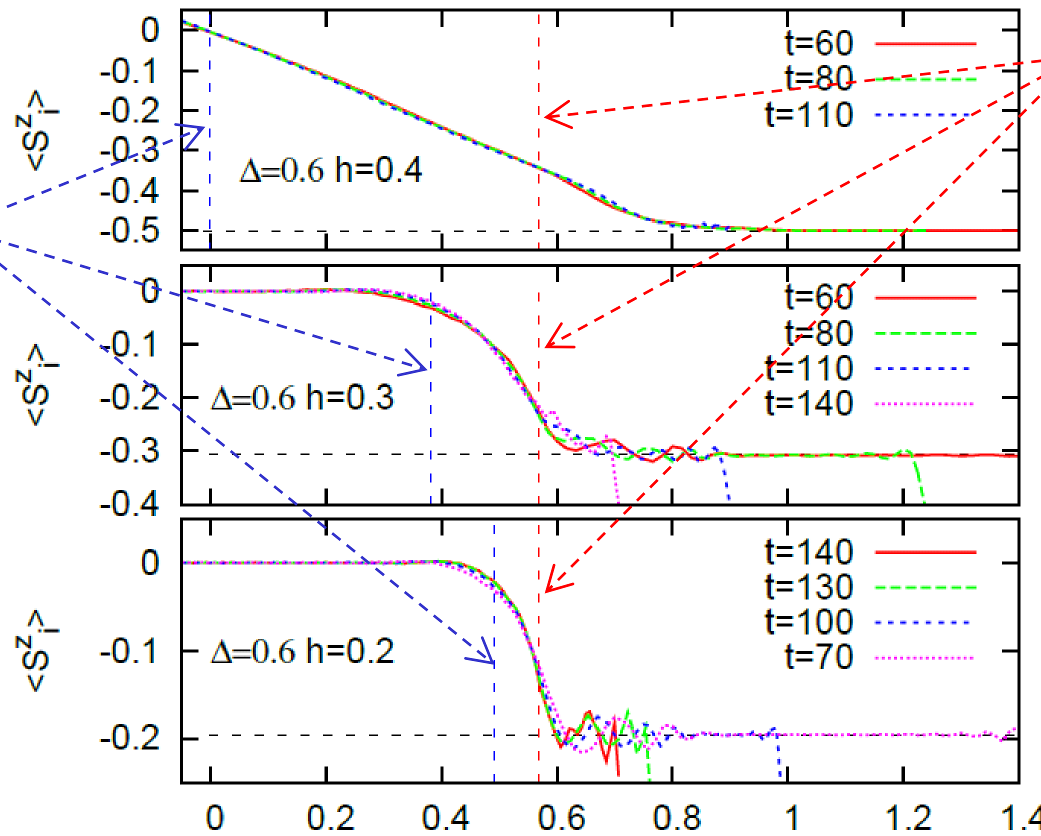

- Velocity(ies) of the front ?
- Shape of the front ?
- Nature of the density oscillations ?

# Front shape & velocities

XXZ spinon velocity at $\langle S^z \rangle = m_0$

v= … solve some integral (Bethe) equations …



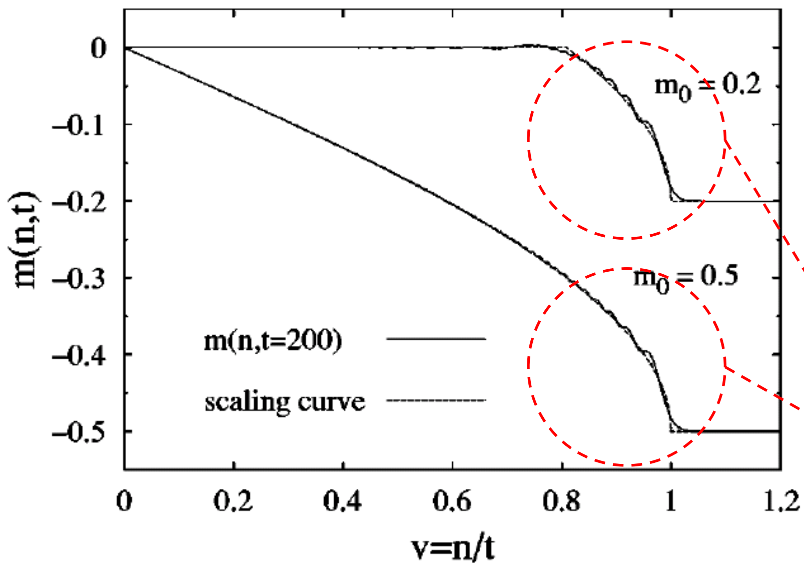




XXZ spinon velocity at $\langle S^z \rangle = 0$

$$v = \frac{\pi}{2} \sin(\gamma)/\gamma$$
$$\cos(\gamma) = -\Delta.$$

Position **i** rescaled with time **t** (velocity)

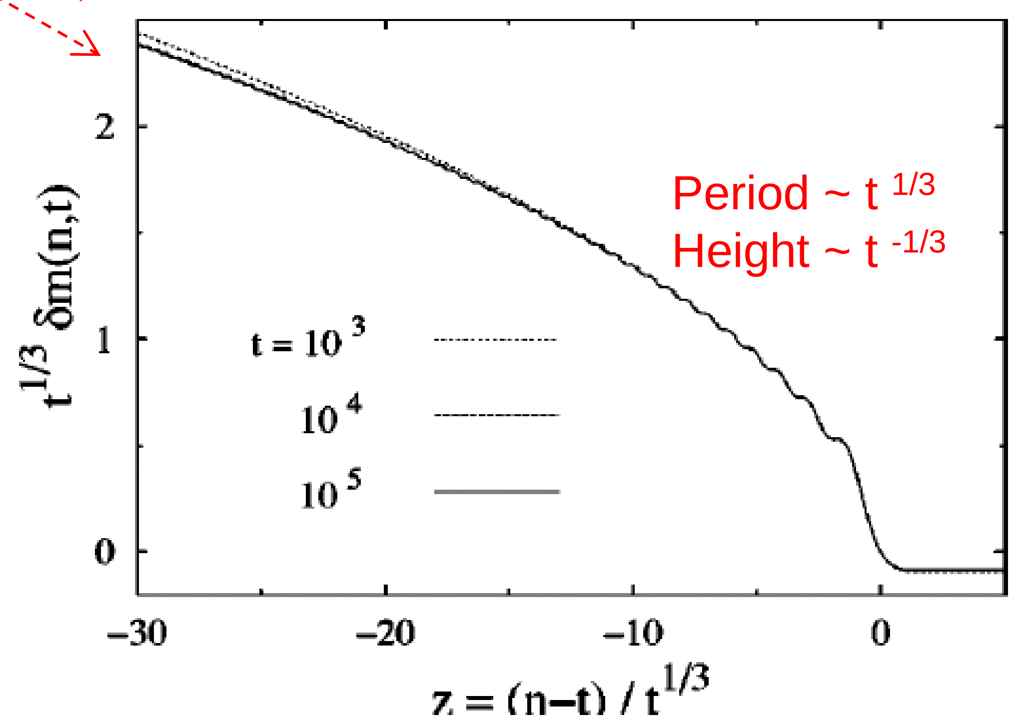
# Density oscillations in the front (Δ=0)



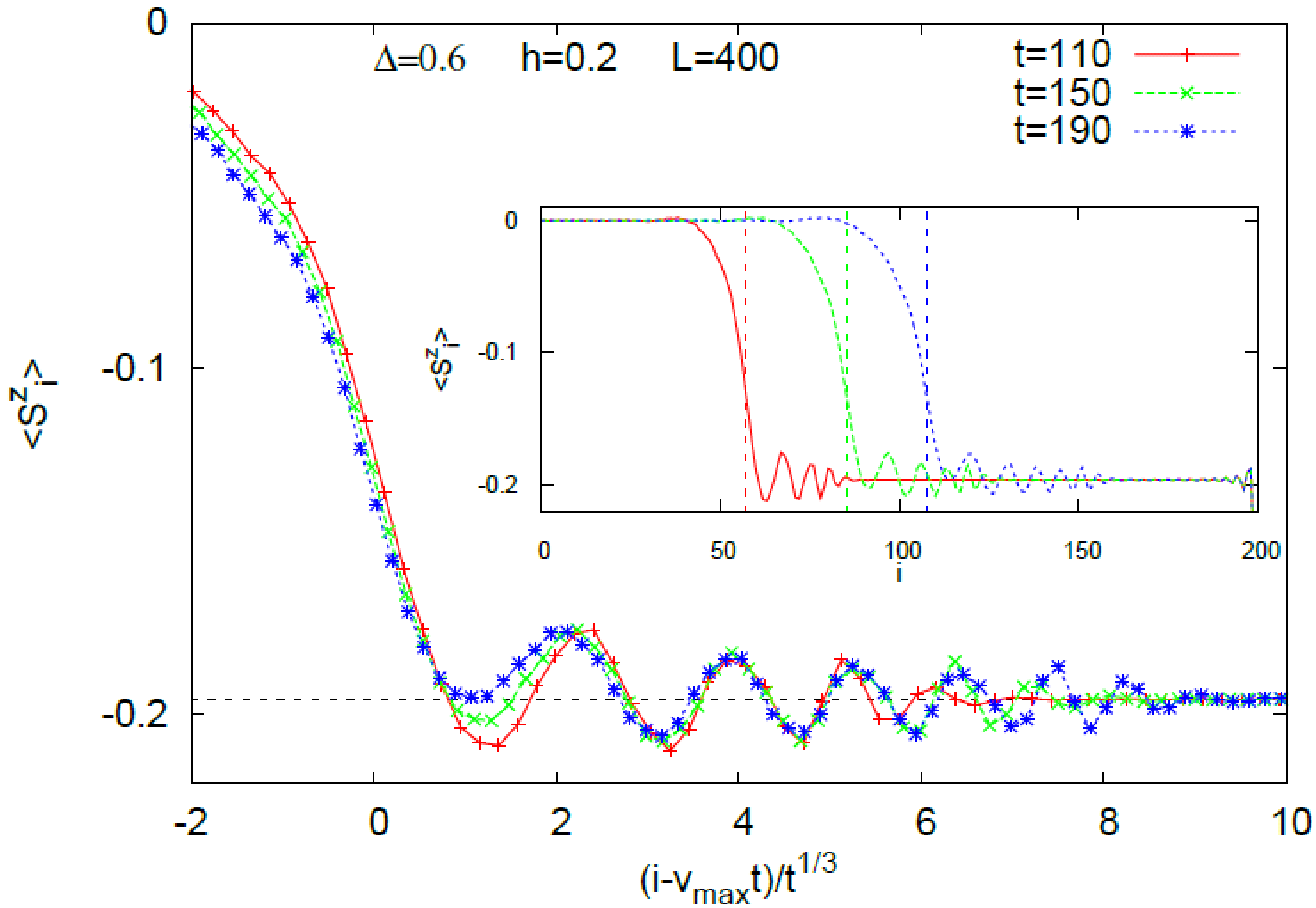

PHYSICAL REVIEW E 69, 066103 (2004)

**Dynamic scaling of fronts in the quantum *XX* chain**

V. Hunyadi,[1] Z. Rácz,[2] and L. Sasvári[1]



# Density oscillations *ahead* of the front (Δ≠0)



# Interating case (Δ≠0): hydrodynamic description ?

PHYSICAL REVIEW A **86**, 033614 (2012)

**Hydrodynamics of cold atomic gases in the limit of weak nonlinearity, dispersion, and dissipation**

Manas Kulkarni[1,2] and Alexander G. Abanov[3]

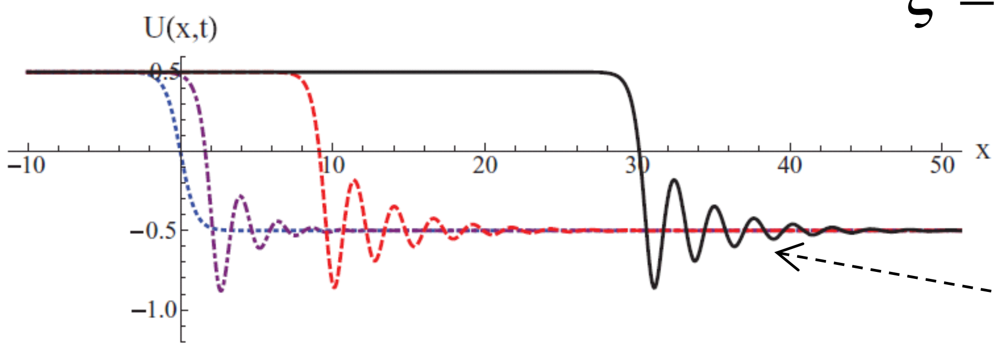
Kortweig - De Vries (KdV) - equation

$$\frac{\partial}{\partial t}u + \zeta u \frac{\partial}{\partial \xi}u - \alpha \frac{\partial^3}{\partial \xi^3}u = 0$$

$$\xi = x - vt$$

Dispersion

Non-linearity

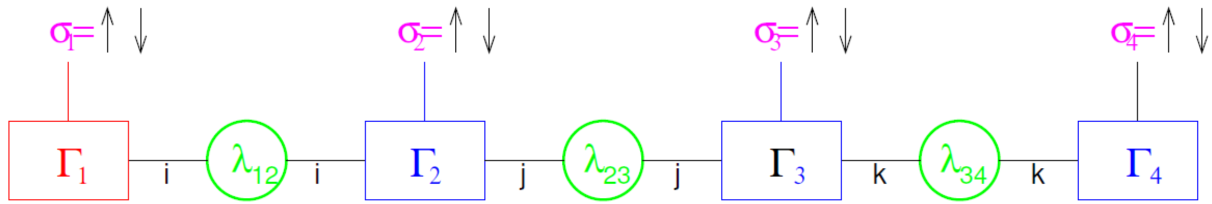


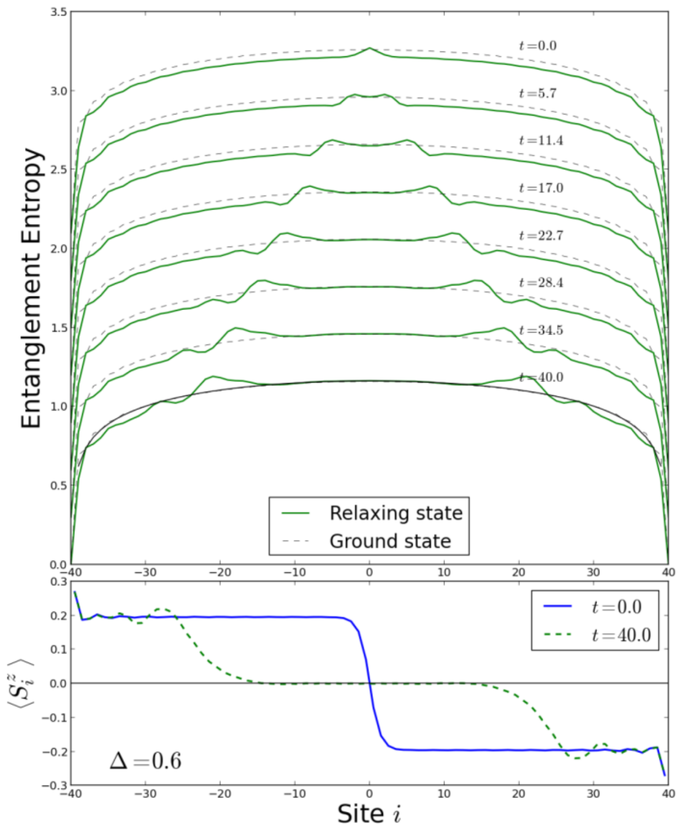

Solitons

FIG. 2. (Color online) The evolution of the initial steplike profile (blue dotted) governed by the KdVB equation (25) in the dispersive shock-wave regime. The dimensions of $x$ and $y$ axes are $\mu$m and

Relation to the front propagation
In the XXZ spin chain ?
Work in progress….

# Summary




- TEBD: computes the real-time dynamics of 1d many-body quantum systems
- Antal's quench: low-entanglement steady-state
- Access to front shape, velocities, oscillations
- Extended linear regime where the current-carrying steady-state is well described by the "boost" picture.
- Front physics ?