Workshop on Theory & Practice of
Adiabatic Quantum Computations & Quantum Simulation

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Universal scaling for a quantum discontinuity critical point and an adiabatic time evolution

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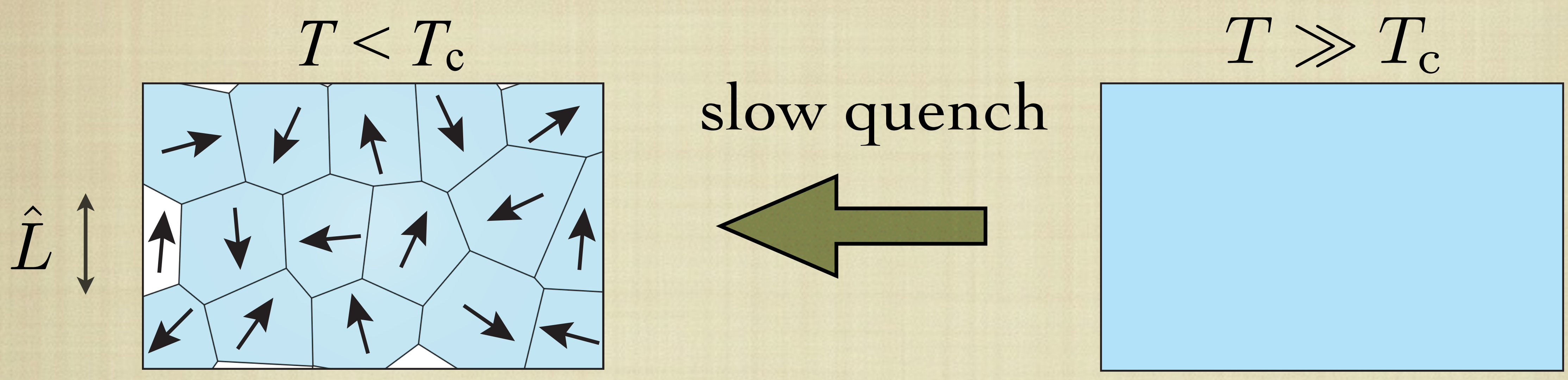
Introduction

- Slow quench across a phase transition



Final state ?

locally ordered

-with inhomogeneity

-defects generated

equilibrium at high T

disordered

Kibble-Zurek mechanism

Introduction

- Kibble-Zurek mechanism

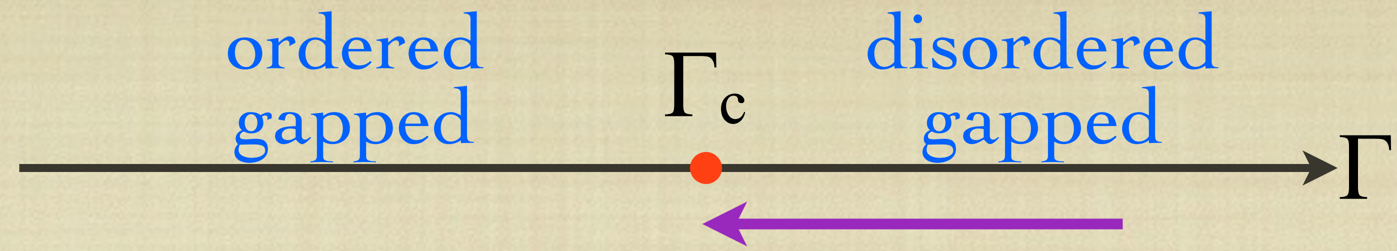
  -originally proposed for the evolution of universe

  -experimentally studied in condensed matter systems (cold atoms, trapped ions, etc.) [Greiner et al (2002), Sadler et al (2006)]

  -dynamics near a quantum phase transition is crucial to quantum annealing

[Zurek et al, Polkovnikov, '05]

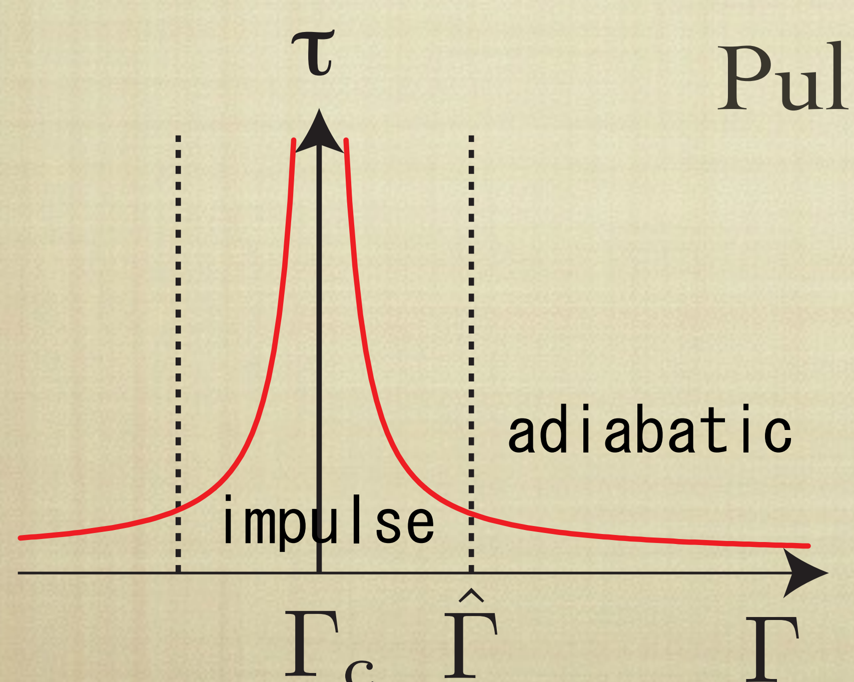
Kibble-Zurek scaling for a continuous (2nd-order) QPT



$$H(\Gamma) = H + \Gamma(t)H' \qquad \Gamma(t) = \Gamma_c - |\Gamma_c|\frac{t}{\tau_Q} \qquad (t : -\infty \to 0)$$

Assume an isolated system and starting from the ground st.

Instantaneous energy gap: $\Delta(t) \sim |\Gamma(t) - \Gamma_c|^{z\nu} \sim \left|\frac{t}{\tau_Q}\right|^{z\nu}$



Pulse-impulse approx.: $\boxed{\tau(t) \sim \Delta(t)^{-1} = |t|}$

$$|\hat{t}| \sim \tau_Q^{z\nu/(z\nu+1)}, \quad \hat{\Delta} \sim \tau_Q^{-z\nu/(z\nu+1)}$$

$$\boxed{\hat{L} \sim \hat{\Delta}^{-1/z} \sim \tau_Q^{\nu/(z\nu+1)}}$$

ν and z are critical exponents

- **Kibble-Zurek scaling** for a discontinuous (1st-order) QPT?

Not known, so far

⇐ -Correlation length remains finite
-Universality is absent

- **Our study focuses on**

1)universality in a particular class of discontinuous PTs

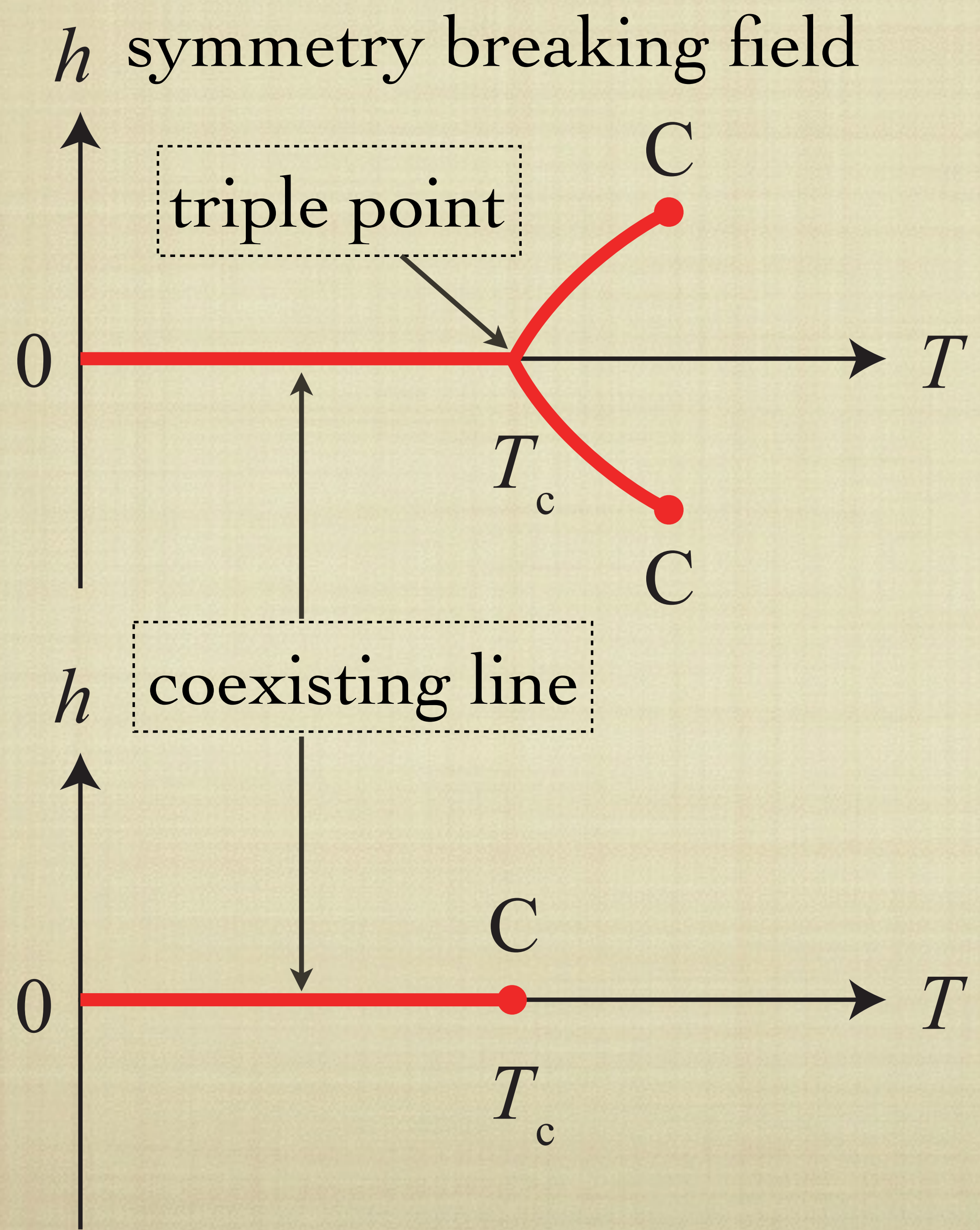
2)Kibble-Zurek scaling for such discontinuous PTs

Discontinuous phase transitions

General picture

[Fisher and Berker, '82]

Assume an Ising-like system



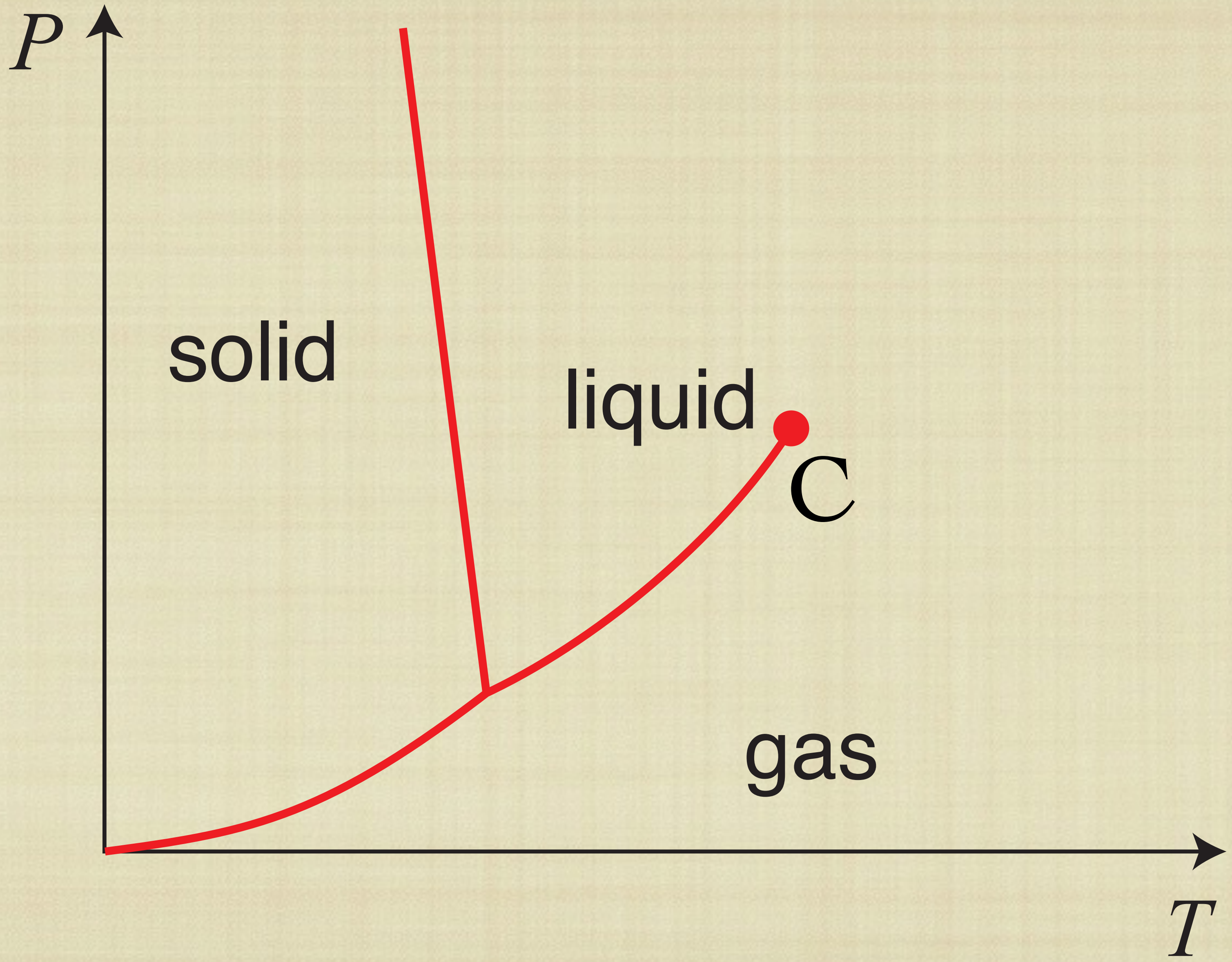
upper picture:

- with metastable states
- Landau picture applies

lower picture:

- without metastable states

Phase diagram of water

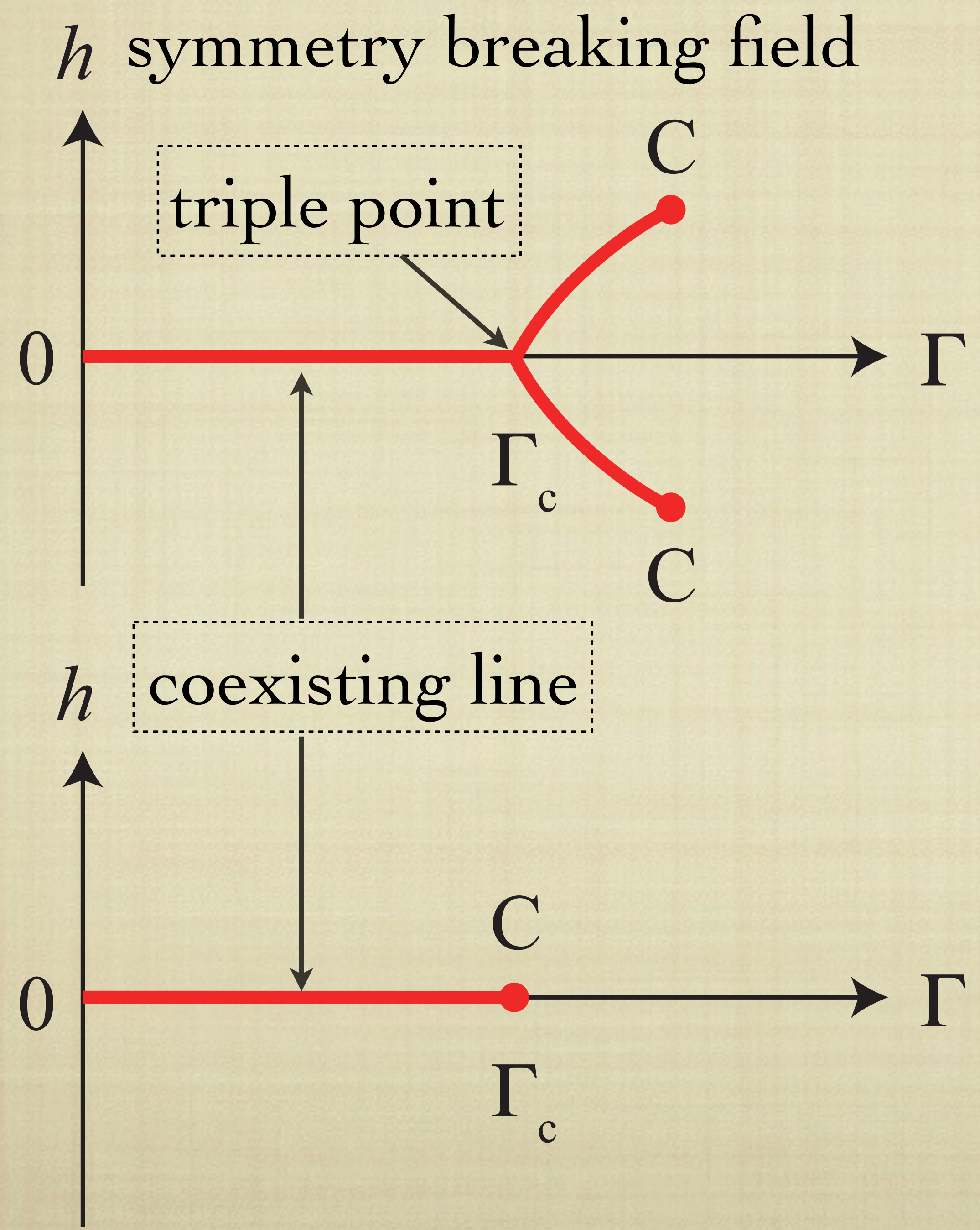


Question: does a discontinuity critical point exist?

Quantum discontinuity critical point

<u>General picture</u> of a discontinuous quantum phase transition

Assume an Ising-like system



upper picture:

- with metastable states
- Landau picture applies

lower picture:

- without metastable states

We focus on the lower one!

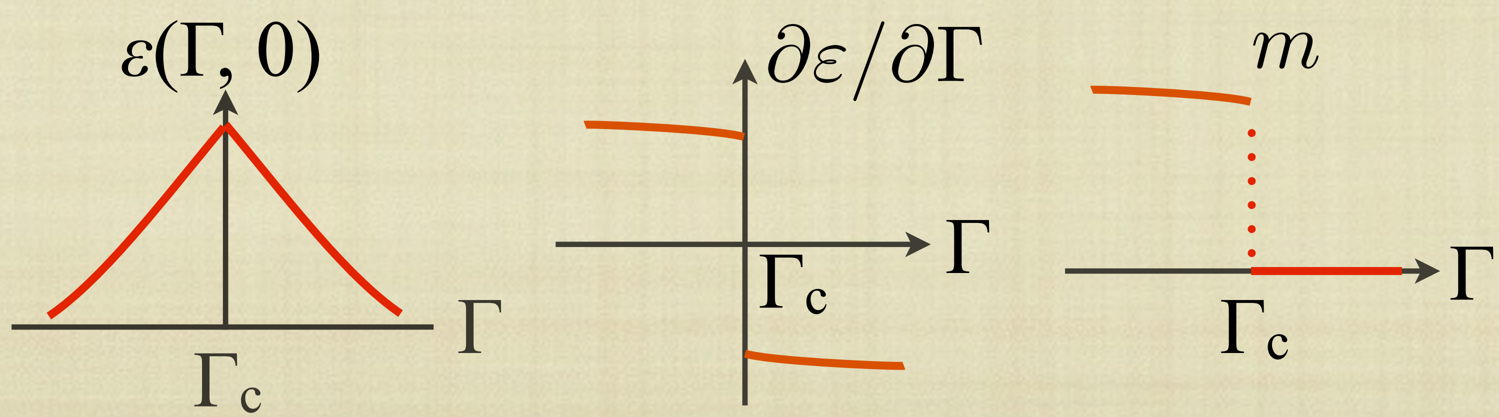
Quantum discontinuity critical point

$\varepsilon_g(\Gamma, h)$: GS energy density Γ: control parameter

h: symmetry breaking field

Let us assume that at $h = 0$

- GS energy density $\varepsilon(\Gamma, 0)$ is continuous
- $\dfrac{\partial \varepsilon(\Gamma,0)}{\partial \Gamma}$ and $m(\Gamma,0) = -\dfrac{\partial \varepsilon(\Gamma,0)}{\partial h}$ are discontinuous at Γ_c



$$\varepsilon(\Gamma,0) - \varepsilon(\Gamma_c,0) \sim |\Gamma - \Gamma_c|^{2-\alpha}, \quad m \sim |\Gamma - \Gamma_c|^{\beta}$$

$$\Rightarrow \quad \boxed{\beta = 0} \quad \boxed{\alpha = 1}$$

Quantum discontinuity critical point

<u>Scaling theory</u>

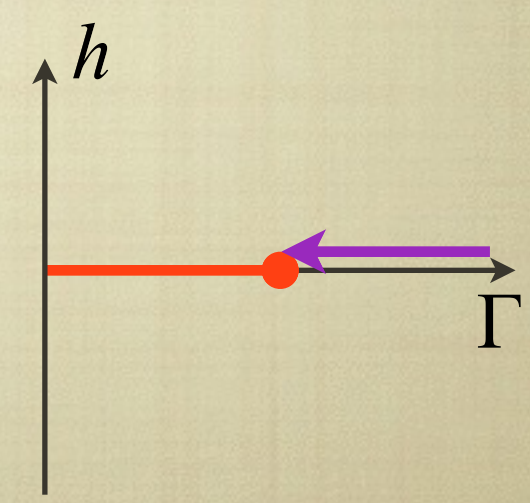
$\boxed{\alpha = 1}$ & scaling relations $\boxed{2 - \alpha = (d + z)\nu}$

(d: spatial dimension)

$\Rightarrow$ $$\boxed{\nu = \frac{1}{d + z}}$$ diverging correlation length!

<u>Kibble-Zurek Scaling</u>

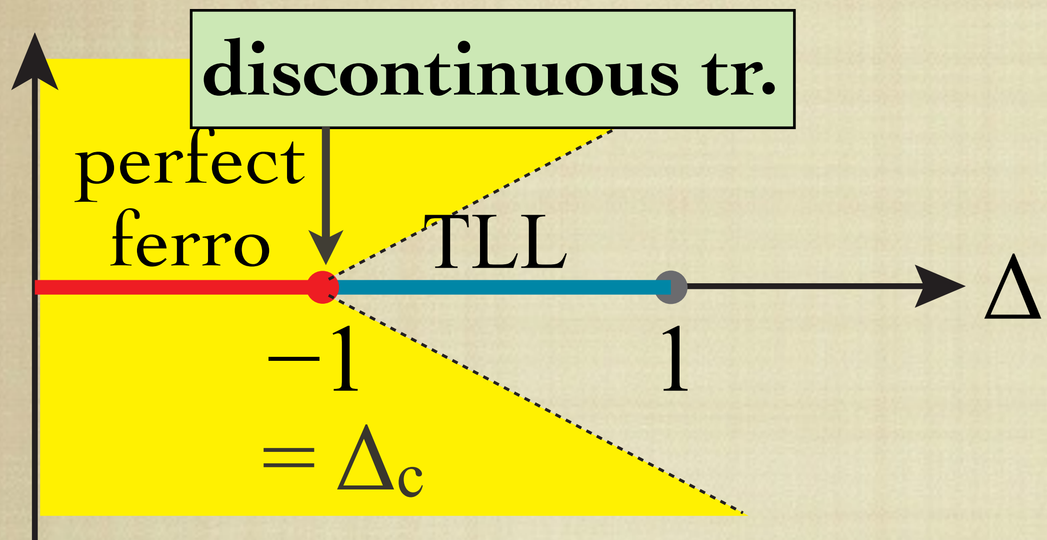
$$\Gamma(t) = \Gamma_{\mathrm{c}}(1 - t/\tau_Q) \text{ with } t : -\infty \to 0$$



$\Rightarrow$ $$\boxed{\hat{L} \sim \tau_{\mathrm{Q}}^{\nu/(z\nu+1)} \sim \tau_{\mathrm{Q}}^{1/(d+2z)}}$$

The XXZ chain

$$H = \sum_i (\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_i^y + \Delta \sigma_i^z \sigma_{i+1}^z)$$



GS energy density near $\Delta = \Delta_c$

$$\varepsilon(\Delta) - \varepsilon(\Delta_c) \sim \begin{cases} \Delta - \Delta_c & (\Delta < \Delta_c) \\ (\Delta - \Delta_c)^{3/2} & (\Delta > \Delta_c) \end{cases}$$

(in the subspace of $\sigma^z_{\mathrm{tot}} = 0$)

Δ_c is a quantum discontinuity critical point!

excitation spectrum at $\Delta = \Delta_c$: $E_k \sim k^2$ ⇒ $\boxed{z = 2}$

excitation gap near $\Delta = \Delta_c$: $\mathit{\Delta} E \sim |\Delta - \Delta_c|^{z\nu}$

⇒ $\boxed{\nu = \frac{1}{2}}$ $\left(\neq \frac{1}{d+z} \right)$ **inconsistent!**

Modified scaling theory for a QDCP

$\alpha_-,\ \nu_-,\ z_- \quad z \quad \alpha_+,\ \nu_+,\ z_+ \quad \Gamma$

Γ_c

Assumptions (− for the left, + for the right, $\delta = \Gamma - \Gamma_c$)

i)excitation spectrum $\boxed{E_k^{(\pm)} \sim |\delta|^{\theta_\pm} k^{z_\pm} + k^z}$ $(z_\pm \le z)$

dimensional consideration $\Rightarrow$ $\theta_\pm + z_\pm \nu_\pm = z\nu_\pm$

ii)GS energy density $\boxed{\varepsilon(\Gamma) - \varepsilon(\Gamma_c) \sim |\delta|^{2-\alpha_\pm} \sim |\delta|^{z\nu_\pm} \xi^{-d}}$

iii)effective correlation length $\boxed{\xi \sim 1 + A_\pm |\delta|^{-\nu_\pm}}$ $(A_\pm \ge 0)$

note that if $A_- = 0$, then $\xi \sim 1$ $\Leftarrow$ the case with **no fluctuation**

iv) $\boxed{\alpha_- = 1}$ (one of $\alpha_\pm$ must be 1, due to the discontinuity of $\partial\varepsilon/\partial\Gamma$ at Γ_c)

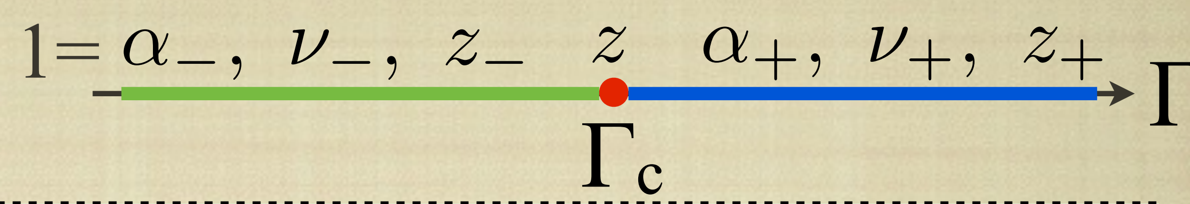
When $A_- = 0$ and $A_+ > 0$ (as t

consistent with XXZ chain (α_+=1/2, z=2, $\nu_\pm$=1/2)

$$\xi \sim \begin{cases} 1 & (\text{for } \Gamma < \Gamma_c) \\ \delta^{-\nu_+} & (\text{for } \Gamma > \Gamma_c) \end{cases} \Rightarrow \quad \nu_- = \frac{1}{z}, \quad \nu_+ = \frac{2-\alpha_+}{d+z}$$

Modified scaling theory for a QDCP

Assumptions



(i) $E_k \sim |\delta|^{\theta_\pm} k^{z_\pm} + k^z$ (ii) $\varepsilon(\Gamma) - \varepsilon(\Gamma_c) \sim |\delta|^{2-\alpha_\pm} \sim |\delta|^{z\nu_\pm} \xi^{-d}$

(iii) $\xi \sim 1 + A_\pm |\delta|^{-\nu_\pm}$ (iv) $\alpha_- = 1$

Results on scaling relations

$$\boxed{\theta_\pm = (z - z_\pm)\nu_\pm}$$

(a) $A_- = 0, \ A_+ = 0$ ⇨ $\nu_- = \dfrac{1}{z}, \quad \nu_+ = \dfrac{2 - \alpha_+}{z}$

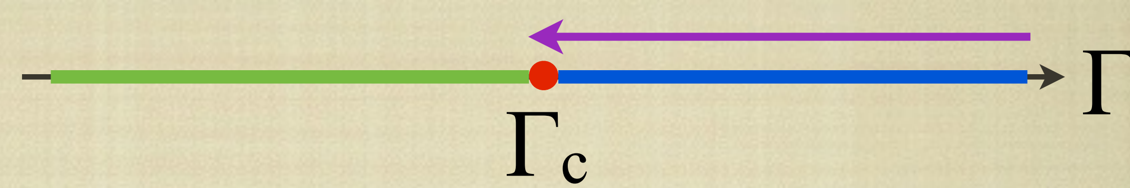
(b) $A_- = 0, \ A_+ > 0$ ⇨ $\nu_- = \dfrac{1}{z}, \quad \nu_+ = \dfrac{2 - \alpha_+}{d + z}$

(c) $A_- > 0, \ A_+ = 0$ ⇨ $\nu_- = \dfrac{1}{d + z}, \quad \nu_+ = \dfrac{2 - \alpha_+}{z}$

(d) $A_- > 0, \ A_+ > 0$ ⇨ $\nu_- = \dfrac{1}{d + z}, \quad \nu_+ = \dfrac{2 - \alpha_+}{d + z}$

Quantum quench

$$\frac{\Gamma(t) - \Gamma_\mathrm{c}}{|\Gamma_\mathrm{c}|} = -t/\tau_Q$$



Assume that a quench starts from the right(+) side

Kibble-Zurek Scaling of residual-energy density after a quench (ending at Γ_c)

$$\varepsilon_\mathrm{res} \sim \hat{L}^{-(d+z)} \sim \tau_Q^{-(d+z)\nu_+/(z\nu_+ +1)}$$

When $A_- = 0$ and $A_+ > 0$ as in XXZ chain

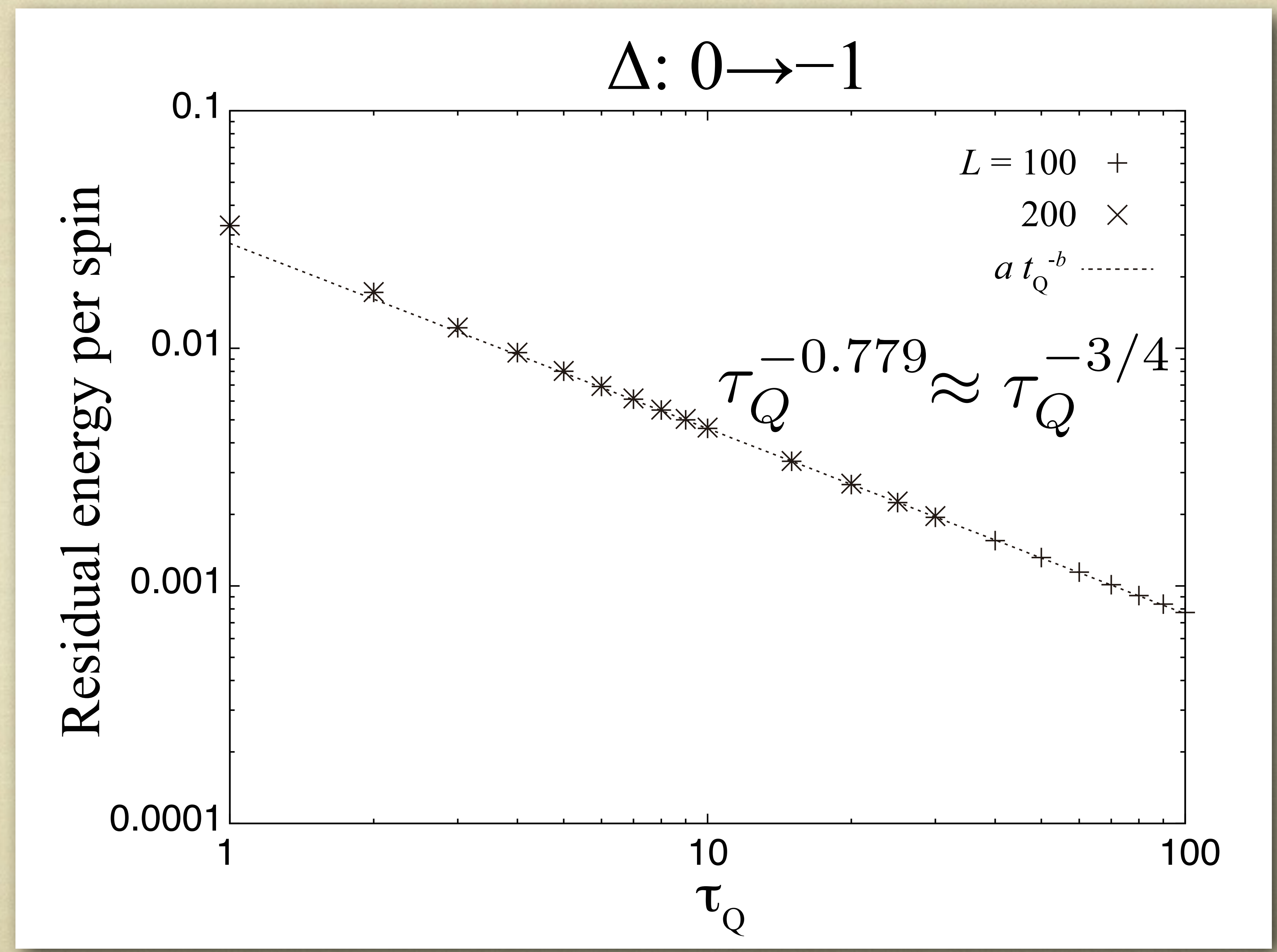
$$\nu_+ = \frac{2-\alpha_+}{d+z} \Rightarrow \boxed{\varepsilon_\mathrm{res} \sim \tau_Q^{-(d+z)(2+\alpha_+)/(d+3z-z\alpha_+)}}$$

For the XXZ chain, one has

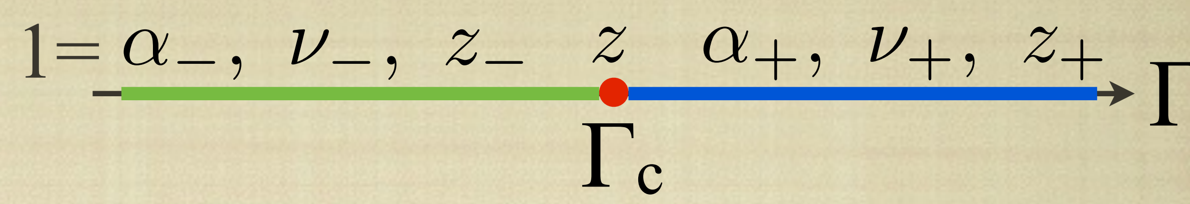
$$d = z_+ = 1, z = 2, \alpha_+ = \tfrac{1}{2} \Rightarrow \boxed{\varepsilon_\mathrm{res} \sim \tau_Q^{-3/4}}$$

Numerical confirmation

Result on the XXZ chain using *t*-DMRG



Kibble-Zurek scaling for a QDCP



Assumptions (same as before)

(i) $E_k \sim |\delta|^{\theta_\pm} k^{z_\pm} + k^z$ (ii) $\varepsilon(\Gamma) - \varepsilon(\Gamma_c) \sim |\delta|^{2-\alpha_\pm} \sim |\delta|^{z\nu_\pm} \xi^{-d}$

(iii) $\xi \sim 1 + A_\pm |\delta|^{-\nu_\pm}$ (iv) $\alpha_- = 1$

Results on the Kibble-Zurek scaling

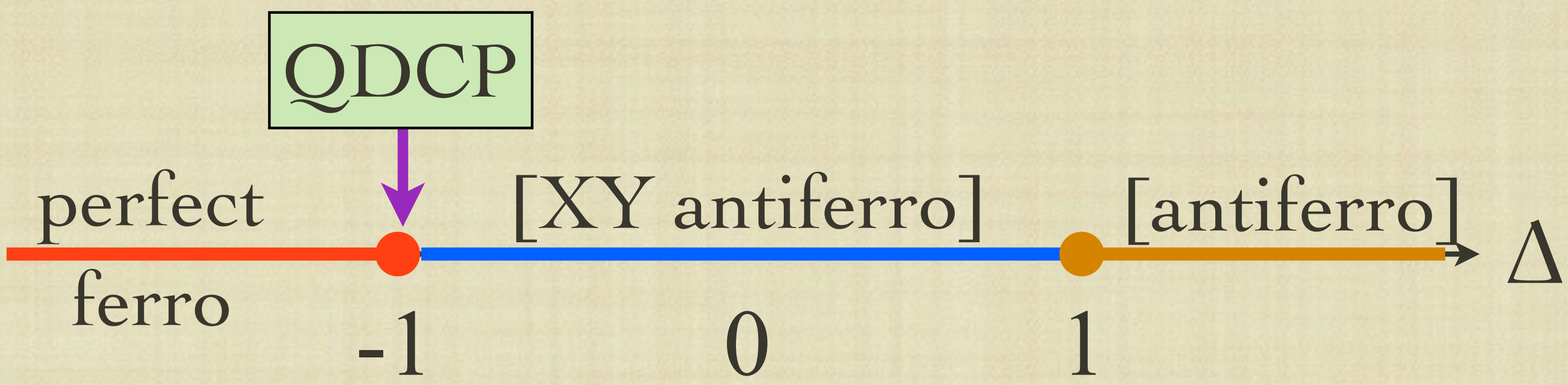
If a quench starts from the right side

(a) $A_- = 0,\ A_+ = 0$ ⇒ $\varepsilon_{\text{res}} \sim \tau_Q^{-(d+z)(2+\alpha_+)/z(3-\alpha_+)}$

(b) $A_- = 0,\ A_+ > 0$ ⇒ $\varepsilon_{\text{res}} \sim \tau_Q^{-(d+z)(2+\alpha_+)/(d+3z-z\alpha_+)}$

Other candidates for QDCP

1. The XXZ models in 2D and 3D



$\alpha_{-}=1$ $z=2$ $\alpha_{+}=?$

$A_{-}=0$ $[A_{+}>0]$

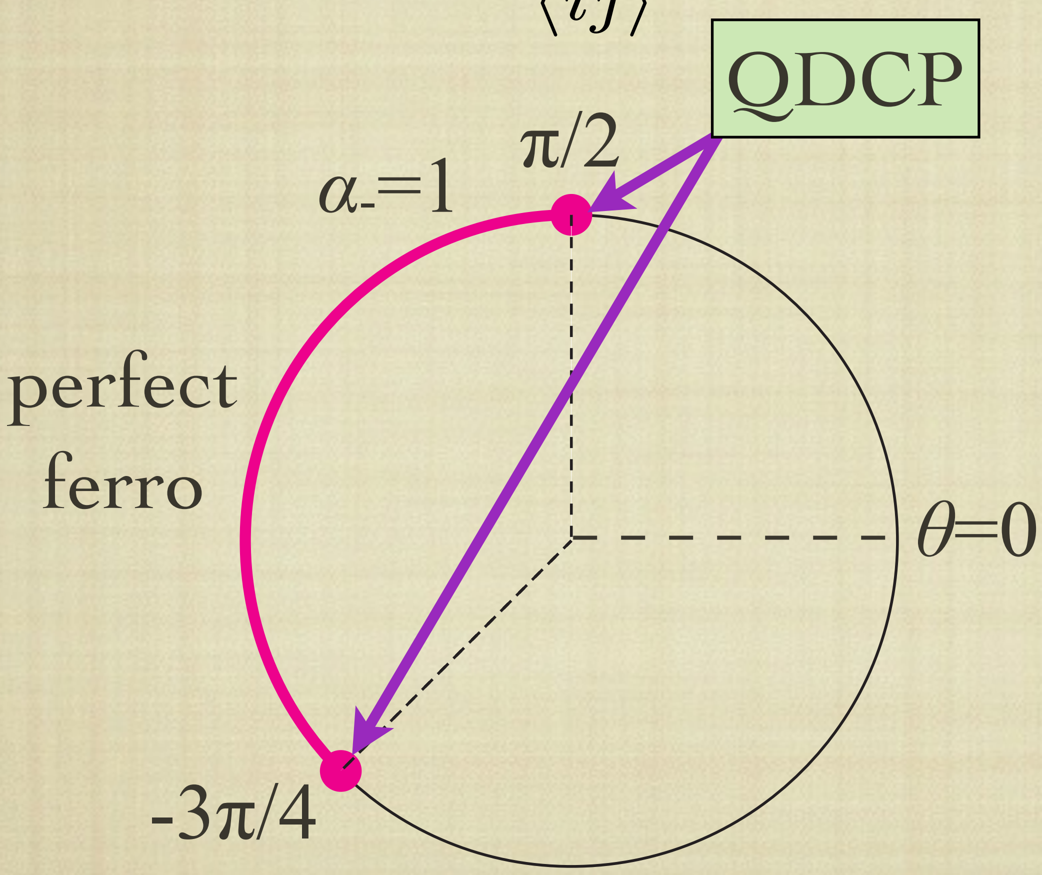
$z_{-}=0$ $[z_{+}=1]$

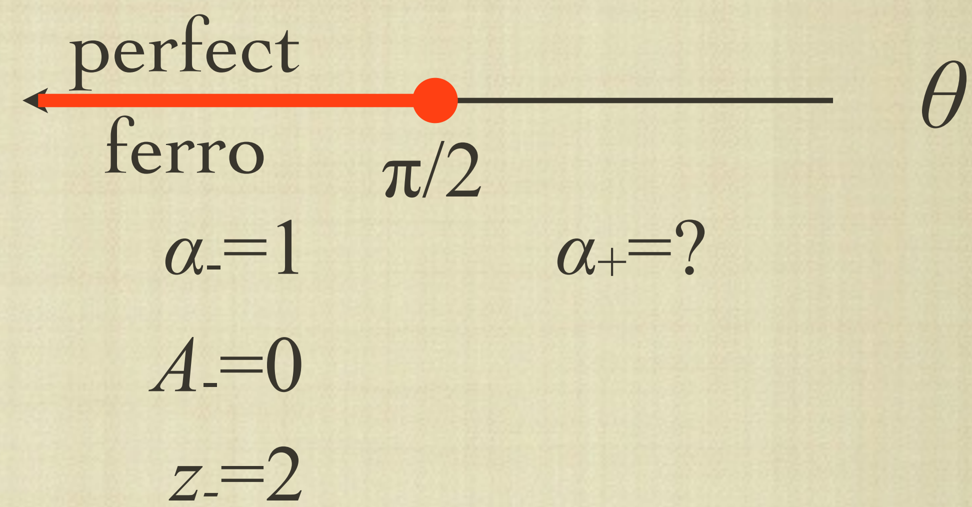
Kibble-Zurek scaling $\Longleftrightarrow$ scaling of GS energy (α_{+})

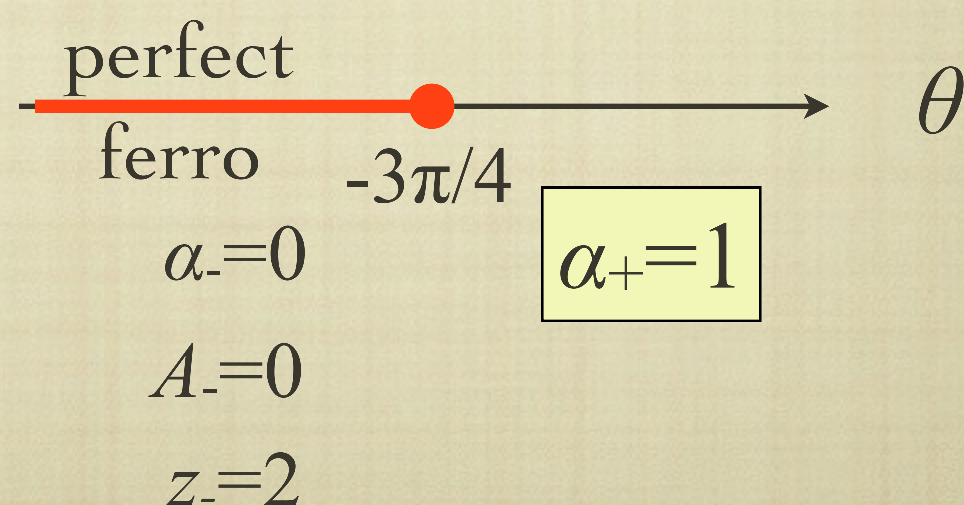
Other candidates for QDCP

2.The S=1 bilinear-biquadratic Heisenberg models

$$H = \sum_{\langle ij \rangle} [\cos\theta \mathbf{S_i} \cdot \mathbf{S_j} + \sin\theta (\mathbf{S_i} \cdot \mathbf{S_j})^{\mathbf{2}}]$$







Conclusion

We studied scaling properties of quantum discontinuity critical points (QDCPs).

Our study might be the first one that discussed them in specific models.

We derived and numerically confirmed the Kibble-Zurek scaling across a QDCP. Although this scaling relation is not valid to a generic 1st order QPT, our study might be a first step to better understanding of dynamics across a 1st order QPT.