High-Temperature Criticality in Strongly Constrained Quantum Systems

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PRB 2006
Ann. of Phys. 2005, 2006

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Correlated Quantum Systems

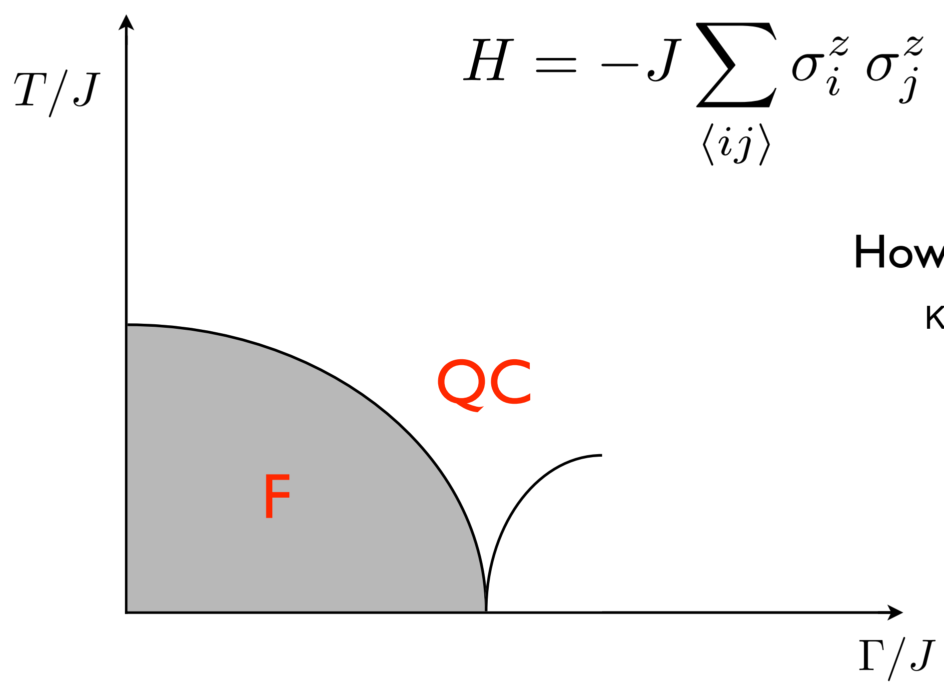
For a system to be in the quantum regime:

$$T \ll \Gamma, J, U$$

Couplings in the quantum Hamiltonian

Ex.: transverse field Ising model

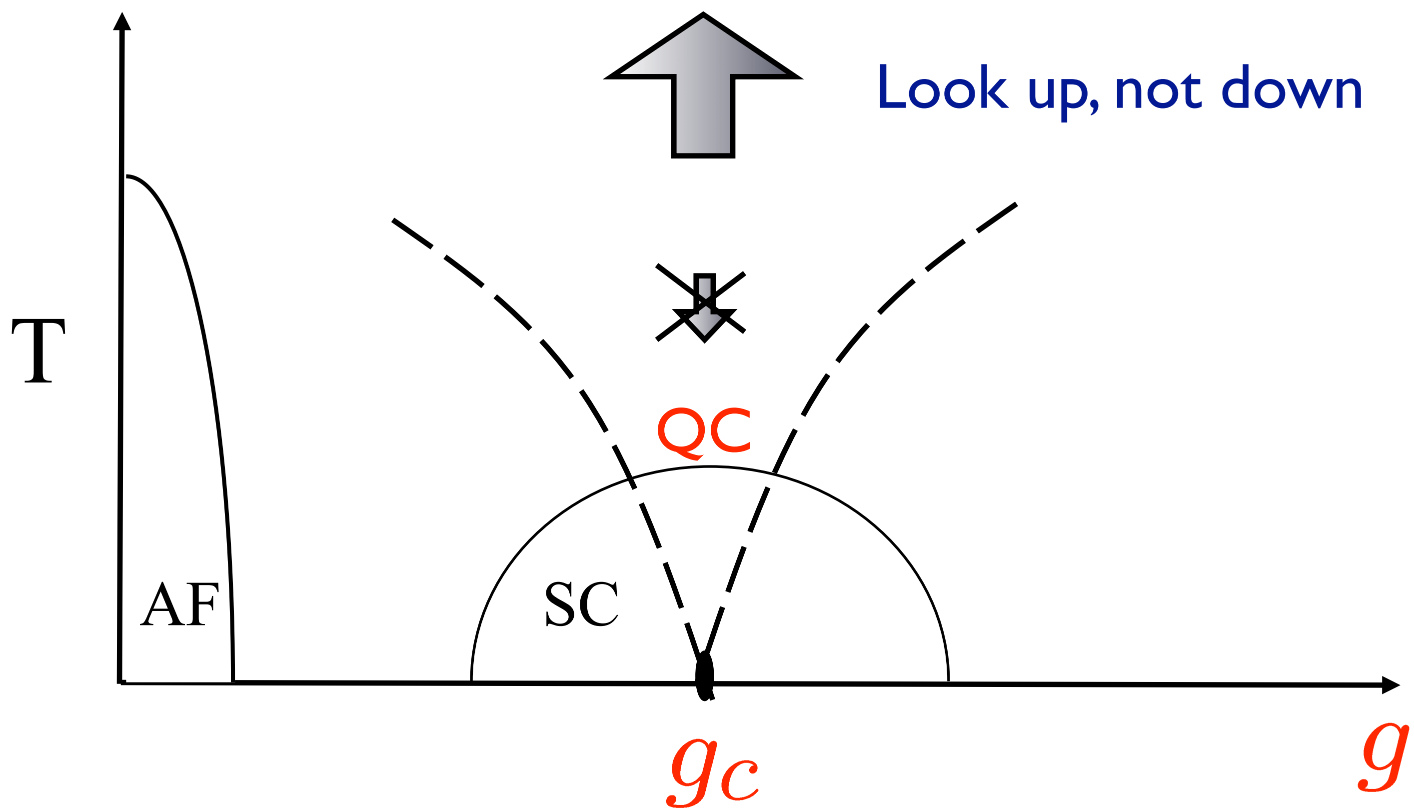
$$H = -J \sum_{\langle ij \rangle} \sigma_i^z \sigma_j^z - \Gamma \sum_i \sigma_i^x$$



How far does the QC regime extend?

Kopp & Chakravarty, Nature Phys. 2006

Quantum criticality here, there, everywhere?



Scaling of optical conductivity?
van der Marel *et al* , Nature 2004

Not with single parameter scaling
Phillips & Chamon, PRL 2005

Electrons interacting with a broad spectrum of bosons
Norman & Chubukov, PRB 2006

Anderson, cond-mat/0512471
Gutzwiller projection

Strongly Constrained Quantum Systems

If there is a dominant, very high energy scale in the problem that imposes a severe kinematic constraint in the system:

$$T \ll \Gamma, J \ll U$$

then, we find that

A hierarchy of scales can open such that:

A) the constrained thermodynamics becomes classical even at low temperatures

B) the dynamics is quantum in origin

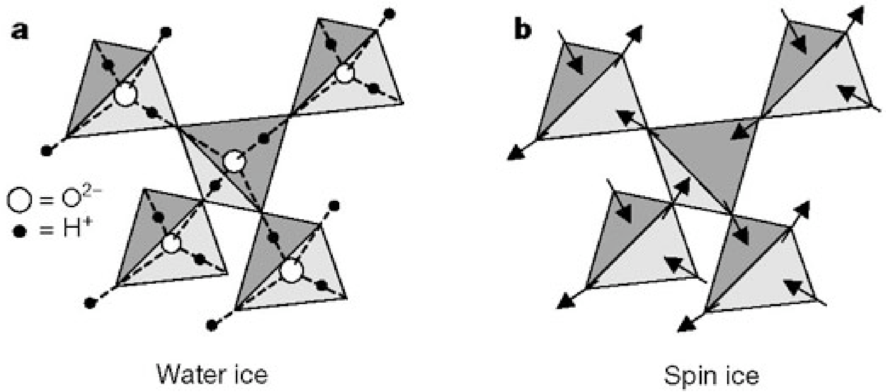
C) the system can display critical behavior at very high temperatures, which is unrelated to quantum criticality

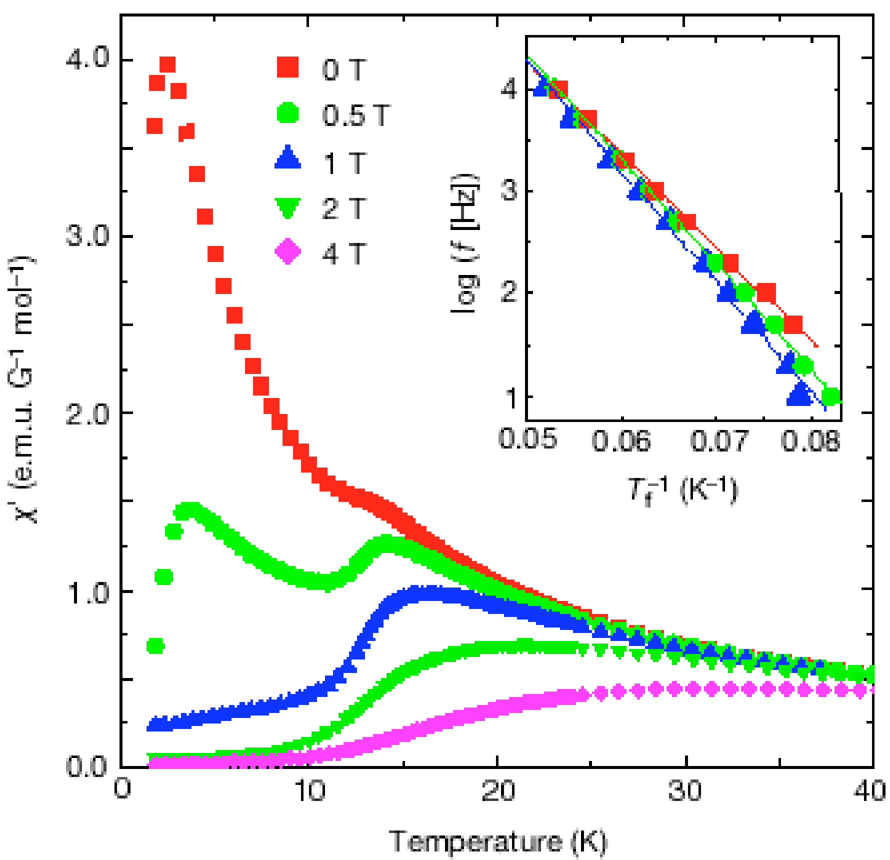
Examples of constrained models

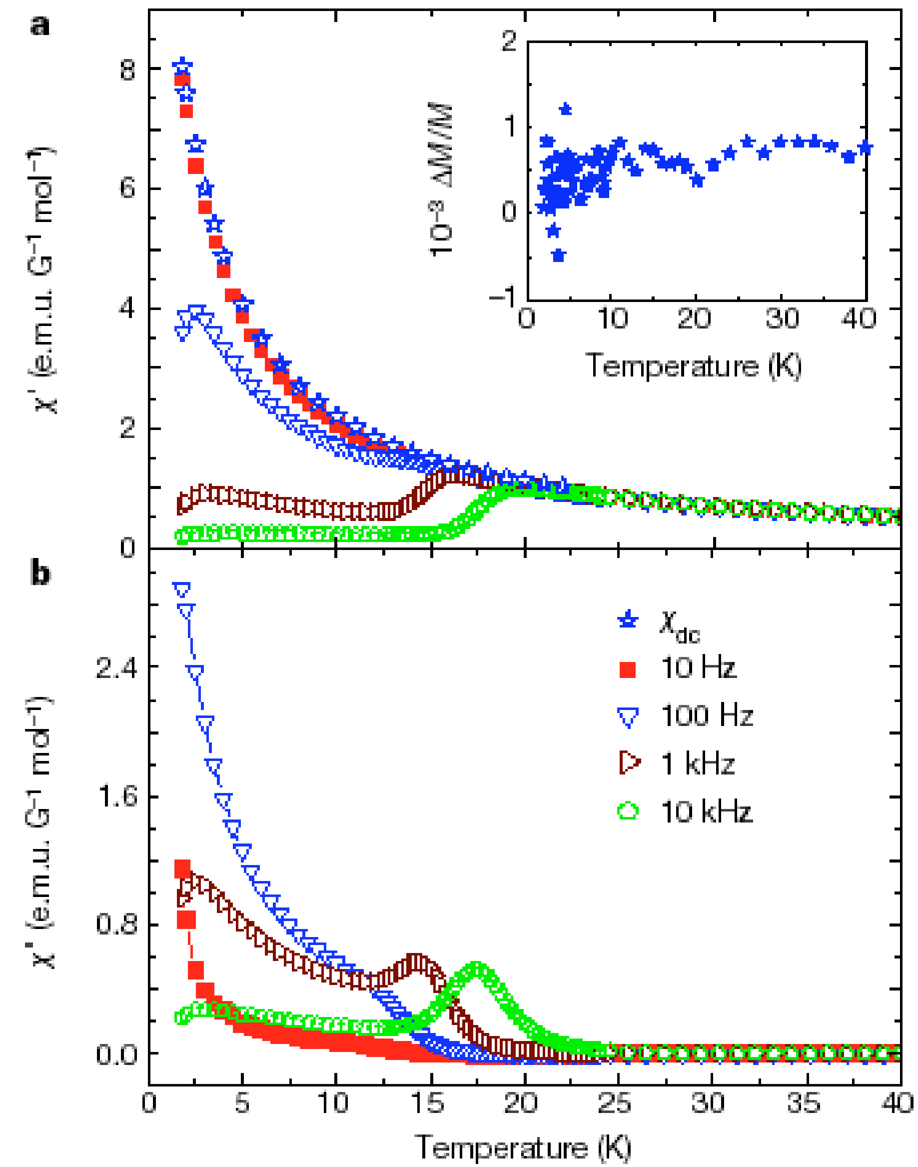
Spin Ice

$Dy_2Ti_2O_7$ ($Ho_2Ti_2O_7$)

Snyder *et al*, Nature (2001)



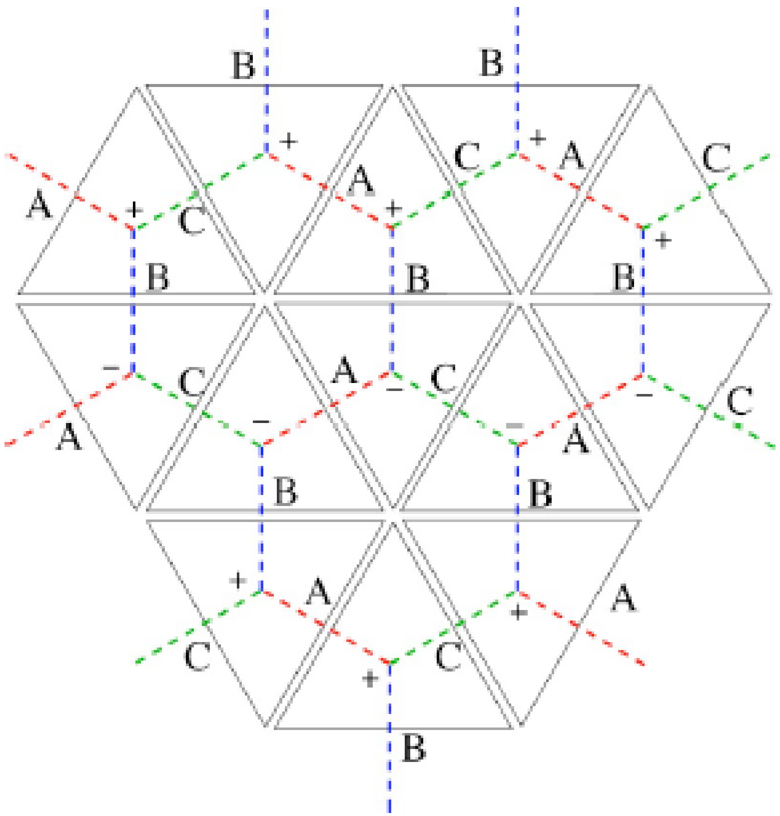




Source: Snyder *et al*, Nature (2001)

Josephson junction arrays of T-breaking superconductors

Sr_2RuO_4 $\quad p_x \pm i p_y$



Moore & Lee, PRB (2004)
Castelnovo, Pujol, and Chamon, PRB (2004)

Constrained Ising model

$\sigma_i = \pm 1$ chirality $p_x \pm i p_y$

$$\Phi_P^{\hexagon} = 2\pi/3 \sum_{i \in P} \sigma_i$$

$$= 2\pi/3 \, \sigma_P^{\hexagon}$$

$$\Rightarrow \sigma_P^{\hexagon} = \sum_{i \in P} \sigma_i = \pm 6, 0$$

$$H = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j \quad \text{with} \quad \sigma_P^{\hexagon} = \pm 6, 0$$

Generic constrained systems

$$\hat{H} = -J\hat{H}_J - \Gamma\hat{H}_\Gamma - U\hat{H}_U \qquad U \gg |J|, |\Gamma| \qquad \text{with} \quad [\hat{H}_U, \hat{H}_J] = 0 \quad \text{and} \quad [\hat{H}_U, \hat{H}_\Gamma] \neq 0$$

For $T \ll U$ the system is effectively constrained to a restricted Hilbert space $\mathcal{H}_U$ spanned by the eigenvectors of $\hat{H}_U$.

$\mathcal{H}_U$ is extensive in the system size

$\mathcal{H}_U$ is not extensive

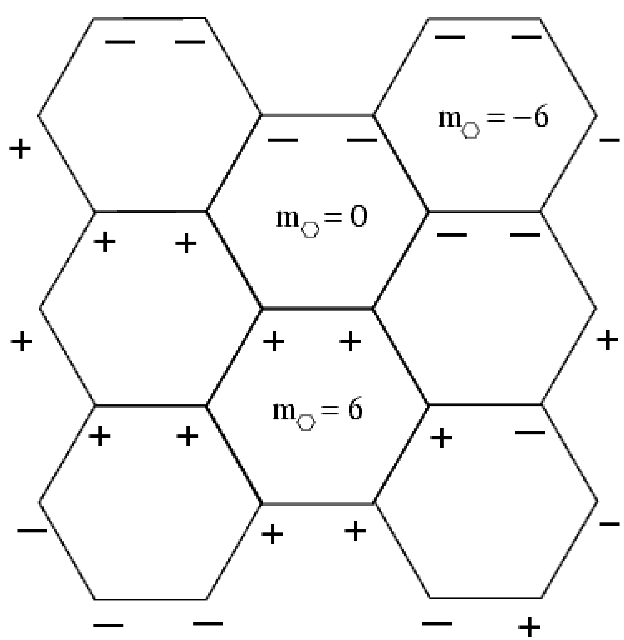
The non-interacting $\Gamma = J = 0$ system exhibits power-law correlations (criticality) when restricted to $\mathcal{H}_U$ (e.g., dimer models, ice models, constrained Ising models)

The correlations of the purely projected system are trivial (e.g., Hubbard model)

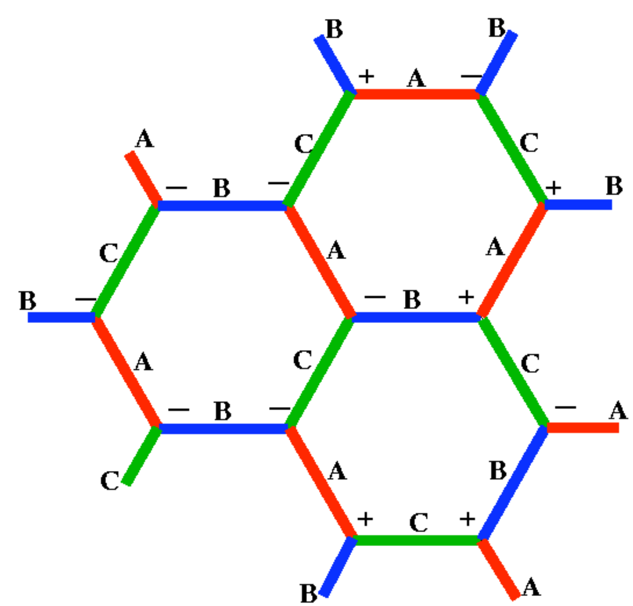
A spin-1/2 example:

$$\hat{H} = -J \sum_{\langle ij \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z - \Gamma \sum_{i=1}^{N} \hat{\sigma}_i^x - U \sum_{\text{hex}} \cos\left(2\pi \sum_{i \in \text{hex}} \hat{\sigma}_i^z / 3\right)$$

with $U \gg |J|, |\Gamma|$, and for temperatures $T \ll U$ the systems is mostly confined to a superposition of GS eigenvectors of $\widehat{H}_U$



$\Leftrightarrow$



The non-commuting $\widehat{H}_\Gamma$ term has a vanishing first-order contribution and needs to be expanded in (degenerate) perturbation!

Introducing the constraint in a quantum system: projection by a large energy coupling $U \gg |J|, |\Gamma|$ onto its (highly-degenerate) ground states.

$$\hat{H} = -J \sum_{\langle ij \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z - \Gamma \sum_{i=1}^{N} \hat{\sigma}_i^x - U \sum_{\text{hex}} \cos\left(2\pi \sum_{i \in \text{hex}} \hat{\sigma}_i^z / 3 \right)$$

(at temperatures much $\Downarrow$ *smaller than U)*

$$\widehat{H}_{\text{eff}} = -J \sum_{\langle i,j \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z - \sum_{n=1}^{\infty} \frac{\Gamma^n}{U^{n-1}} \hat{H}_{\Gamma/U}^{(n)}$$

on the restricted Hilbert space
$\equiv$
span of GS basis vectors of U term

First non-vanishing contributions of the (degenerate) perturbation theory appear only at sixth order (third order if we used Heisenberg Hamiltonian instead of Ising Hamiltonian):

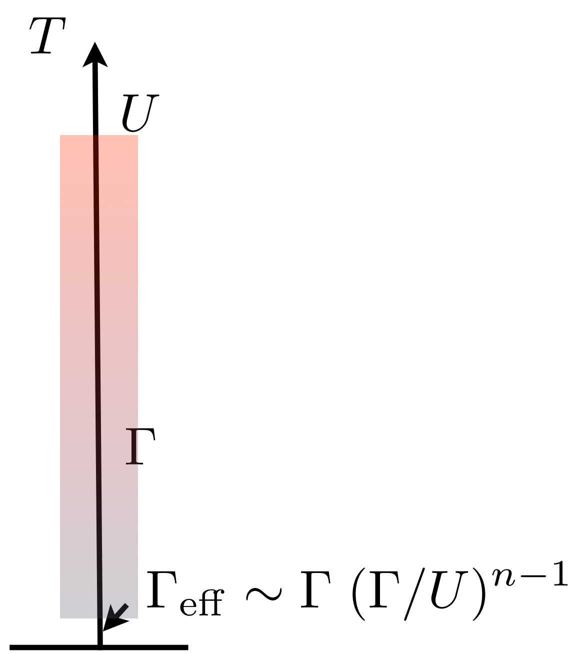
$$n = 6 \qquad \Longrightarrow \qquad \Gamma_{\text{eff}} = \frac{\Gamma^6}{U^5} \ll \Gamma$$

Different temperature regimes

- $T \gg U$ - all terms in the Hamiltonian become negligible, free-spin paramagectic phase
- $T \ll \Gamma_{\mathrm{eff}}$ - "quantum regime"
- $T \gg \Gamma_{\mathrm{eff}}$ - classical hard-constrained regime with infinitesimal perturbation J and *quantum dynamics*

A classical ordered phase can appear depending on the effects of J

Hierarchy opens a large window in which the *thermodynamics is classical*



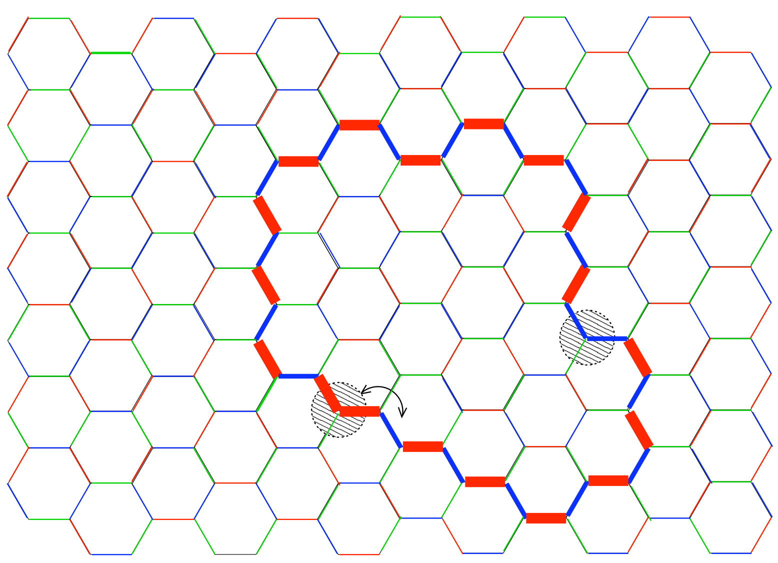
Dynamics is still quantum: why?

consider coupling the system to a thermal bath, e.g., a la Caldeira-Leggett:

$$\sum_{i,\lambda_i} \gamma\, \hat{\sigma}_i^{\mathrm{x}} \left(\hat{a}_{\lambda_i} + \hat{a}^{\dagger}_{\lambda_i} \right),$$

with

$$0 < \gamma \text{ (bath coupling) } \ll |\Gamma| \text{ (kinetic energy)}$$



Relaxation time for thermally activated processes (over the defect-creation barrier $\sim \exp(U/T)$):

$$\tau_T = \gamma^{-1} e^{(U/T)}$$

Relaxation time for virtual processes (via quantum tunneling of at least 6-th order in perturbation):

$$\tau_Q = \min(|\Gamma_{\text{eff}}^{-1}|, \gamma_{\text{eff}}^{-1}),$$

where

$$\begin{cases} \gamma_{\text{eff}} \sim \gamma(\gamma/U)^{n-1} \ll \gamma \\ \Gamma_{\text{eff}} \sim \Gamma(\Gamma/U)^{n-1} \end{cases}$$

$\tau_Q \ll \tau_T \Longrightarrow$ phantom of quantum mechanics in the form of sporadic tunneling events between which coherence is lost provides the fastest mechanism for the system to reach classical thermodynamic equilibrium when $|\Gamma_{\text{eff}}| \ll T \ll U$.

Effects of the constraint at the classical behavior

$$\hat{H} = -J\sum_{\langle ij\rangle}\hat{\sigma}_i^z\hat{\sigma}_j^z - \sum_{i=1}^{N}\left[h + (-1)^i h_s\right]\hat{\sigma}_i^z - \Gamma\sum_{i=1}^{N}\hat{\sigma}_i^x - U\sum_{\text{hex}}\cos\left(2\pi\sum_{i\in\text{hex}}\hat{\sigma}_i^z/3\right)$$

How does the constraint alters the Ising model?

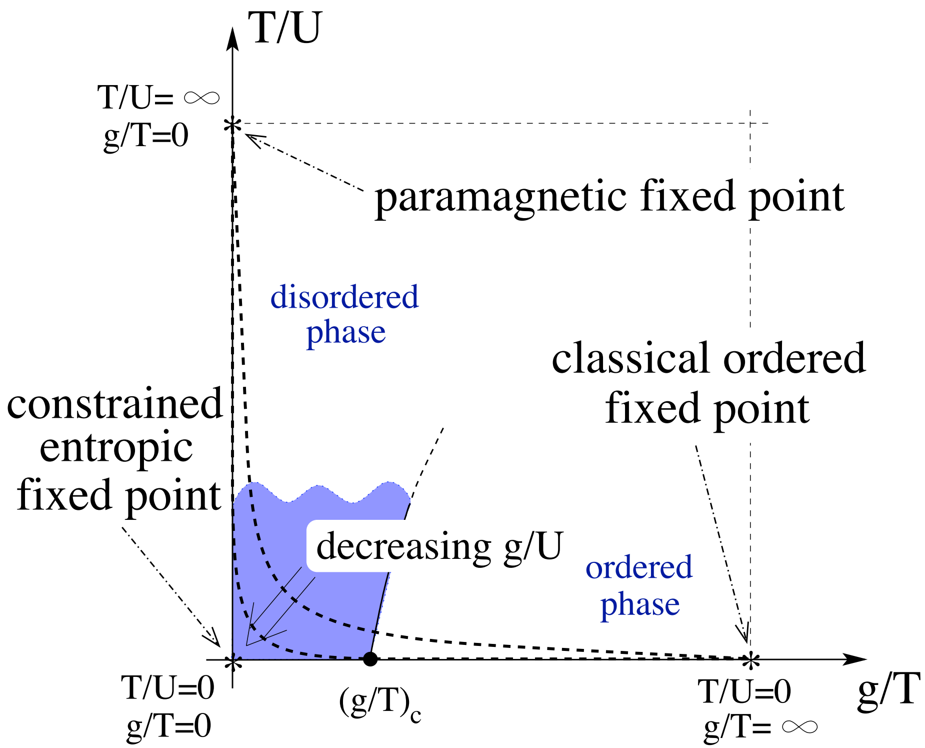
- The model is critical in the absence of interactions (Baxter), and its long distance behavior is captured by an $SU(3)|_{k=1}$ Wess-Zumino-Novikov-Witten conformal field theory

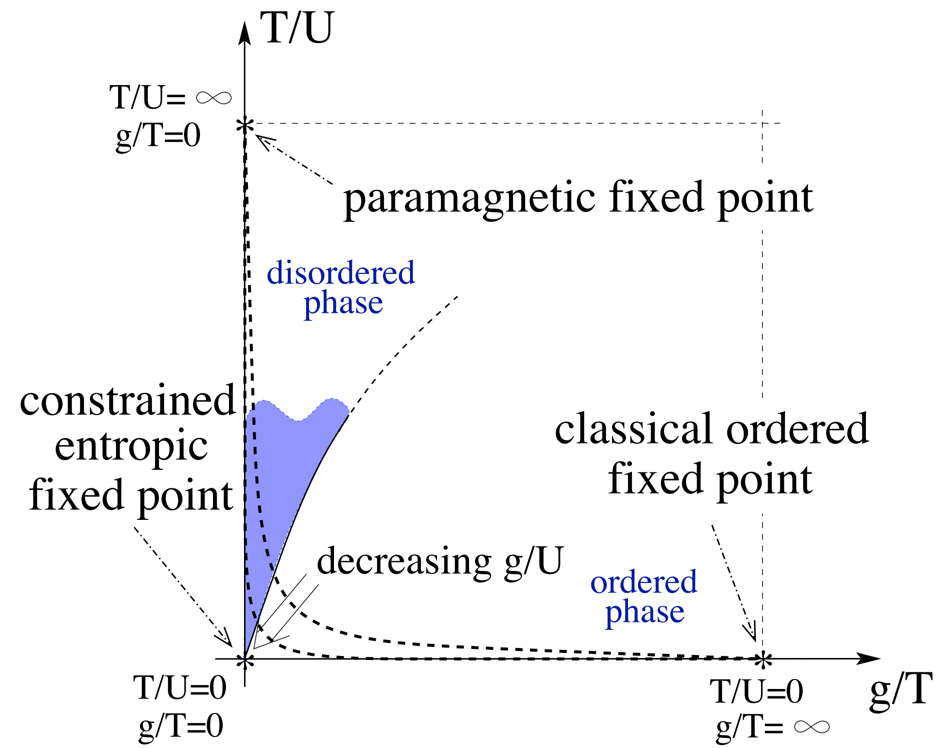
$$S = \int d^2x\left(\frac{\pi}{2}||\nabla\vec{h}||^2 + V(\vec{h})\right)$$

2 component height field

- What are now the effects of J, h, h_s in the constrained model?

Qualitative phase diagram



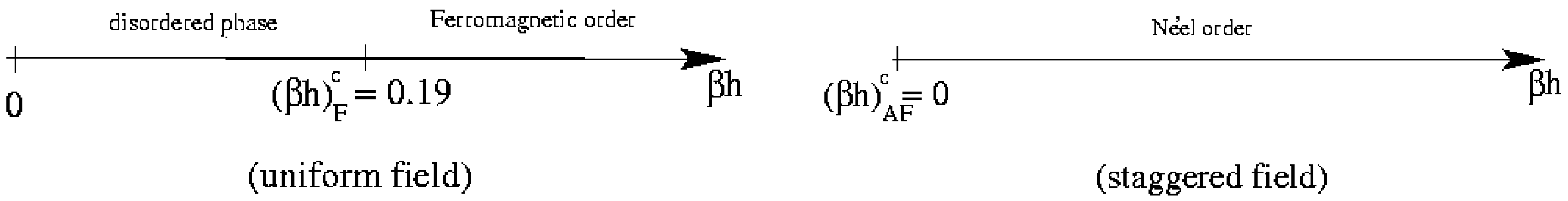


$g = h$ or h_s or J

1) The (staggered/uniform) magnetic field case

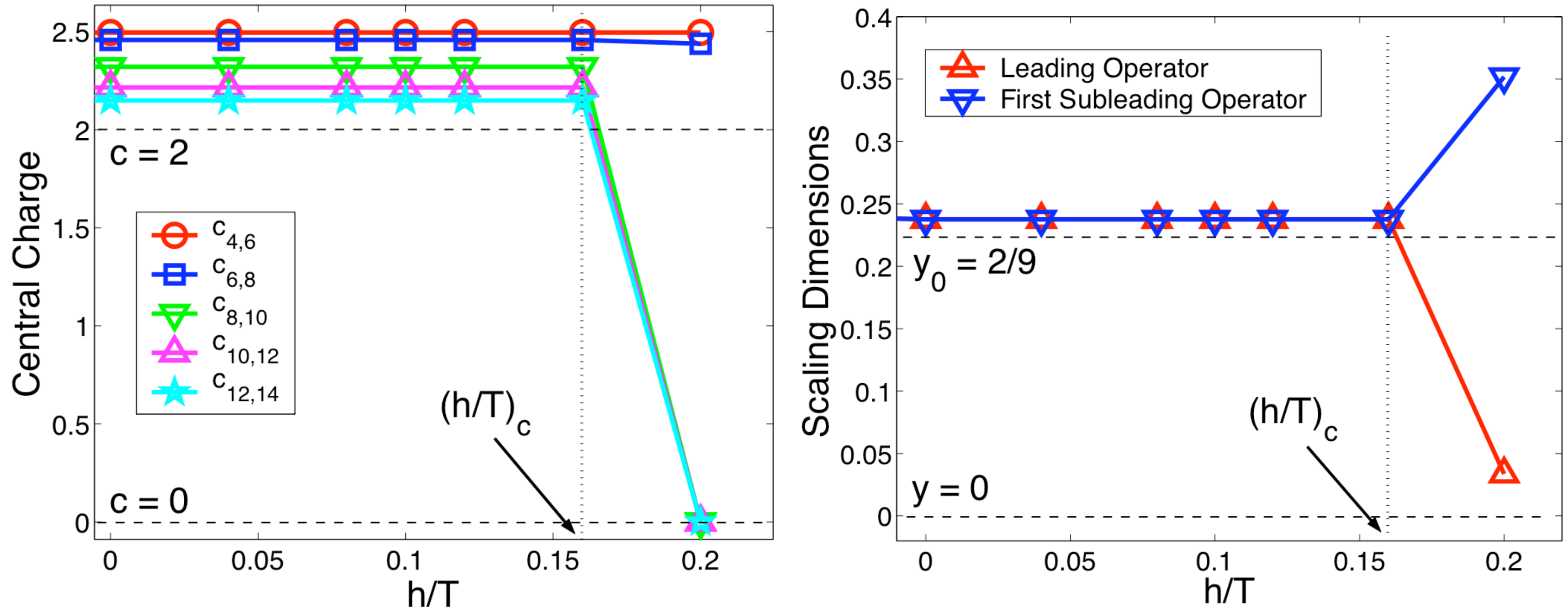
From Monte Carlo simulations, Cluster Mean Field Method results, and Transfer Matrix calculations of the free energy and magnetization of the system, as well as analytical results in the staggered field case (Baxter, Kondev):

$$E = -\sum_i h_i \sigma_i \qquad \sum_{i \in \mathrm{hex}} \sigma_i = \pm 6, 0$$



- The uniform magnetic field case exhibits an exotic first order phase transition to the ferromagnetically ordered phase where the magnetization per spin jumps discontinuously from 0 to 1

- The staggered magnetic field case exhibits an infinite order phase transition at infinite temperature to the Néel phase



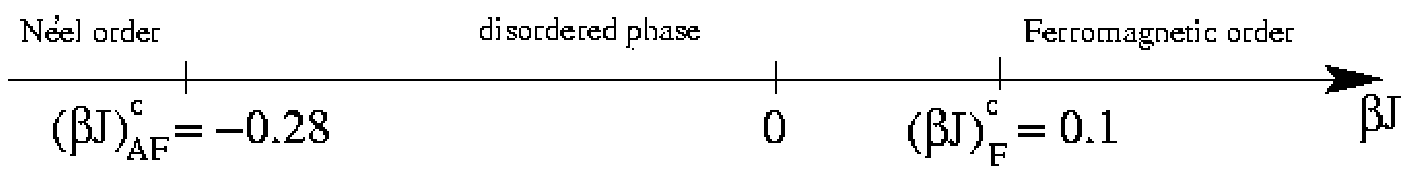
Characteristic features:

- the criticality is robust in presence of a uniform magnetic field up to the first order phase transition
- the $SU(3)$ symmetry is preserved up to the first order transition (same central charge $c = 2$ and same exponents)!

2) The nearest-neighbor interaction case

From Monte Carlo simulations, Cluster Mean Field Method results, and Transfer Matrix calculations of the free energy and magnetization of the system:

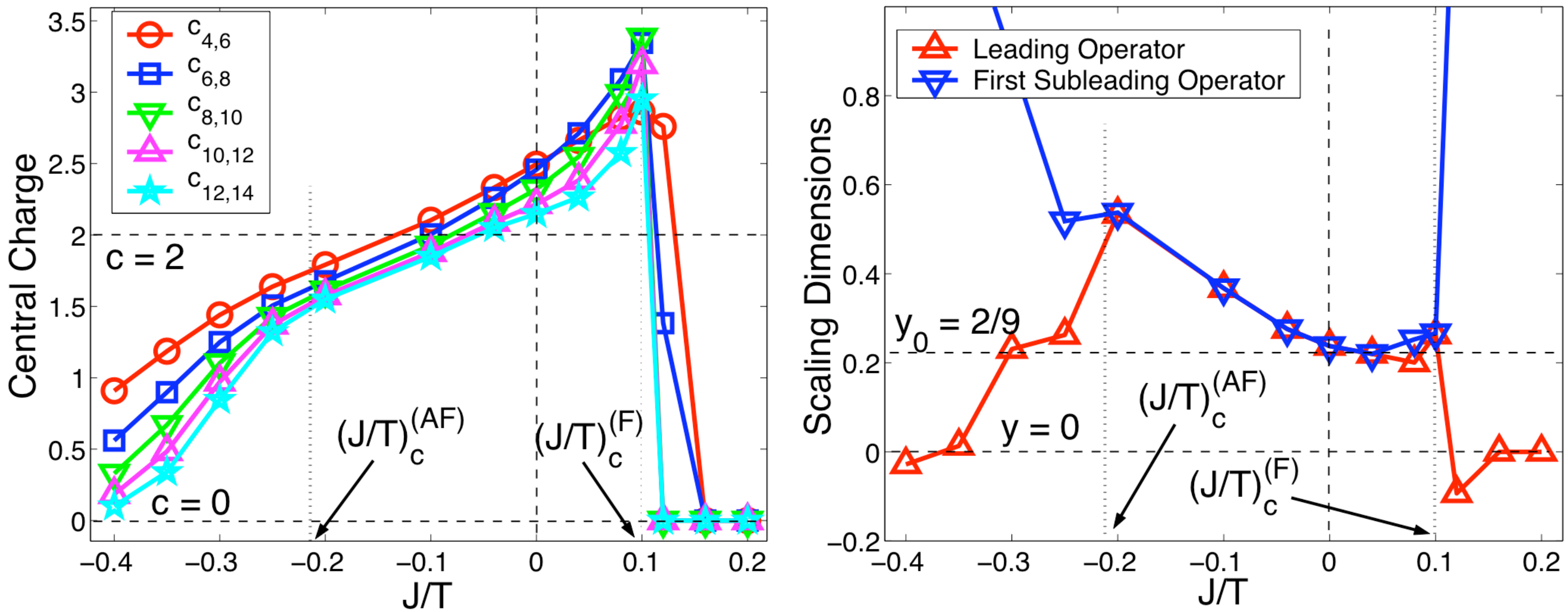
$$E = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j \qquad\qquad \sum_{i \in \mathrm{hex}} \sigma_i = \pm 6, 0$$



- In the case of ferromagnetic interactions, the system undergoes an exotic first order phase transition to the ferromagnetically ordered phase where the magnetization per spin jumps discontinuously from 0 to 1

- In the case of antiferromagnetic interactions, the system undergoes a "*second order*" phase transition to the Néel phase

- Monte Carlo simulations are incapable of detecting the AF transition



Characteristic features:

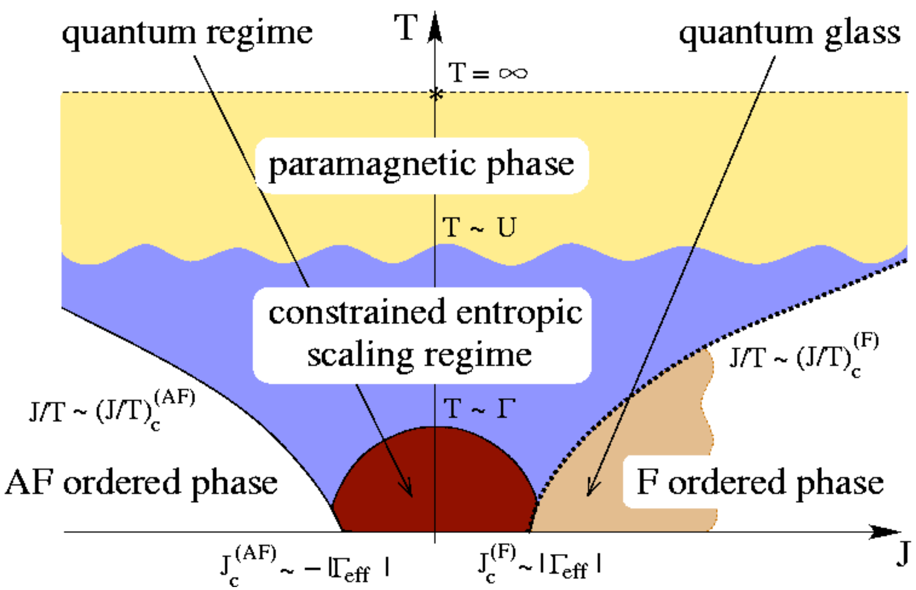
- criticality with $c = 2$ for a ferromagnetic coupling J until the first order phase transition is reached ($\exp(-L/\xi)$ finite size correction close to the transition)
- criticality with a varying central charge on the antiferromagnetic side approximately from $\beta J = (\beta J)^c_{\mathrm{AF}}$ ($c \approx 1.5$) to $\beta J = 0$ ($c = 2$)

HiTc (High-temperature criticality) in strongly constrained quantum systems

Static properties of the effective Hamiltonian

$$\widehat{H}_{\text{eff}} = -J \sum_{\langle i,j \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z - \Gamma_{\text{eff}} \widehat{H}^{\text{eff}}_{\Gamma/U}$$

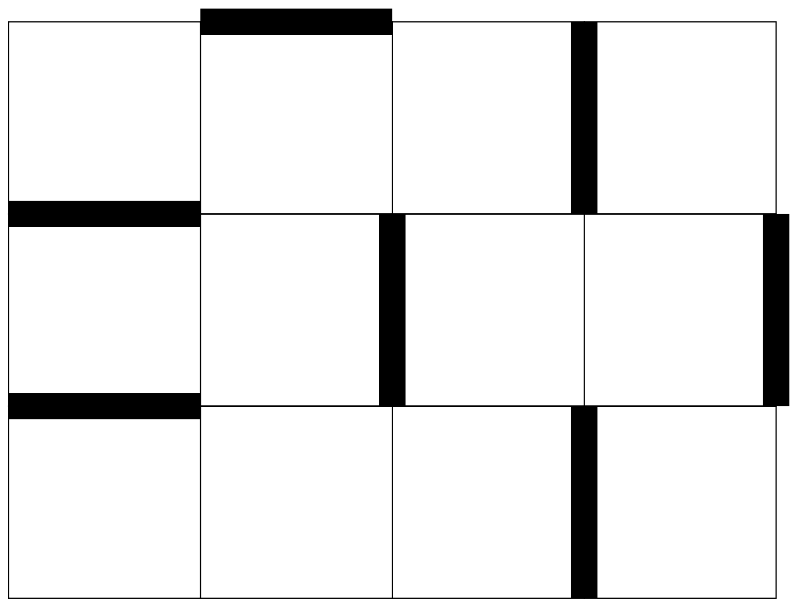
where $\Gamma_{\text{eff}} = \frac{\Gamma^6}{U^5}$ and $\widehat{H}^{\text{eff}}_{\Gamma/U}$ is at most of order 1 in $\frac{\Gamma}{U}$.

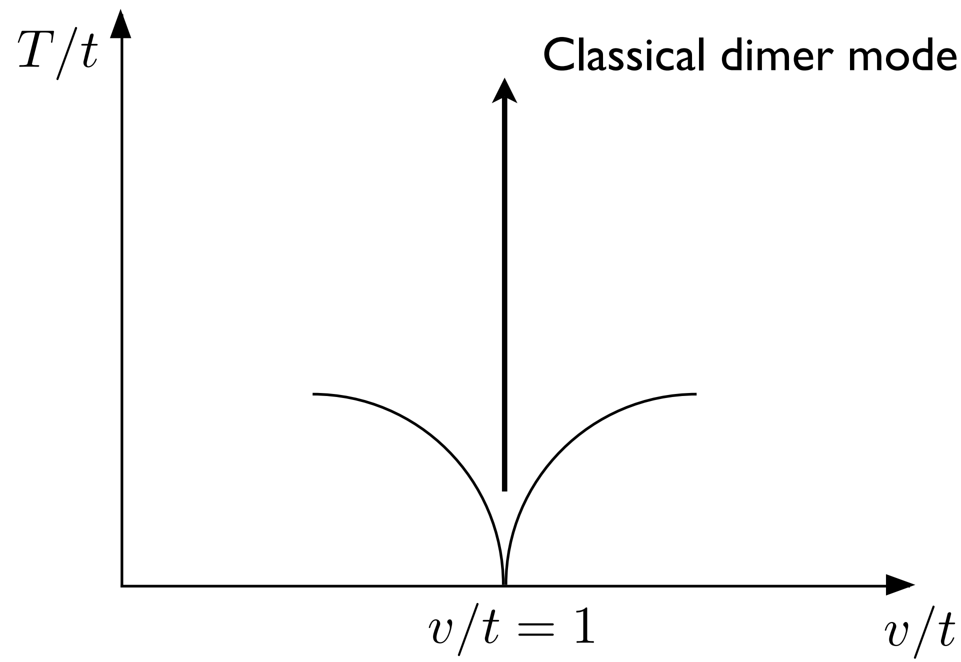


- $U \ll T \longrightarrow$ classical paramagnetic phase (U relevant)
- $|J|, |\Gamma_{\text{eff}}| \ll T \ll U \longrightarrow$ constraint fully enforced; classical phase equivalent to classical constrained model with nearest-neighbor interaction J: universal critical behavior at large enough temperature!
- $T \ll |J|, |\Gamma_{\text{eff}}| \longrightarrow$ ordered phases that depend on the model-specific Hamiltonian details

Large temperature universal scaling regime with no required underlying critical point!

More hard-constrained systems





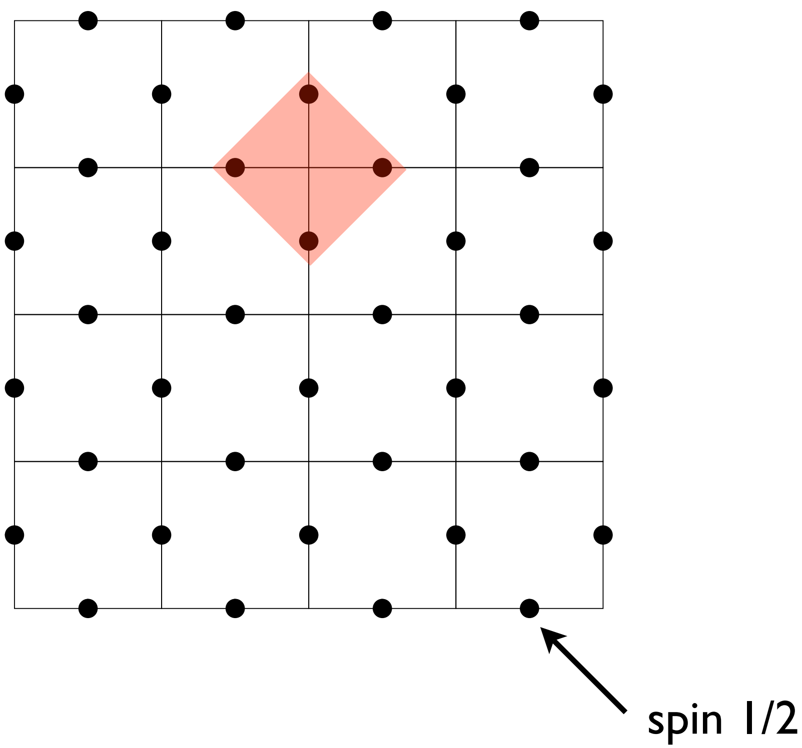
$$\hat{H}_{RK} = \sum_{\square_P} v \; \left(|=\rangle\langle=| + |\,\|\,\rangle\langle\,\|\,| \right) - t \; \left(|\,\|\,\rangle\langle=| + |=\rangle\langle\,\|\,| \right)$$

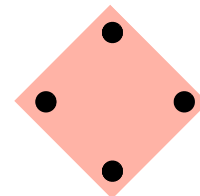
Rokhsar & Kivelson, PRL 1988

$$|\Psi\rangle = \frac{1}{\sqrt{\mathcal{N}}} \sum_{\mathcal{C}} |\mathcal{C}\rangle \quad \text{at} \quad v = t$$

$$\hat{\rho} = \frac{1}{\mathcal{N}} \sum_{\mathcal{C},\mathcal{C}'} |\mathcal{C}\rangle\langle\mathcal{C}'| \quad \xrightarrow{\text{increase T}} \quad \hat{\rho}_{\text{classical}} = \frac{1}{\mathcal{N}} \sum_{\mathcal{C}} |\mathcal{C}\rangle\langle\mathcal{C}|$$

$\mathbb{Z}_2$ gauge theory





Constraint: $\prod_{i \in S} \sigma_i^z = 1$

$$\hat{H}_U = -U \sum_S \hat{A}_S \quad \text{with} \quad \hat{A}_S = \prod_{i \in S} \sigma_i^z$$

$$\hat{H} = -\Gamma \sum_i \sigma_i^x - U \sum_S \hat{A}_S$$

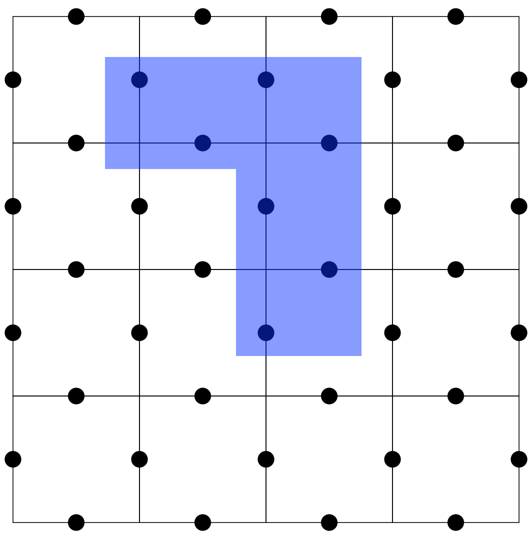
$$\hat{H}_{\text{eff}} = -\Gamma_{\text{eff}} \sum_P \hat{B}_P - U \sum_S \hat{A}_S \quad \text{with} \quad \hat{B}_P = \prod_{i \in P} \sigma_i^x$$

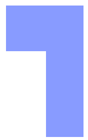
Kitaev, Ann. Phys. 2003
Wen, PRL 2003

$$|\Psi\rangle = \frac{1}{\sqrt{\mathcal{N}}} \sum_{\mathcal{C}} |\mathcal{C}\rangle \qquad \hat{\rho} = \frac{1}{\mathcal{N}} \sum_{\mathcal{C},\mathcal{C}'} |\mathcal{C}\rangle\langle\mathcal{C}'|$$

$$\hat{\rho}_{\text{classical}} = \frac{1}{\mathcal{N}} \sum_{\mathcal{C}} |\mathcal{C}\rangle\langle\mathcal{C}|$$

Classical correlation entropy of constrained systems
vs.
von Neumann entropy



A:  $S_A = -\mathrm{tr}_A \left(\rho_A \;\ln \rho_A \right)$ $\qquad \rho_A = \mathrm{tr}_B \; \hat{\rho}$

where

B: the rest $S_B = -\mathrm{tr}_B \left(\rho_B \;\ln \rho_B \right)$ $\qquad \rho_B = \mathrm{tr}_A \; \hat{\rho}$

The von Neumann entropy depends on the boundary for pure states, but on the bulk as well for mixed states

To subtract the bulk term, we define

$$S_{\mathrm{boundary}} = \frac{1}{2} \left(S_A + S_B - S_{A \cup B} \right)$$

$$S^{\mathrm{mixed}}_{\mathrm{boundary}} = \frac{1}{2} \; S^{\mathrm{pure}}_{\mathrm{boundary}}$$

Non-trivial correlation entropy even at large T!

Summary

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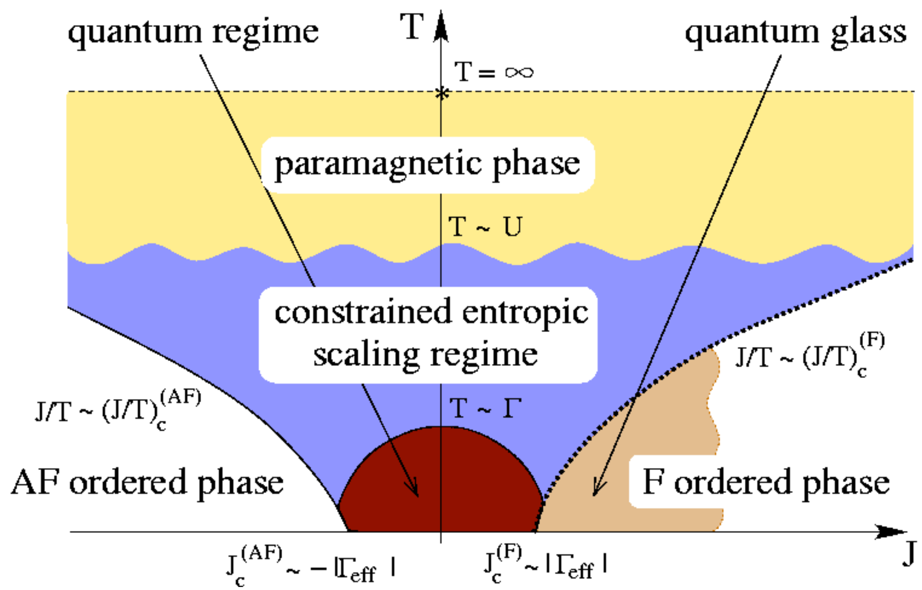

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