Title: Bound on the dynamical exponent of frustration-free Hamiltonians and Markov processes

Speakers: Tomohiro Soejima

Collection/Series: Quantum Matter

Subject: Condensed Matter

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Abstract:

Exactly solvable models have tremendously helped our understanding of condensed matter systems. A notable number of them are "frustration-free" in the sense that all local terms of the Hamiltonian can be minimized simultaneously. It has been particularly successful at describing the physics of gapped phases of matter, such as symmetry protected topological phases and topologically ordered phases. On the other hand, relatively little has been understood about gapless frustration-free Hamiltonians, and their ability to teach us about more generic systems. In this talk, we derive a constraint on the spectrum of frustration-free Hamiltonians. Their dynamical exponent z, which captures the scaling of the energy gap versus the system size, is bounded from below to be z >= 2. This proves that frustration-free Hamiltonians are incapable of describing conformal critical points with z = 1. Further, by a well-known mapping from Markov processes to frustration-free Hamiltonians, we show that the relaxation time for many Markov processes also scale with z >=2. This improves the previously known bound on the relaxation time scaling of z >= 7/4. The talk is based on works with Rintaro Masaoka and Haruki Watanabe.

Bound on the dynamic critical exponent of frustration-free Hamiltonians and Markov processes

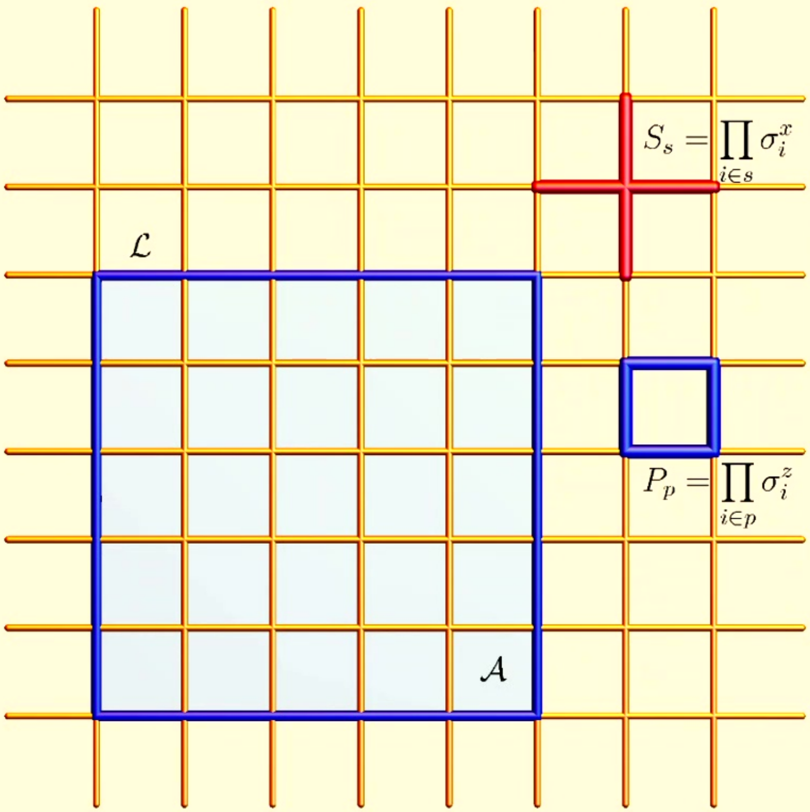
Tomo Soejima

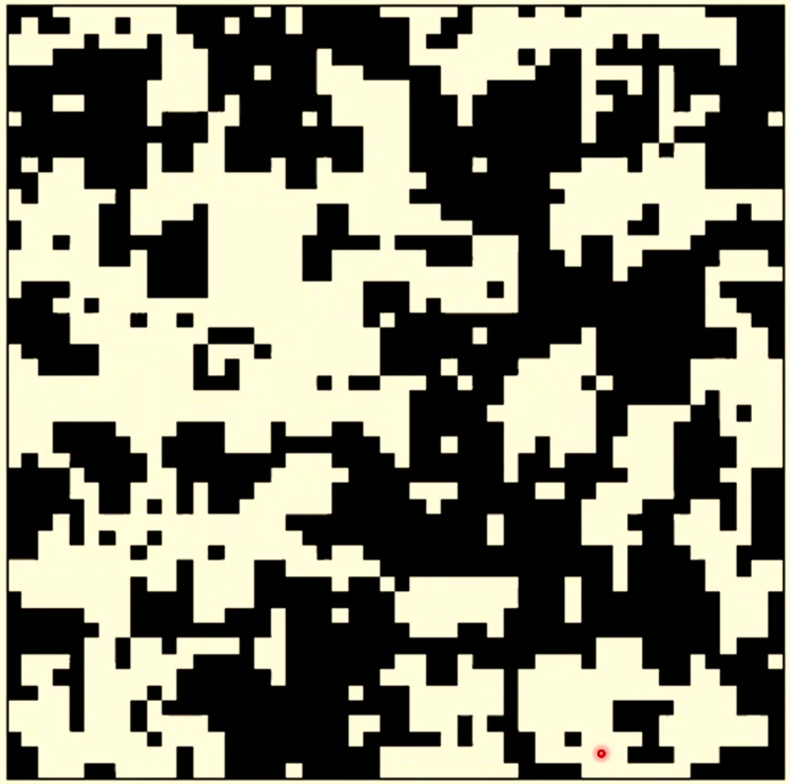
Postdoctoral fellow, Harvard University

based on works with Rintaro Masaoka and Haruki Watanabe

arXiv: 2406.06414, 2406.06415, 2502.09908

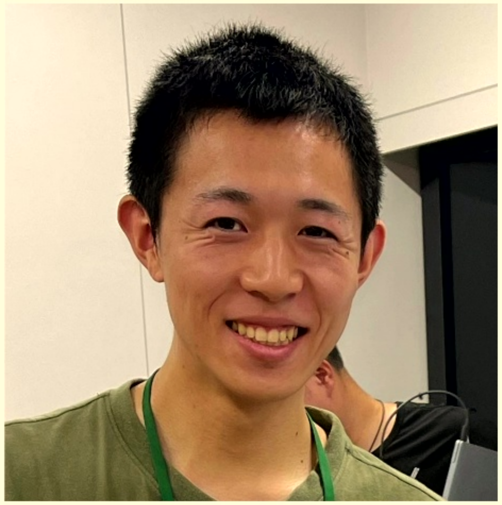
What do they have in common?



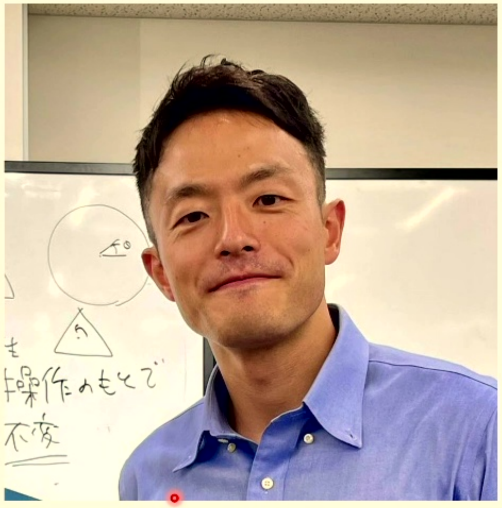


Toric code Figure from Savary, Balents 2017

Collaborators

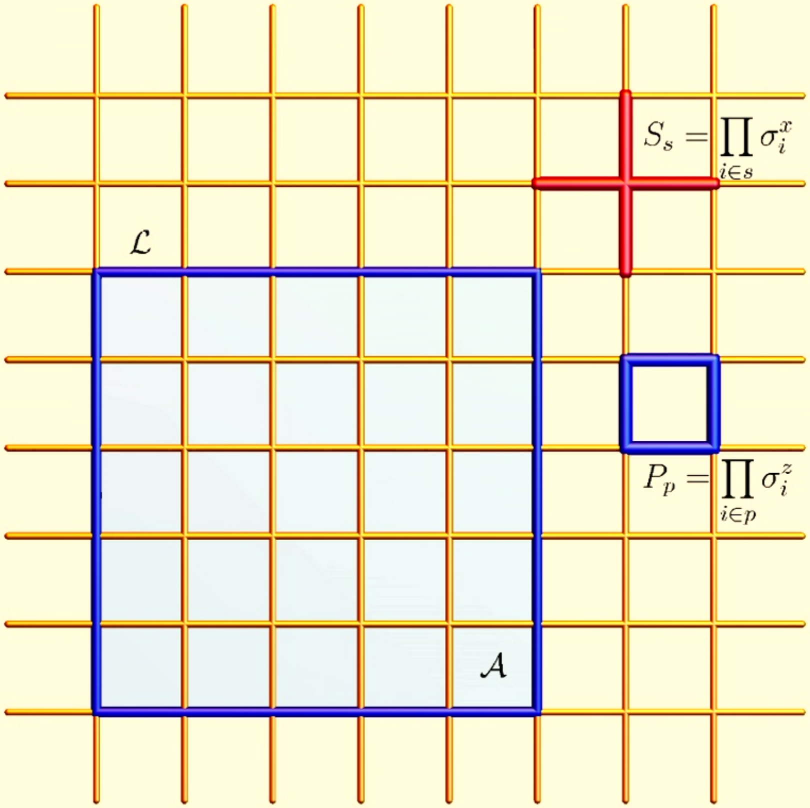


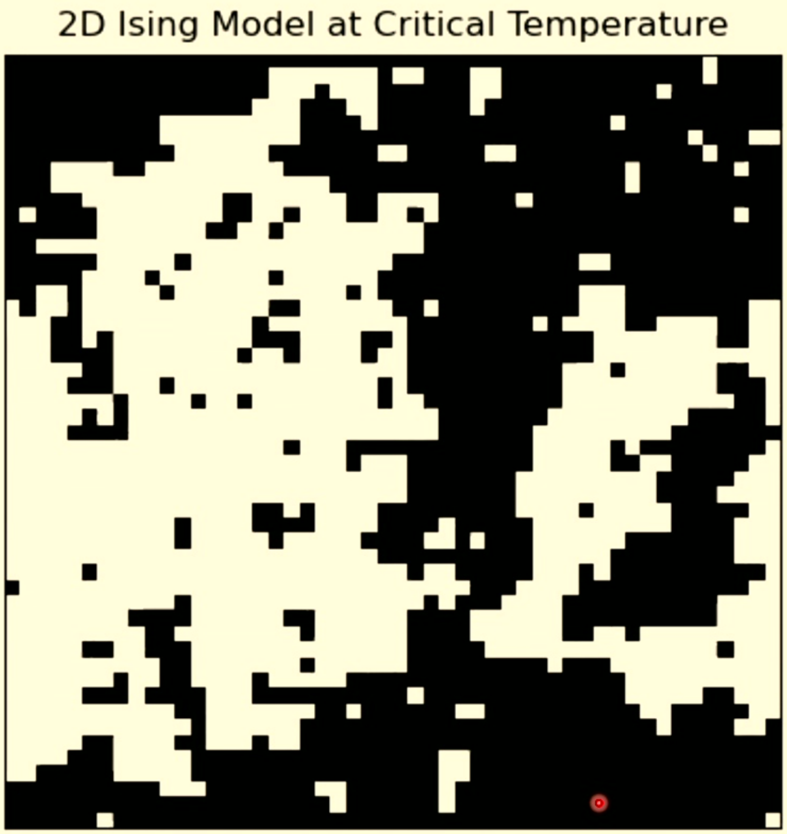
Ryotaro Masaoka
University of Tokyo



Haruki Watanabe
University of Tokyo

What do they have in common?





Toric code Figure from Savary, Balents 2017

Gapless Hamiltonians are ubiquitous in nature

Gapless Hamiltonian (informal)

A Hamiltonian whose ground state has gapless excitations

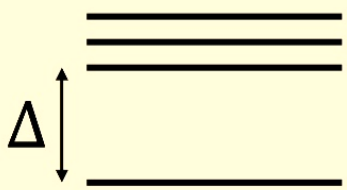
Example	Gapless excitations
Metal	Electrons
Magnet	Nambu-Goldstone bosons
Critical point	Critical fluctuations

Gapless Hamiltonians are ubiquitous in nature

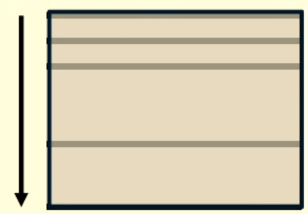
Gapless Hamiltonian (formal)

$\epsilon(L)$: the spectral gap at system size L.
The Hamiltonian is gapless if $\epsilon(L) \to 0$ as $L \to \infty$

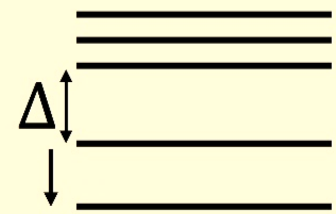
Gapped



Gapless



Metal, magnet, critical point



Note: Often "gapless" means the rightmost scenarios, but we include both cases.

Frustration-free Hamiltonians by example

Paramagnet	$H = \sum_i Z_i$
Ising model	$H = \sum_i Z_i Z_{i+1}$
FM Heisenberg model	$H = -\sum_i \overrightarrow{S_i} \cdot \vec{S}_{i+1}$
AKLT model	$H = \sum_i \overrightarrow{S_i} \cdot \vec{S}_{i+1} + \frac{1}{3}\left(\vec{S}_i \cdot \vec{S}_{i+1}\right)^2$
Toric code	$H = \sum_s A_s + \sum_p B_p$

Frustration-free Hamiltonians by example

Trivial	Paramagnet	$H = \sum_i Z_i$
Discrete SSB	Ising model	$H = \sum_i Z_i Z_{i+1}$
Continuous SSB	FM Heisenberg model	$H = -\sum_i \overrightarrow{S_i} \cdot \vec{S}_{i+1}$
SPT	AKLT model	$H = \sum_i \overrightarrow{S_i} \cdot \vec{S}_{i+1} + \frac{1}{3}\left(\vec{S}_i \cdot \vec{S}_{i+1}\right)^2$
Topological order	Toric code	$H = \sum_s A_s + \sum_p B_p$

Frustration-free Hamiltonians

Frustration-free Hamiltonian

Let $H = \sum_i H_i$ with *local* H_i. Then

H is frustration-free < = > The ground state minimizes H_i simultaneously

Remark:
Sometimes we impose $H_i \geq 0$, in which case we can write $H_i|GS\rangle = 0$

Commuting projector Hamiltonians are frustration-free

$$H = \sum_s S_s + \sum_p A_p \,, [S_s, A_p] = 0$$

Simultaneously diagonalize all terms
=> Frustration free

Note:
Stabilizer Hamiltonians for quantum computation are all frustration free

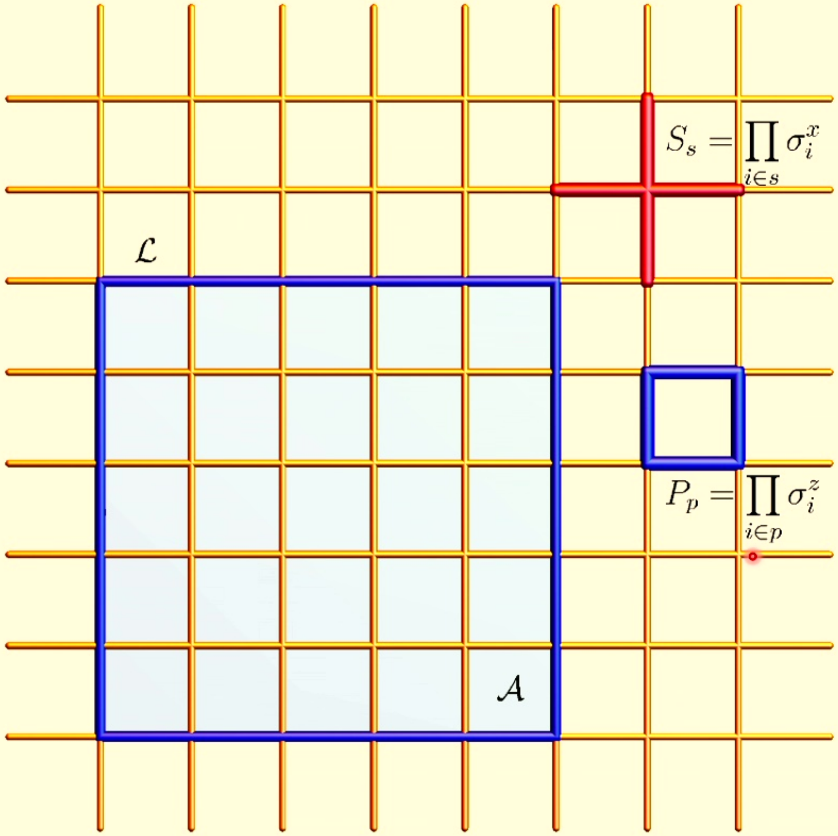


Figure from Savary, Balents 2017

Non- commuting frustration-free Hamiltonians

AKLT Hamiltonian

$$H = \sum_i \vec{S}_i \cdot \vec{S}_{i+1} + \frac{1}{3}\left(\vec{S}_i \cdot \vec{S}_{i+1}\right)^2 = \underbrace{\sum_i P_{i,i+1}^{S=2}}_{\text{Non-commuting projector}}$$

Valence bond solid state

 $= \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$

Note:

All matrix product states admit frustration-free parent Hamiltonian

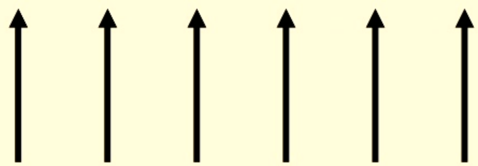
Ferromagnet Heisenberg is gapless and frustration-free

$$H = -\sum_i \vec{S}_i \cdot \vec{S}_{i+1}$$

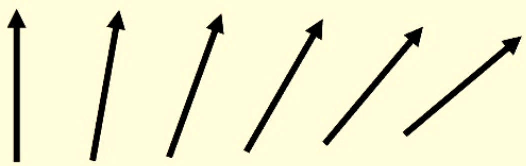
Ground states: spin $S = \frac{N}{2}$ states

$|\Psi\rangle = |\uparrow\rangle^{\otimes N}$

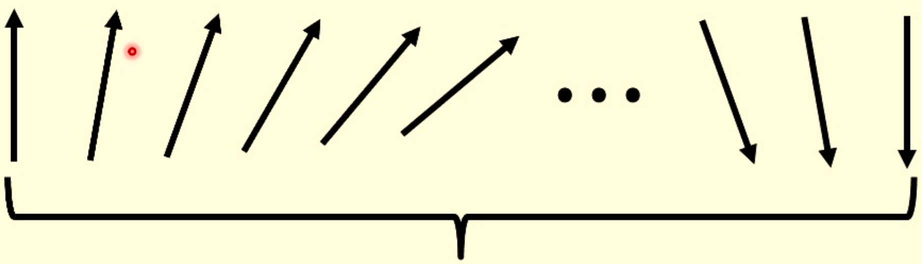
$S_-^m \, |\Psi\rangle$



Excited states: Magnons

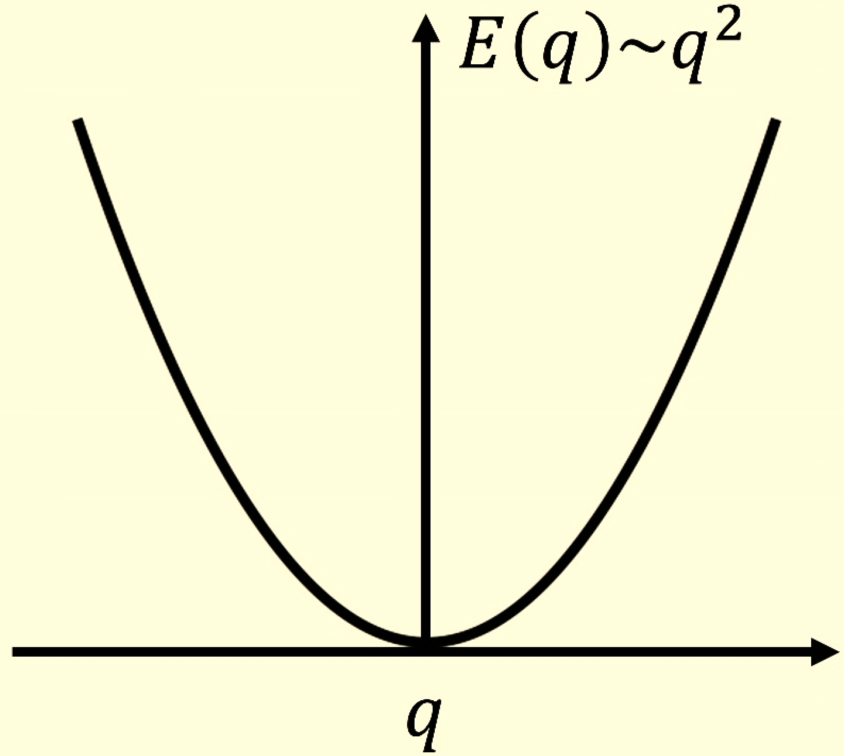


Magnon dispersion is gapless and quadratic



$\sim \frac{1}{q}$

$$T_x|\Psi_q\rangle = e^{iqa}|\Psi_q\rangle$$

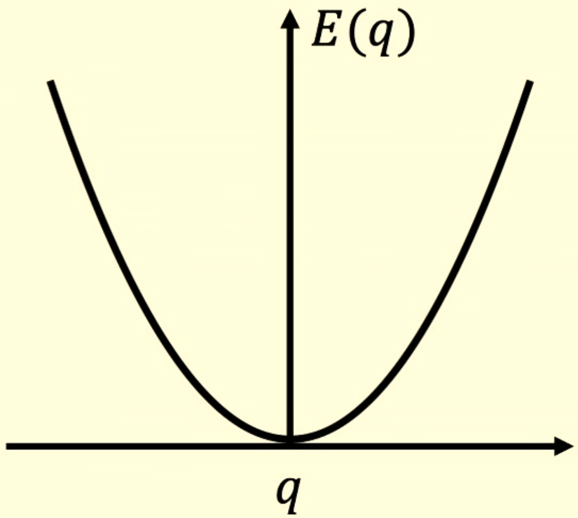


Ferromagnet and antiferromagnet comparison

Ferromagnet

$$H = -\sum_i \vec{S}_i \cdot \vec{S}_{i+1}$$

Frustration free

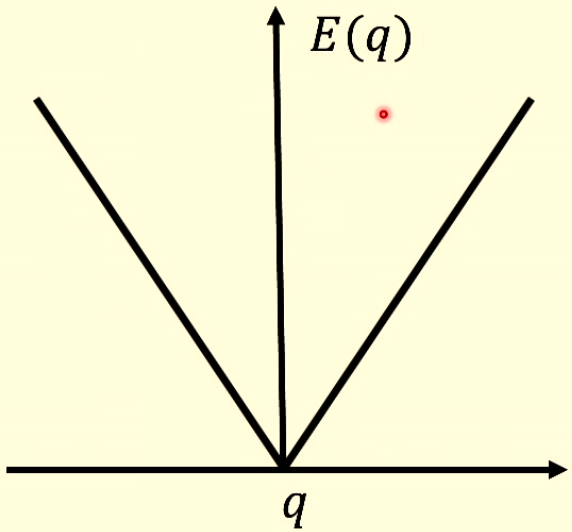


Quadratic

Antiferromagnet

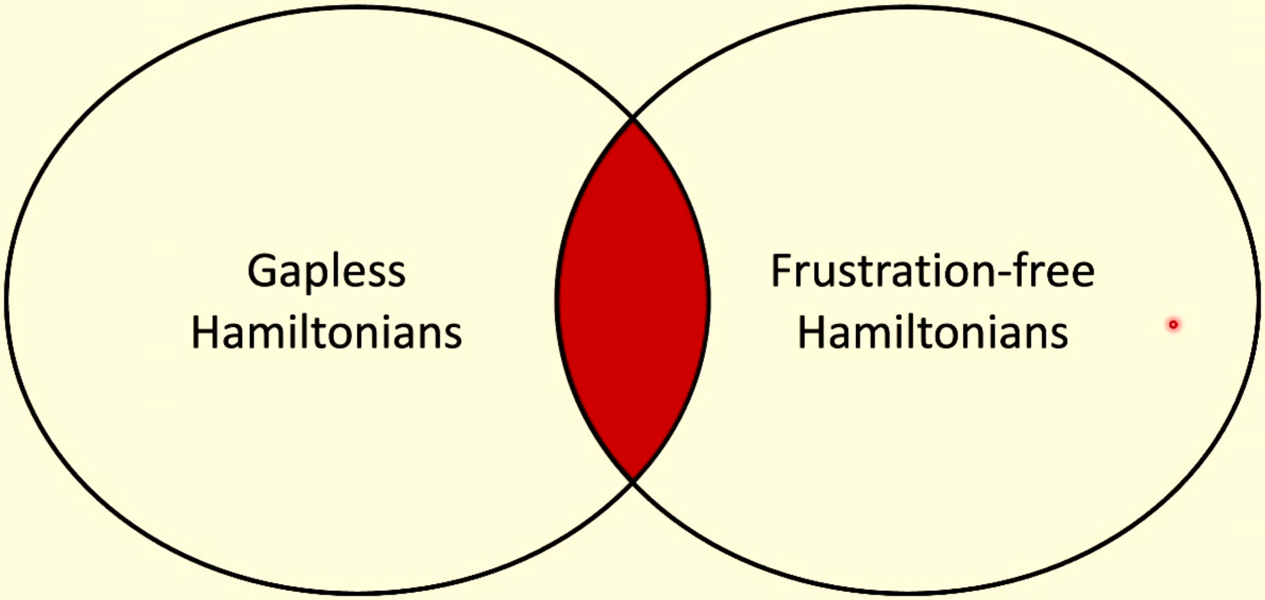
$$H = \sum_i \vec{S}_i \cdot \vec{S}_{i+1}$$

Not Frustration free



Linear

The aim of this talk



Frustration-free imposes nontrivial constraints on the spectrum

↓

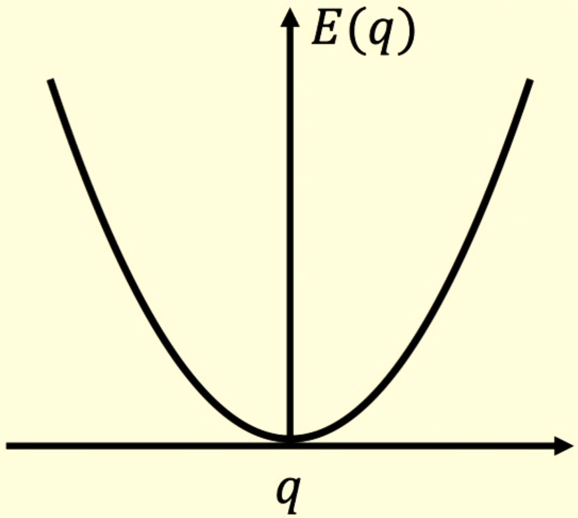
Frustration-free gapless Hamiltonians are not generic

Outline

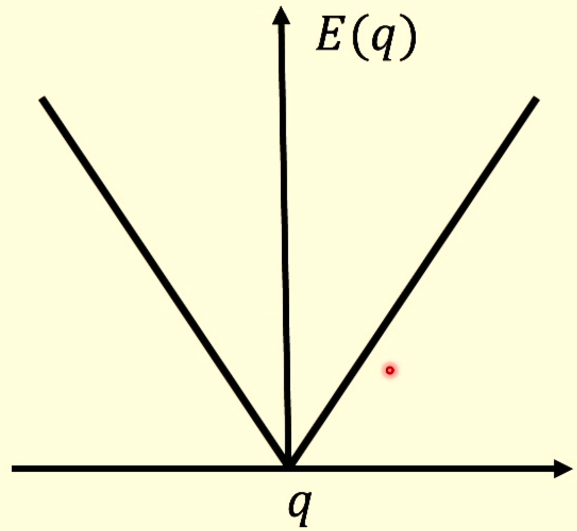
1. Dispersion relation for frustration-free Hamiltonians
2. Dynamic critical exponent for frustration-free Hamiltonians
3. Markov process as frustration-free Hamiltonians

Quadratic dispersion in frustration-free Hamiltonians

Frustration free



Not Frustration free



Is this a generic feature in frustration-free Hamiltonians?

- Partial proof in 1D
- Partial proof in nD

Partial proof for 1D case

1D FF Hamiltonian with $S = \frac{1}{2}$ and NN interactions are fully characterized

RESEARCH ARTICLE | JUNE 18 2015

Gapped and gapless phases of frustration-free spin-$\frac{1}{2}$ chains

Sergey Bravyi; David Gosset

We can use this to prove quadratic dispersion in 1D

Masaoka, **TS**, Watanabe, arXiv: 2406.06414

Proof strategy in 1D

One of the ground states take the form

$$|\Phi_0\rangle := \bigotimes_{x=1}^{L} |0\rangle_x = |0 \cdots 0\rangle$$

A magnon-type ansatz can be constructed as

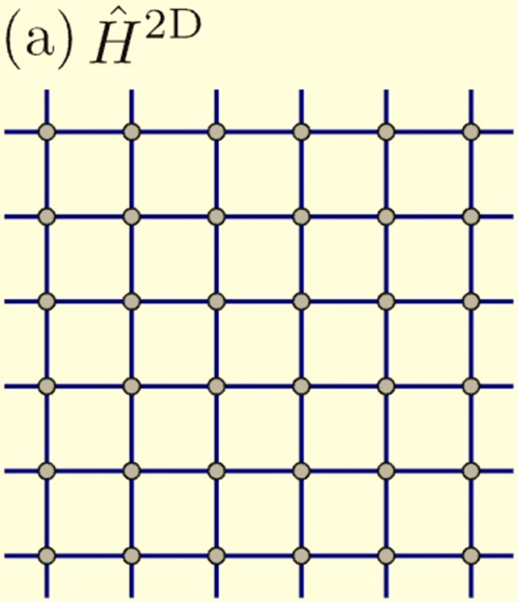
$$|\Psi_k\rangle := \frac{1}{\sqrt{L}} \sum_{x=1}^{L} e^{ikx} \hat{s}_x^- |\Phi_0\rangle$$

Evaluate the variational energy explicitly

$$\langle \Psi_k | \hat{H} | \Psi_k \rangle$$

Partial proof in 2D

Consider nD FF Hamiltonian with $S = \frac{1}{2}$ and NN. Then



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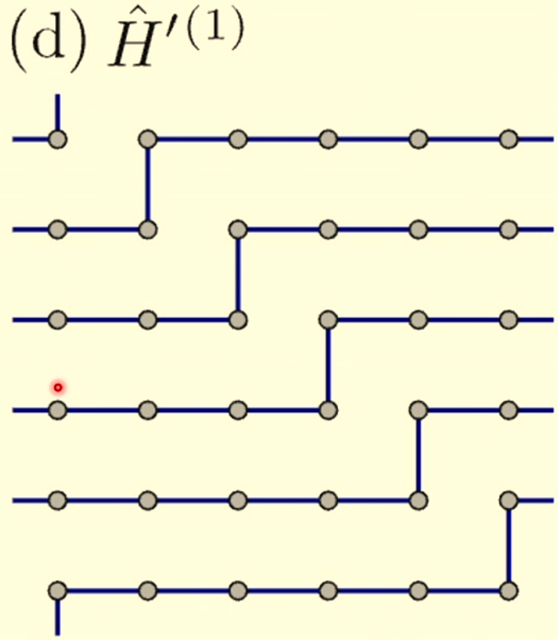
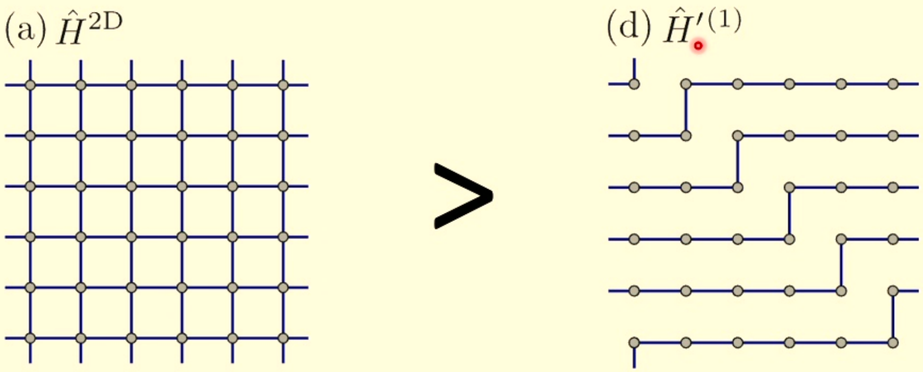


Partial proof in 2D

Min-Max principle

If $H' > H$, then $E_n' > E_n$



If $\widehat{H}^{2D}$ is gapless, so is $\widehat{H}^{1D}$

↓

We can use classification result for 1D

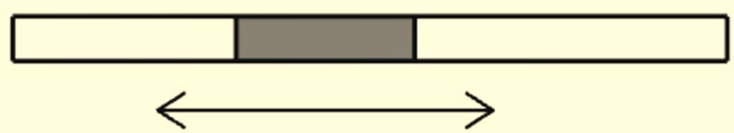
↓

nD Hamiltonians also have quadratic dispersion

Nontrivial examples outside Bravyi-Gosset

$$\hat{H}_{\boldsymbol{r}} = \frac{1}{2\cosh(J\sum_{\boldsymbol{r}'\in B_{\boldsymbol{r}'}} \hat{\sigma}^z_{\boldsymbol{r}'})}\left(\underbrace{e^{-J\hat{\sigma}^z_{\boldsymbol{r}}\sum_{\boldsymbol{r}'\in B_{\boldsymbol{r}}}\hat{\sigma}^z_{\boldsymbol{r}'}}}_{\text{Three-body interaction goes beyond the assumptions}} - \hat{\sigma}^x_{\boldsymbol{r}}\right)$$

- Magnon-type excitation is high-energy
- ”Moving domain wall”-type excitation is low energy
- Can be used to create quadratic states



Summary of Part I

- Conjectured quadratic dispersion for FF Hamiltonians
- Proved it for 1D S=1/2 NN Hamiltonians by explicit construction
- Proved it for subclass of nD NN Hamiltonians on hypercubic lattice
- The general version is still open!

Outline

1. Dispersion relation for frustration-free Hamiltonians

2. Dynamic critical exponent for frustration-free Hamiltonians

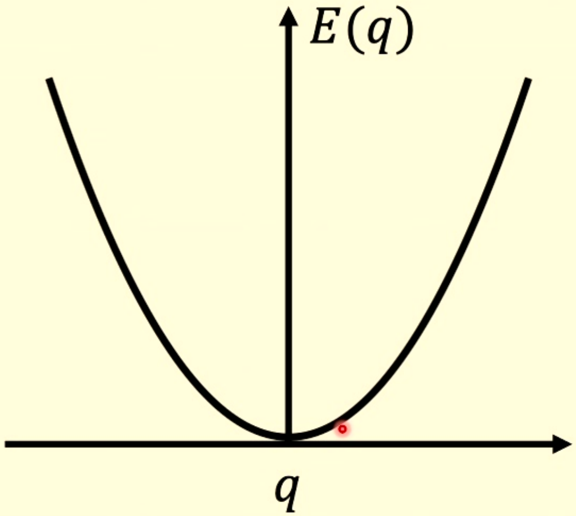
3. Markov process as frustration-free Hamiltonians

Dynamic critical exponent

Dynamic critical exponent

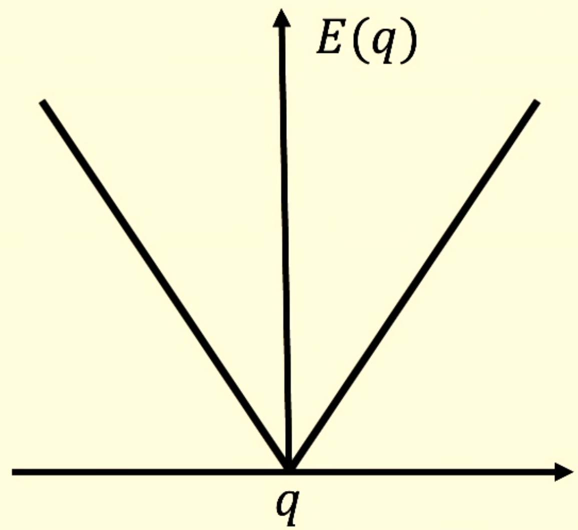
Exponent $\boldsymbol{z}$ such that $\epsilon(L) \sim L^{-z}$

Frustration free



$z = 2$

Not Frustration free



$z = 1$

We can bound dynamic critical exponent

Theorem (Masaoka, TS, Watanabe)

If the ground state subspace of FF Hamiltonian has *critical* correlations,

$$z \geq 2$$

Remarks:

1. Critical correlations ~ power law correlations. To be defined precisely later.
2. Shows FF Hamiltonian cannot give CFT, which has $z = 1$.
3. Goes beyond [Gosset, Mozgunov, 2016], which applied to OBC.

Gosset-Huang inequality

Gosset-Huang inequality

$$\frac{|\langle\Psi|\hat{\mathcal{O}}_{\boldsymbol{x}}^{\dagger}(\hat{\mathbb{1}}-\hat{G})\hat{\mathcal{O}}'_{\boldsymbol{y}}|\Psi\rangle|}{\|\hat{\mathcal{O}}_{\boldsymbol{x}}|\Psi\rangle\|\|\hat{\mathcal{O}}'_{\boldsymbol{y}}|\Psi\rangle\|} \leq 2\exp\left(-g'|\boldsymbol{x}-\boldsymbol{y}|\sqrt{\frac{\epsilon}{g^2+\epsilon}}\right)$$

g, g': constants, ϵ: gap size, $\hat{G}$: Ground state projector

Remarks:

1. For unique ground state, LHS is the connected correlator
2. Heuristically, this means $\xi \sim \epsilon^{-\frac{1}{2}}$, as opposed to $\xi \sim \epsilon^{-1}$

Gosset, Huang, PRL (2016)

Proof of bound on dynamic critical exponent

Assume critical correlations

$$\frac{|\langle\Psi|\hat{\mathcal{O}}_{\boldsymbol{x}}^{\dagger}(\hat{\mathbb{1}}-\hat{G})\hat{\mathcal{O}}'_{\boldsymbol{y}}|\Psi\rangle|}{\|\hat{\mathcal{O}}_{\boldsymbol{x}}|\Psi\rangle\|\|\hat{\mathcal{O}}'_{\boldsymbol{y}}|\Psi\rangle\|}=\Omega(L^{-\Delta})$$

On the other hand, we can write

$$2\exp\left(-g'|\boldsymbol{x}-\boldsymbol{y}|\sqrt{\frac{\epsilon}{g^2+\epsilon}}\right)=2\exp(-\Omega(L^{1-z/2}))$$

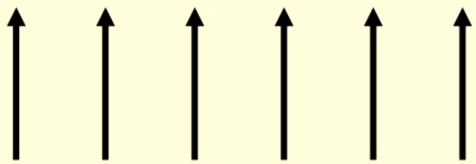
Using Gosset-Huang inequality,

$$\Omega(L^{-\Delta})\leq 2\exp(-\Omega(L^{1-z/2}))$$

This implies

$$z\geq 2$$

Example: Ferromagnetic Heisenberg model



Ground states: spin $S = \frac{N}{2}$ states

$|\Psi\rangle = |\uparrow\rangle^{\otimes N}$

$S_-^m\,|\Psi\rangle$

$\hat{G}$ is nontrivial

There is a critical correlation

$$\frac{|\langle\Psi|\hat{O}_{\boldsymbol{x}}^\dagger(\hat{\mathbb{1}} - \hat{G})\hat{O}'_{\boldsymbol{y}}|\Psi\rangle|}{\|\hat{O}_{\boldsymbol{x}}|\Psi\rangle\|\|\hat{O}'_{\boldsymbol{y}}|\Psi\rangle\|}$$

Many other examples including MPS/PEPS uncle Hamiltonians

Summary of Part II

- A new bound on dynamic critical exponent from Gosset-Huang inequality
- FF precludes generic behavior such as CFT
- Applicable to a wide range of gapless systems

Outline

1. Dispersion relation for frustration-free Hamiltonians

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3. Markov process as frustration-free Hamiltonians

We can bound dynamic critical exponent

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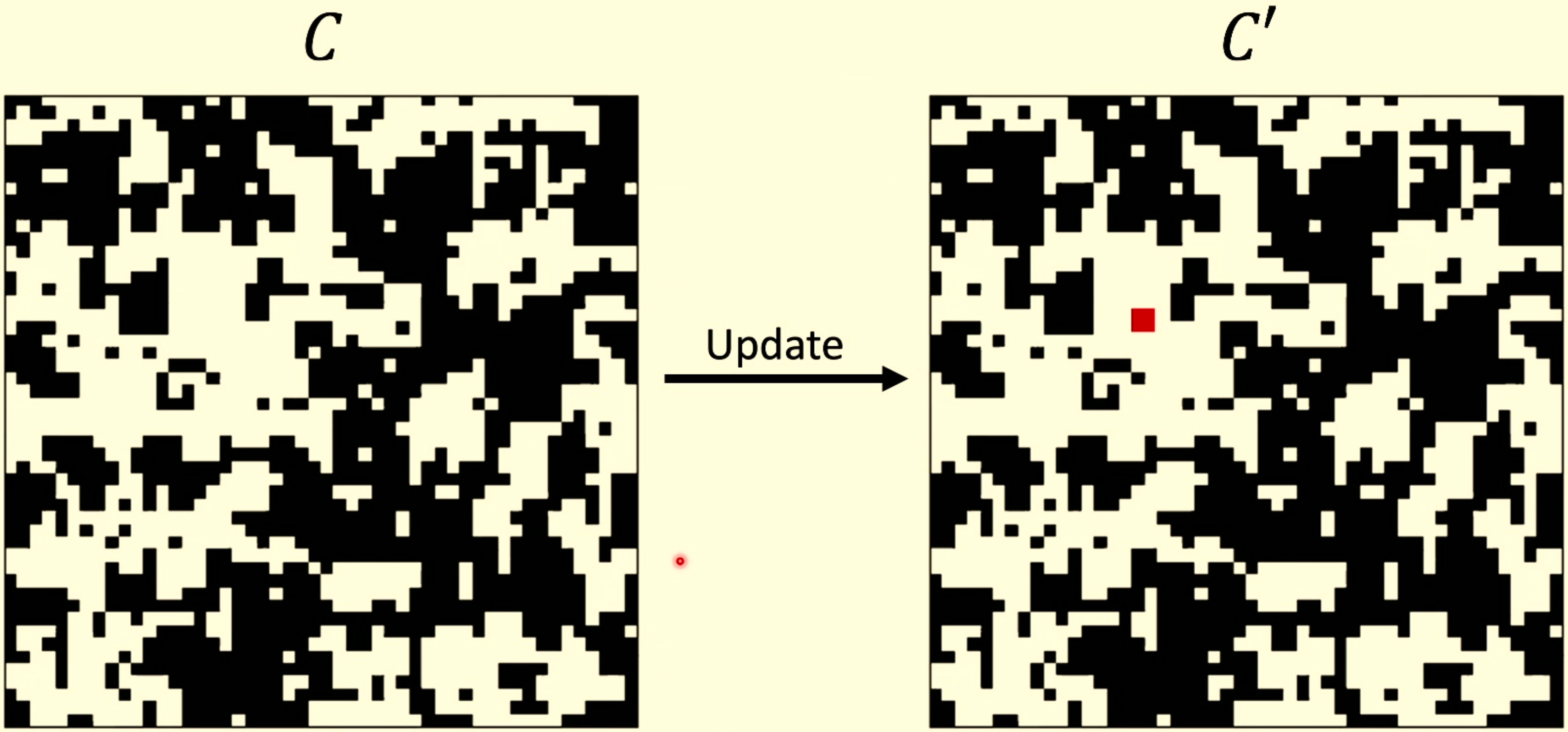
Markov Chain Monte Carlo updates spin configuration



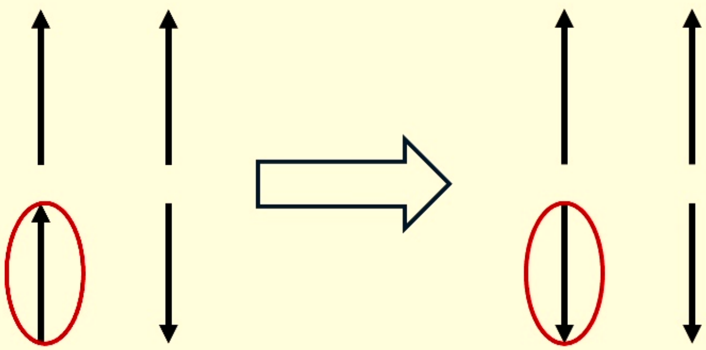
Stochastic time evolution as a Markov process

The transition rate Matrix W

$$\frac{\mathrm{d}}{\mathrm{d}t} p_C = \sum_{C'} W_{CC'} p_{C'}$$

C : (spin) configuration, p_C: Probability of a configuration

Example: Glauber dynamics



- Compute the energy of two configurations
- Evolve according to relative probability of two configurations

Auto correlation time and critical slow down

Autocorrelation time $\boldsymbol{\tau}$ (informal)

Autocorrelation function behaves as

$$\mathrm{A(t)} = \langle O_t \, O_0 \rangle_C \leq \# \, e^{-\frac{t}{\tau}}$$

Given transition rate matrix W, and its spectral gap ϵ,

$$\tau = 1/\epsilon$$

Critical slowdown

At critical point, $\tau \sim L^z$

Can we understand how autocorrelation scales?

Conditions on transition-rate Matrix

Transition rate matrix: W

Equilibrium weight: $w(C)$

Locality: $W = \sum_i W_i$

Probability Conservation: $\sum_C (W_i)_{CC'} = 0$

Balance condition: $\sum_{C'} W_{CC'}\, w(C') = 0$

Detailed balance: $W_{CC'}\, w(C') = W_{C'C}\, w(C)$

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RK Hamiltonian: $H = -S^{-1} W S$

Ground state: $|\Psi_{RK}\rangle = \sum_C \sqrt{w(C)}\ |C\rangle$

Locality: $H = \sum_i H_i$

Left frustration-free: $\langle \Psi_{RK}| H_i = 0$

Right-frustration-free: $H_i |\Psi_{RK}\rangle = 0$

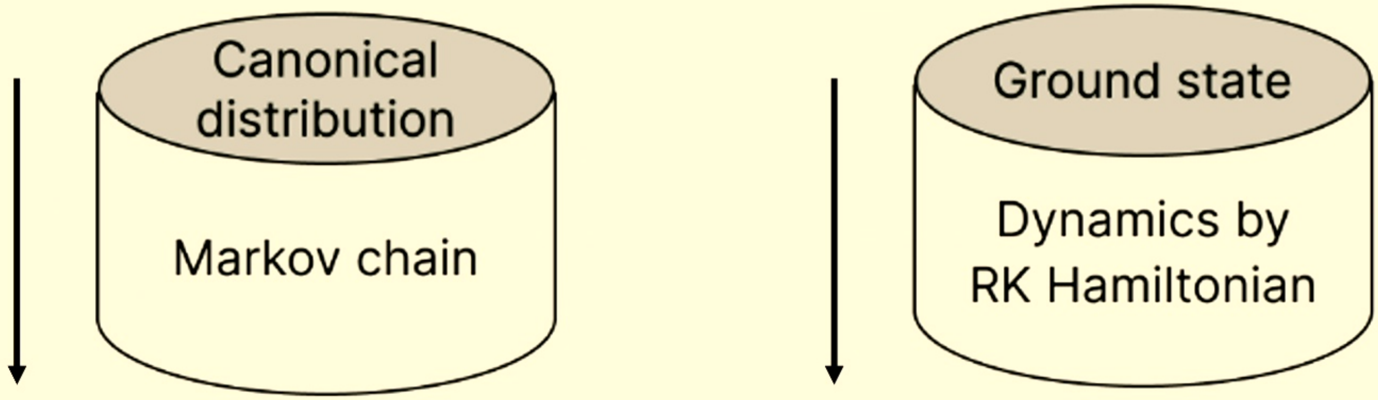
Hermiticity: $H_{CC'} = H_{C'C}$

Rokhsar, Kivelson PRL (1998)

Correspondence between classical and quantum problems

Equilibrium weight: $w(C)$

Ground state: $|\Psi_{RK}\rangle = \sum_C \sqrt{w(C)}\ |C\rangle$



These time evolutions are governed by the same dynamics

Our dynamic critical exponent bound $z \geq 2$ applies!

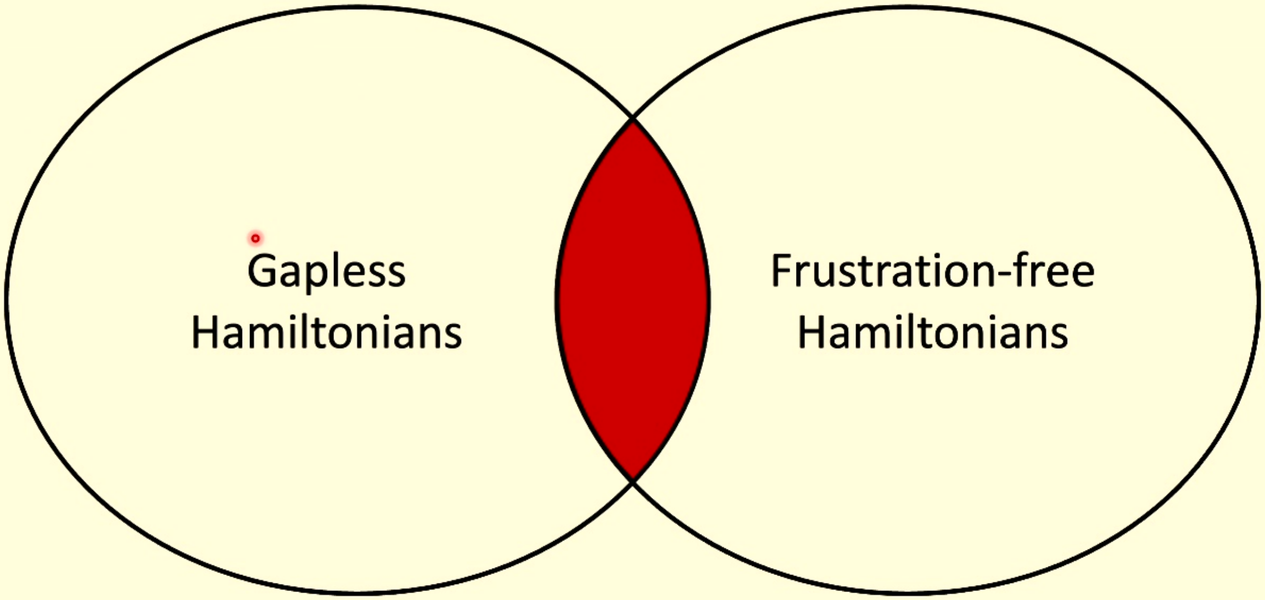
The bound for autocorrelation holds very broadly

Critical points	z (numerical)	References
Ising (2D)	$2.1667(5) \geq 2$	Nightingale, Blöte, PRB 62, 1089 (2000).
Ising (3D)	$2.0245(15) \geq 2$	Hasenbusch, PRE 101, 022126 (2020).
Heisenberg (3D)	$2.033(5) \geq 2$	Astillero, Ruiz-Lorenzo, PRE 100, 062117 (2019).
three-state Potts (2D)	$2.193(5) \geq 2$	Murase, Ito, JPSJ 77, 014002 (2008).
four-state Potts (2D)	$2.296(5) \geq 2$	Phys. A: Stat. Mech. Appl. 388, 4379 (2009).

Summary of Part III

- Analyzed autocorrelation of Markov Chain Monte Carlo
- Mapped MCMC to FF Hamiltonians to bound critical slowdown
- Showed a new bound on classical algorithms from a quantum result

The aim of this talk



Frustration-free imposes nontrivial constraints on the spectrum

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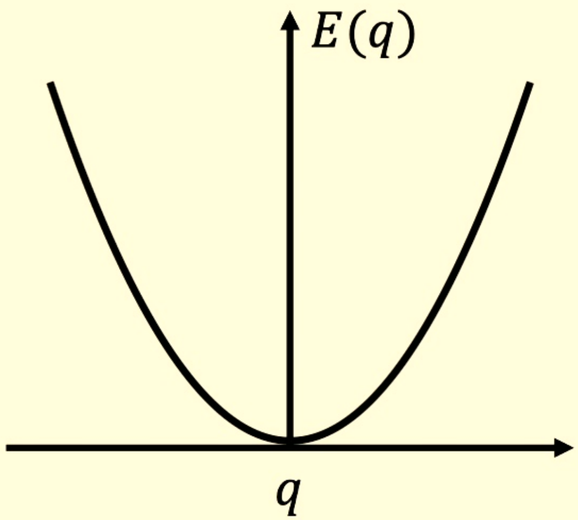
Frustration-free gapless Hamiltonians are not generic

Conclusion

Dispersion of frustration-free systems



Bound on Dynamic critical exponent

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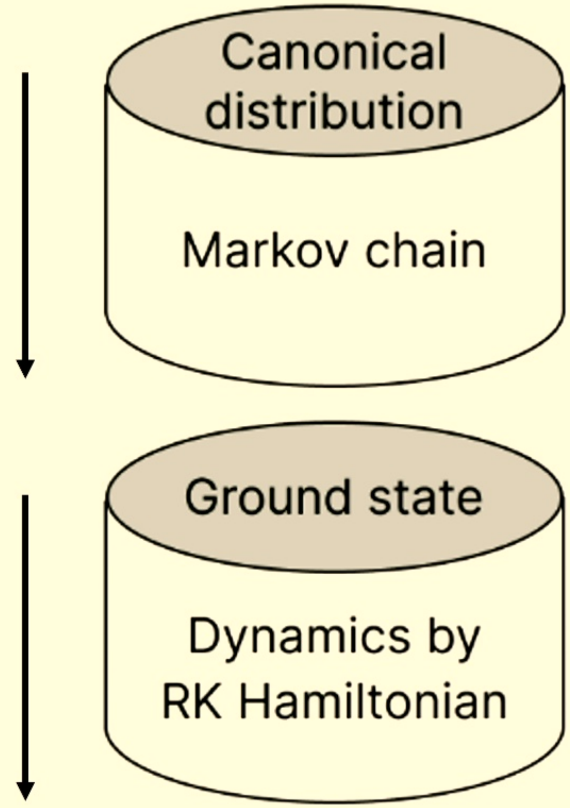
Mapping to Classical statistical models



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Right-frustration-free: $H_i |\Psi_{RK}\rangle = 0$

Hermiticity: $H_{CC'} = H_{C'C}$

Rokhsar, Kivelson PRL (1998)