Frustrated Magnetism in Materials with Kagome Lattice

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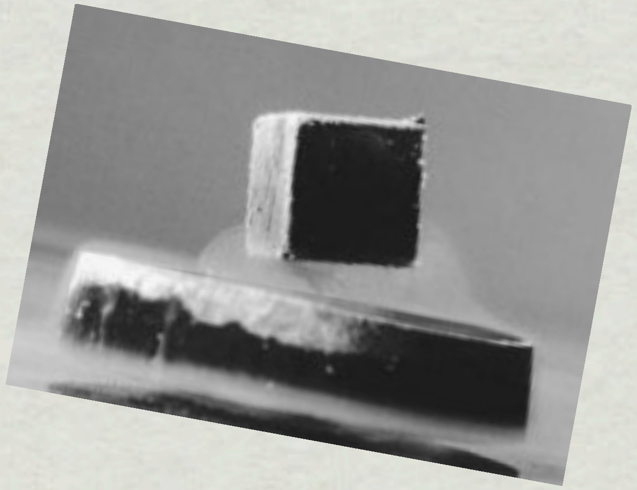
SIMPLE RULES

Emergent Phenomena

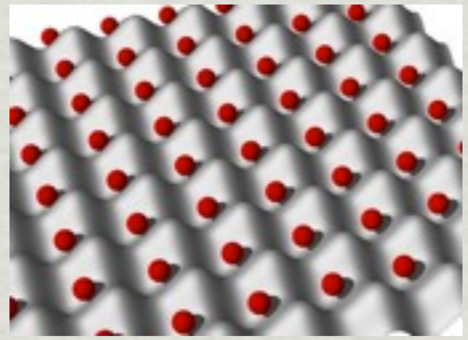


COMPLICATED BEHAVIOR

Strongly Correlated Systems!!

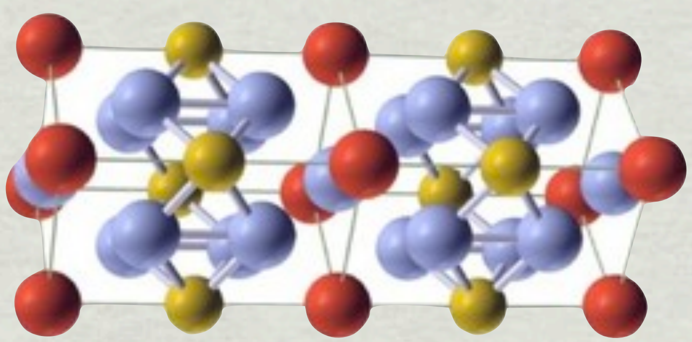
Emergent phenomena is responsible for both ...

INTERESTING PHYSICAL PHENOMENA



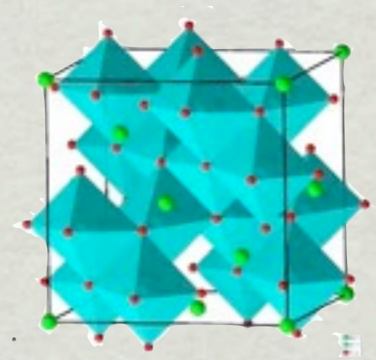
Mott Insulators

Heavy Fermions



Superconductivity

Fractional Quantum Hall



Frustrated Magnets

DIFFICULTY UNDERSTANDING

Nonperturbative ...

Beyond mean field...

Computational methods are one important component to computing properties and better understanding strongly correlated systems.

Computational Methods

Auxiliary Field Quantum Monte Carlo

Diffusion Monte Carlo

Dynamical Mean Field Theory

Density Matrix Renormalization Group

Determinant QMC

Exact diagonalization

Full Configuration Interaction QMC

Path Integral Monte Carlo

(Path Integral) Molecular Dynamics

Numerical linked cluster expansion

Variational Monte Carlo

Computational Methods

Written code and used in previous projects

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Computational Methods

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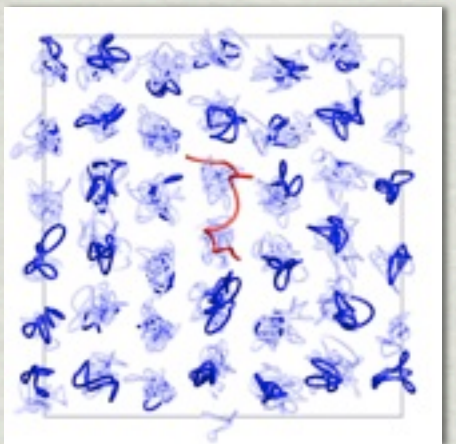
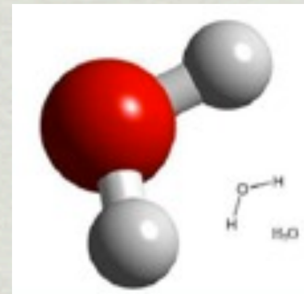
Writing code and using in current projects.

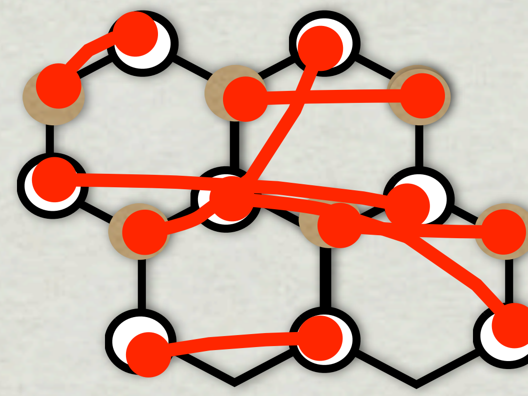
Success of Numerics



Supersolids

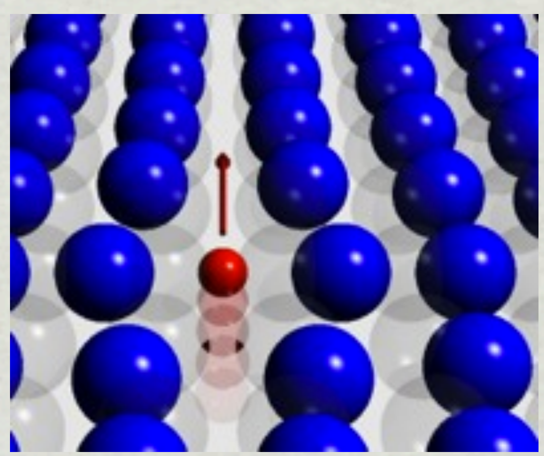


Ab-initio

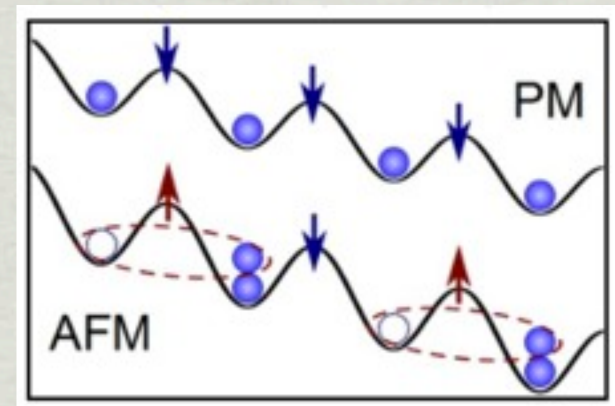


Frustrated Magnetism

Fractional Quantum Hall

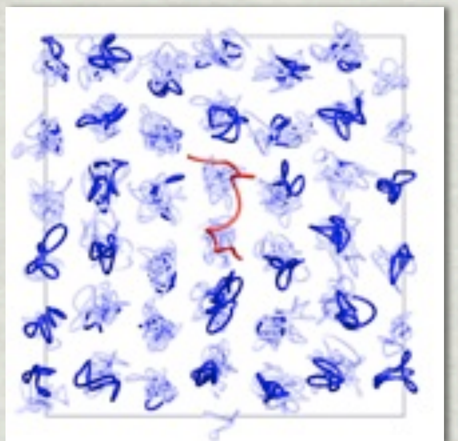


Cold Atoms



Non-equilibrium

Success of Numerics



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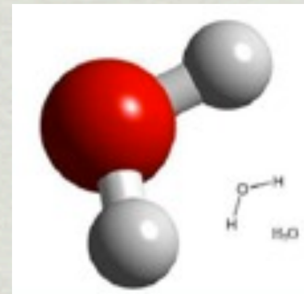

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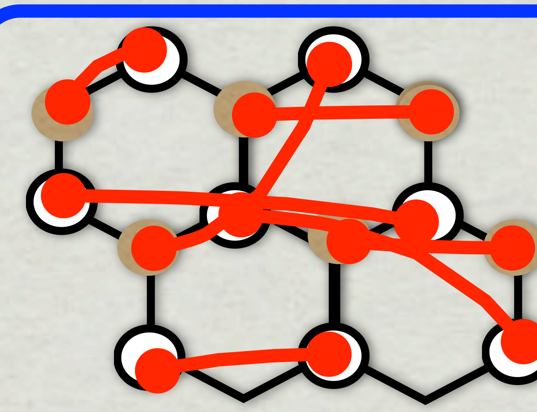

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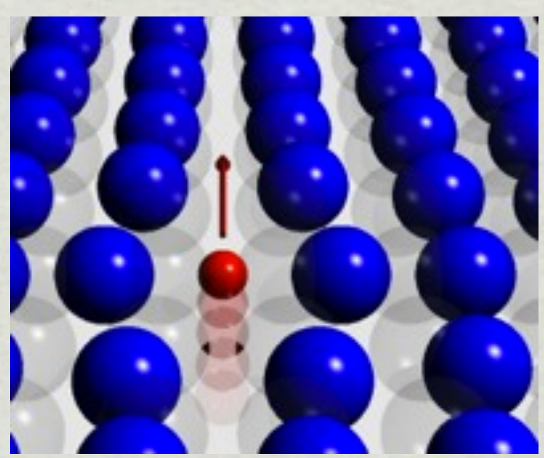
Fractional Quantum Hall



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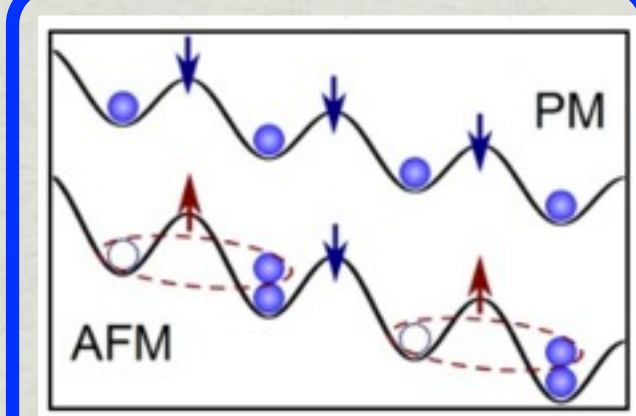

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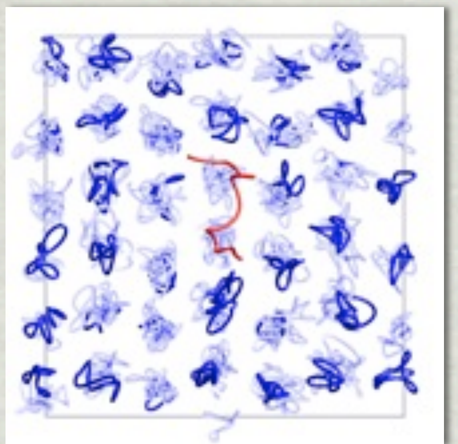
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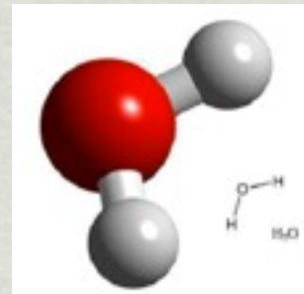
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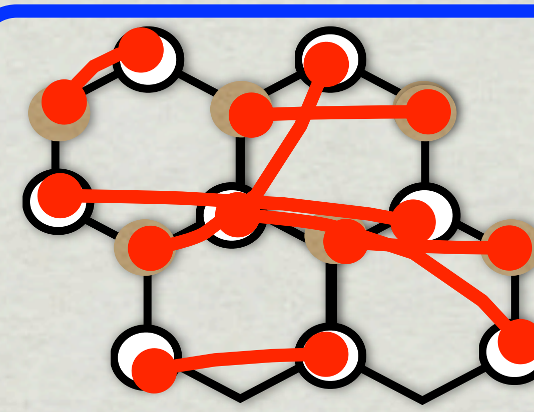
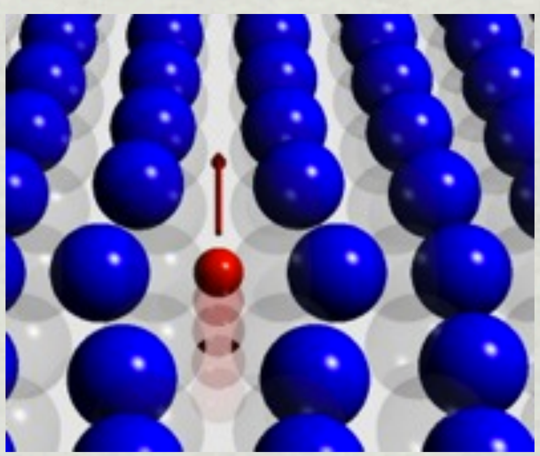

Frustrated Magnetism


Fractional Quantum Hall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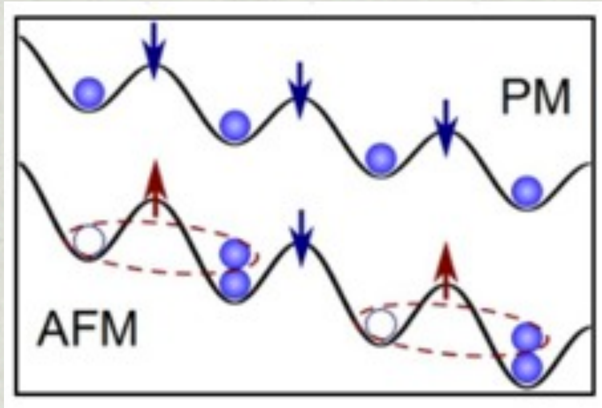

Non-equilibrium

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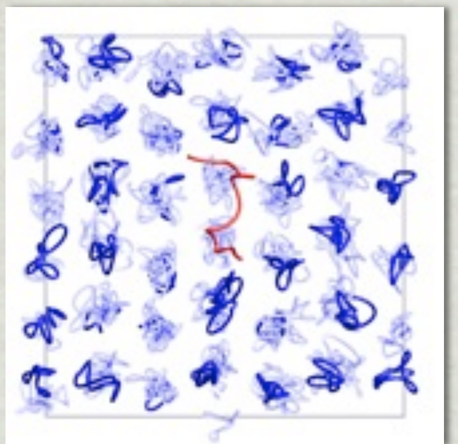

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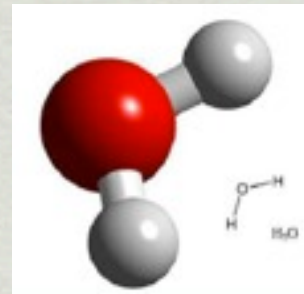

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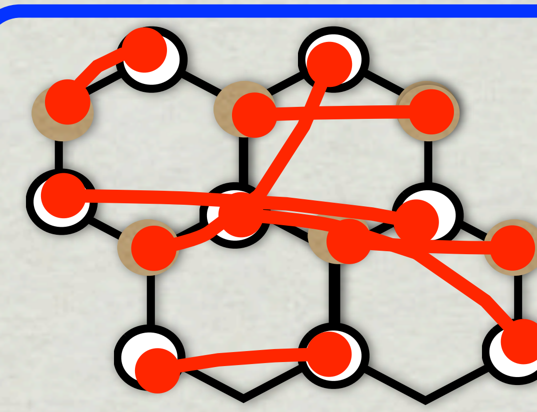

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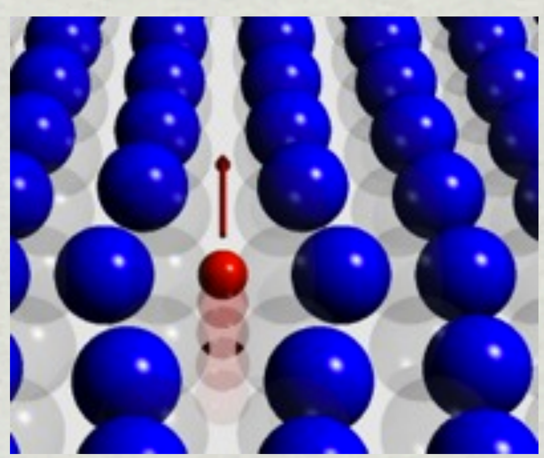

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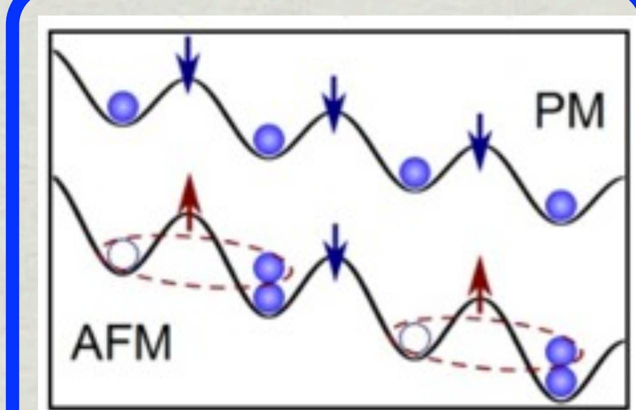
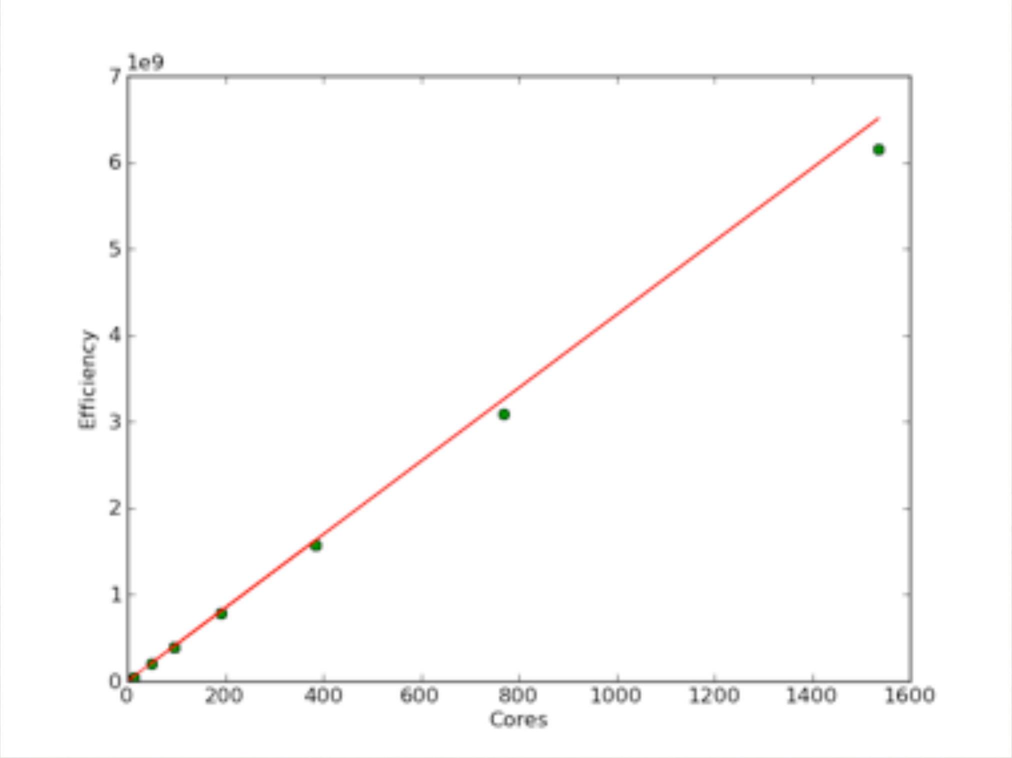


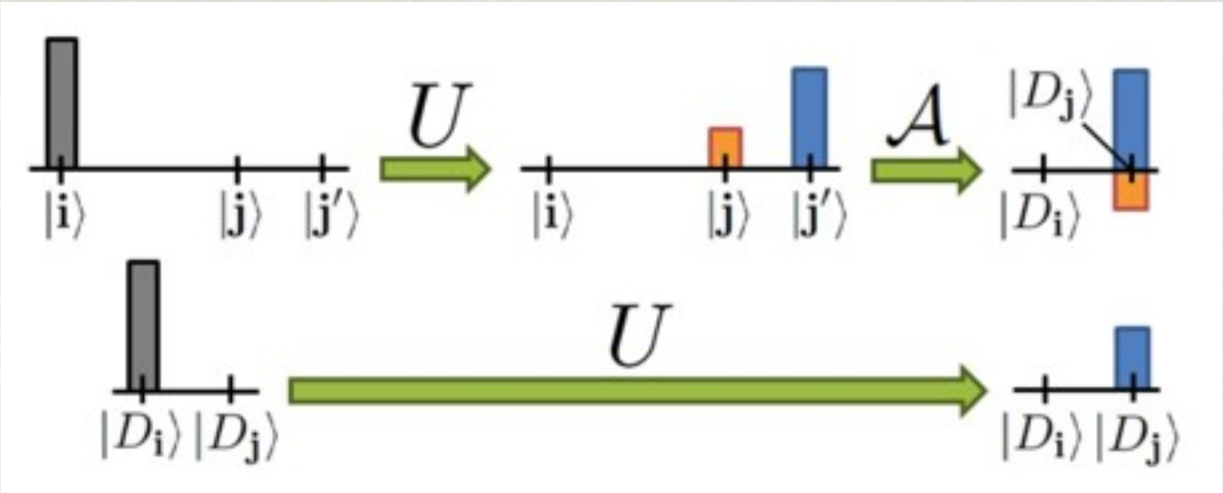
Non-equilibrium

Driving computational condensed matter

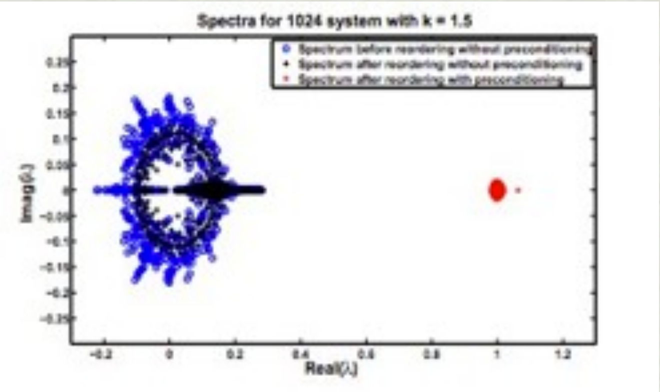
Massively Parallel Supercomputers



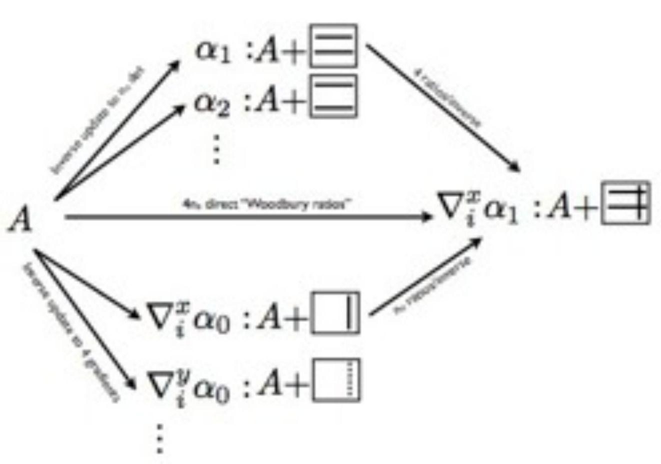
New Algorithms



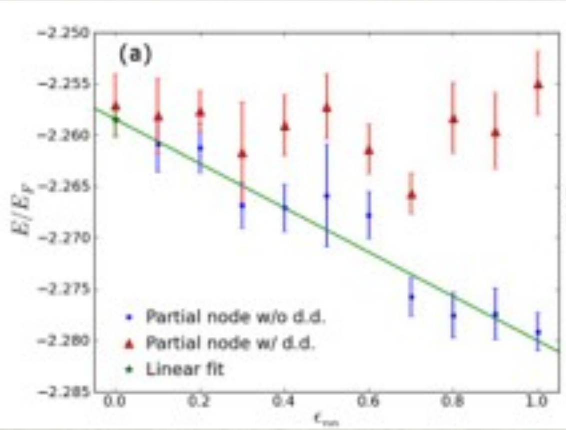
Working in an antisymmetric basis help.



O(n³) -> O(n²)



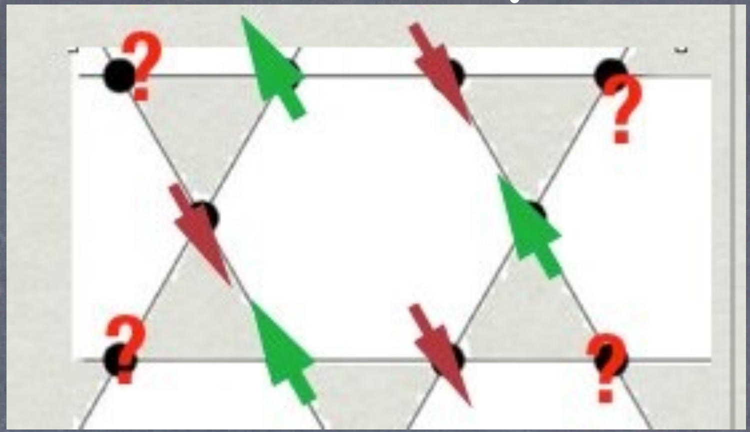
Determinants for constant cost



Attenuate the sign problem

We want to find interesting phases (like spin liquids)

A good place to search for spin liquids are frustrated lattices.



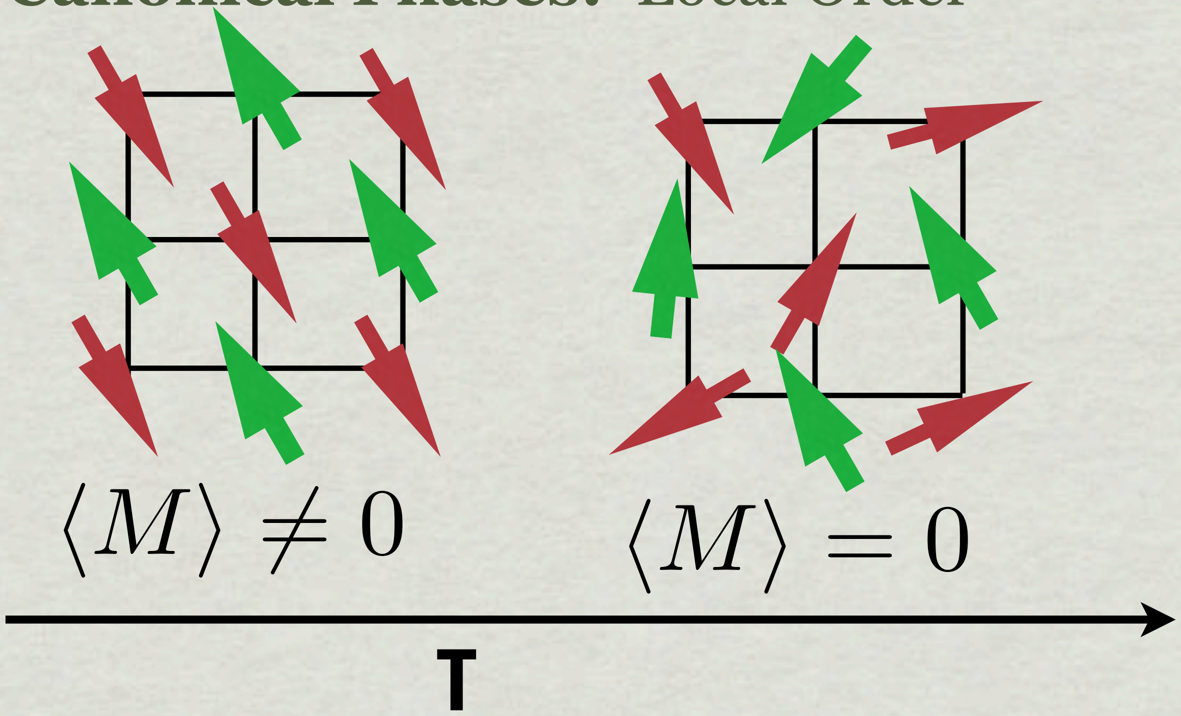
Use a variational approach to find likely spin-liquids

Use long history of theoretical work on spin-liquids to motivate the variational space to work in.

Find a new phase this way; connect to experiment

Spin Liquids

Canonical Phases: Local Order



Spin Liquids: No local order parameter

The typical viewpoint: Featureless

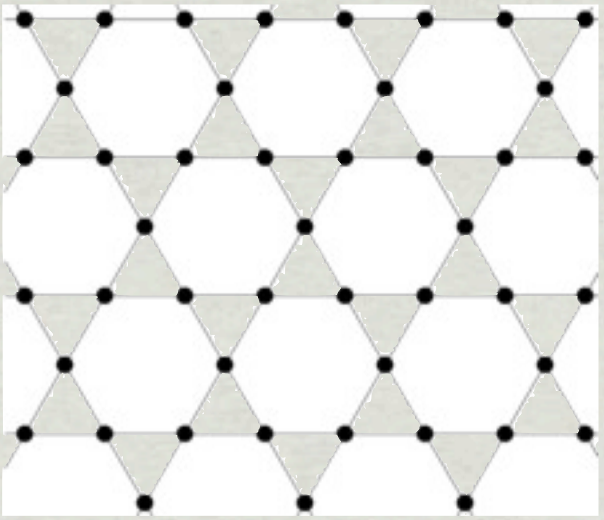
A better viewpoint:

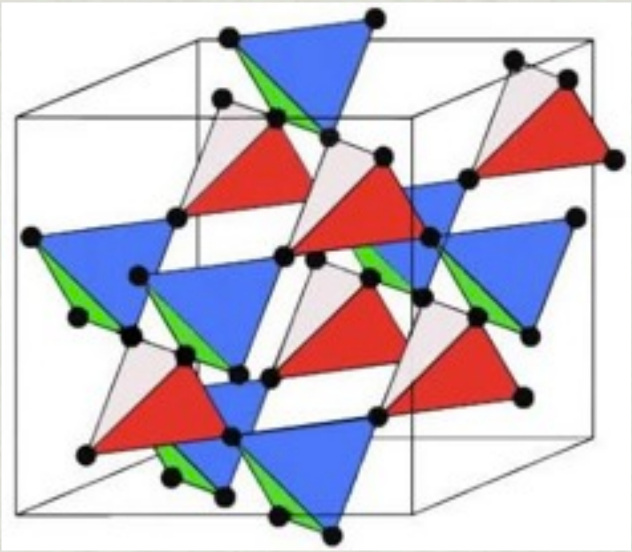
Insulator + Long Range Entanglement

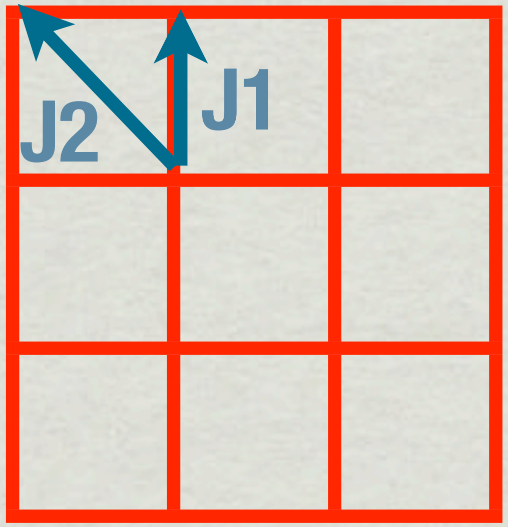
Very far from a product state - quantum circuits take a long time to build them.

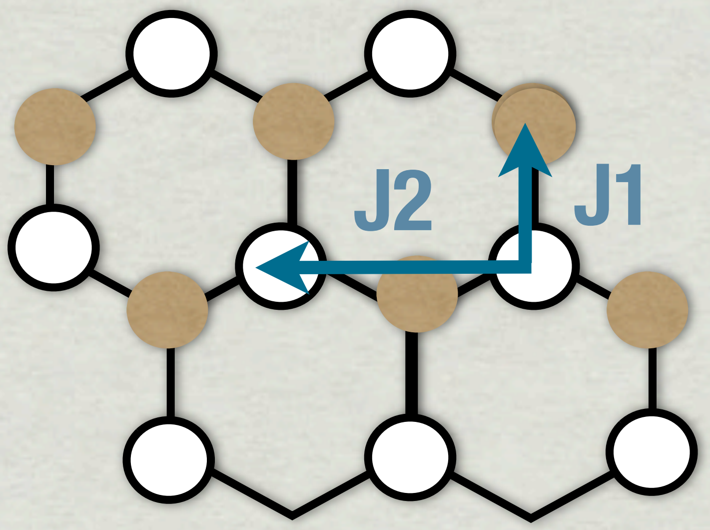
Fractionalized excitations: Spinons = Spin 1/2 fermionic excitations but no charge

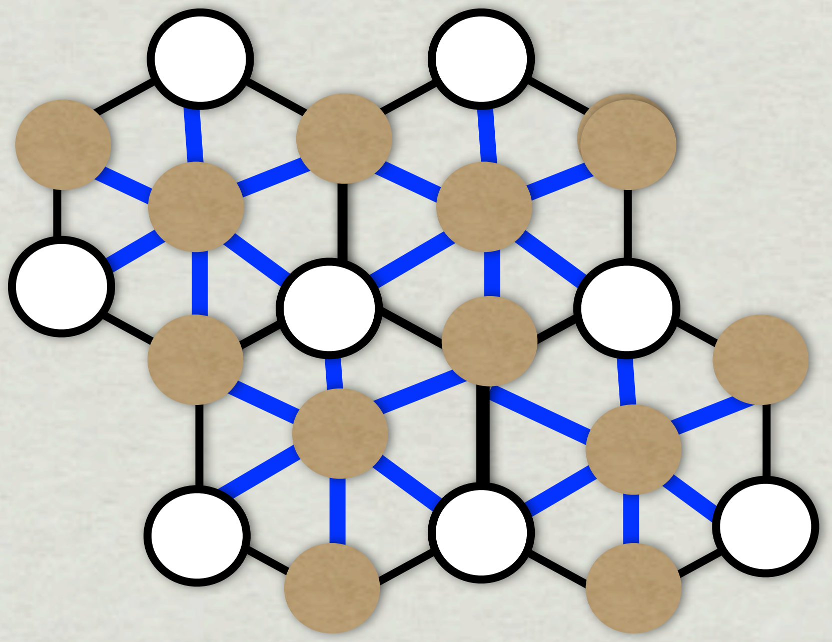
Frustrated Magnets...

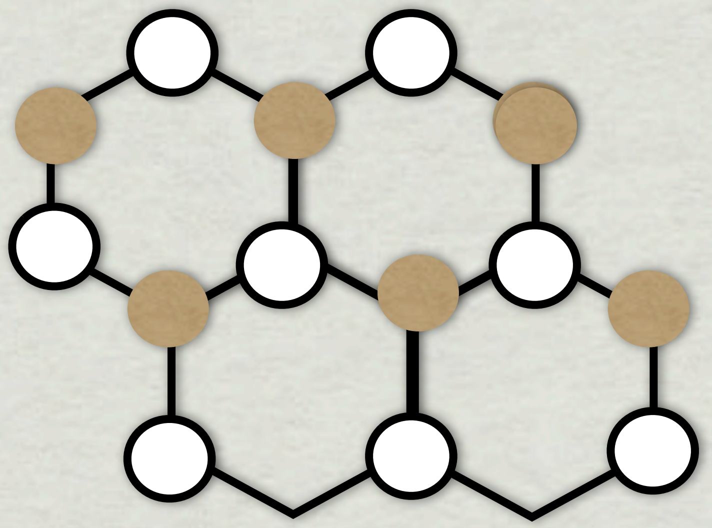






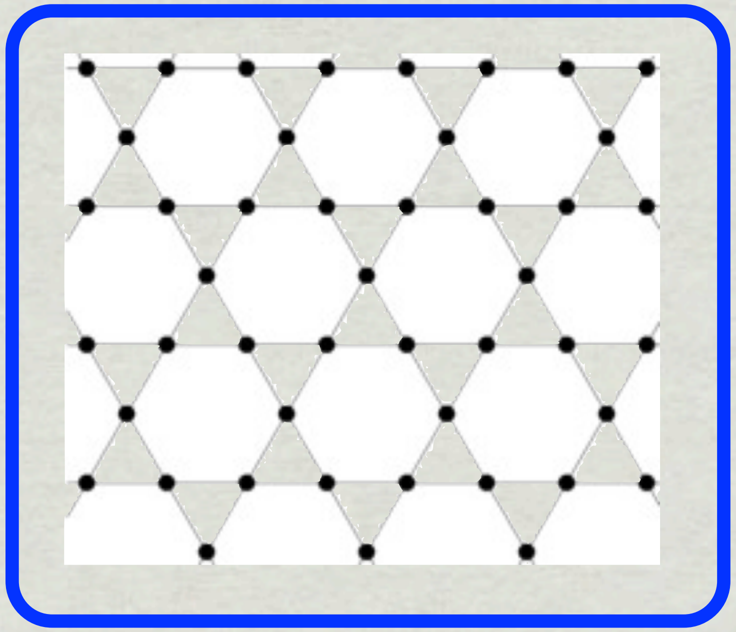


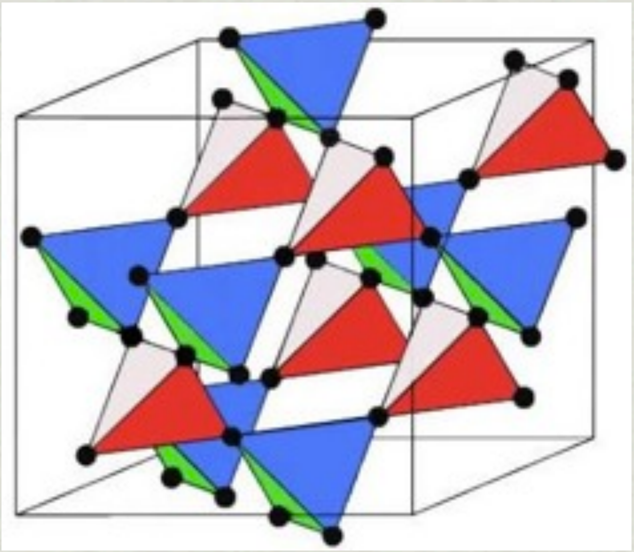


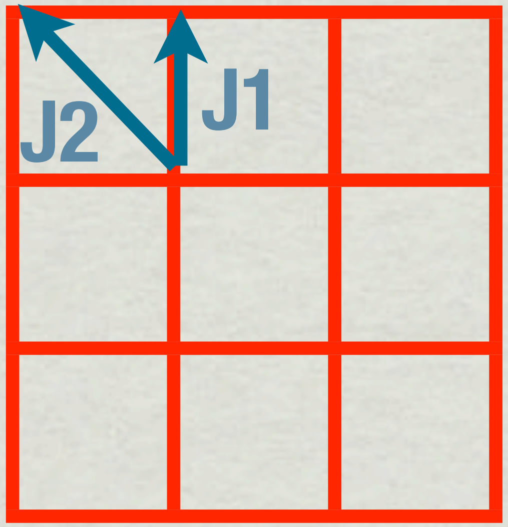


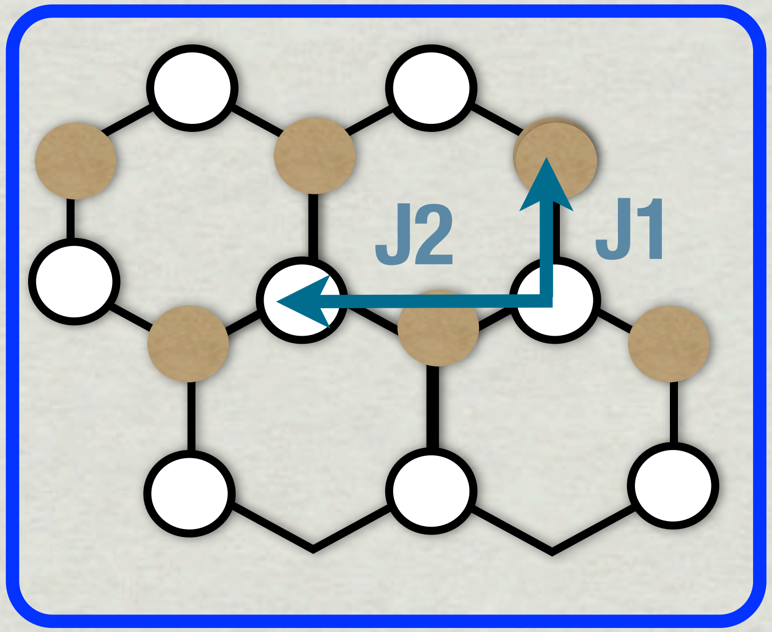
HUBBARD

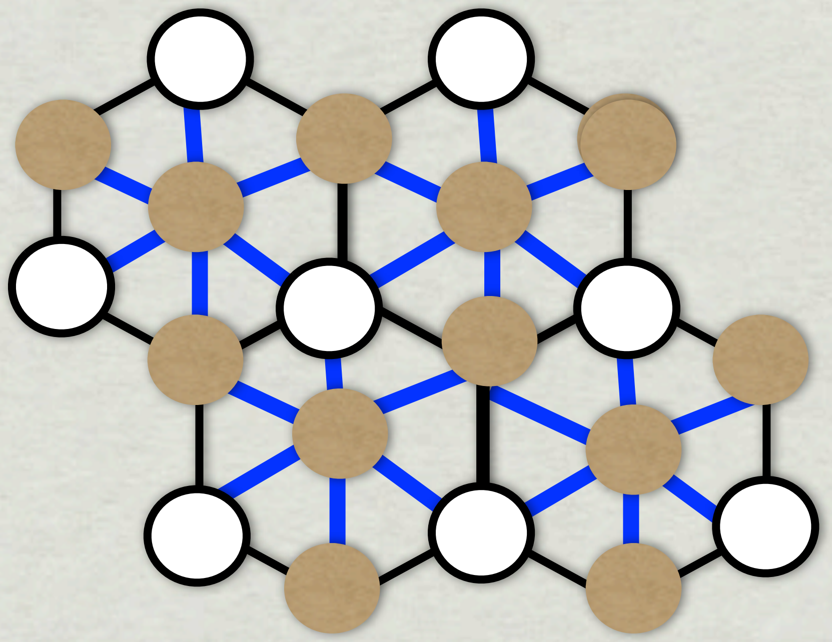
Frustrated Magnets...

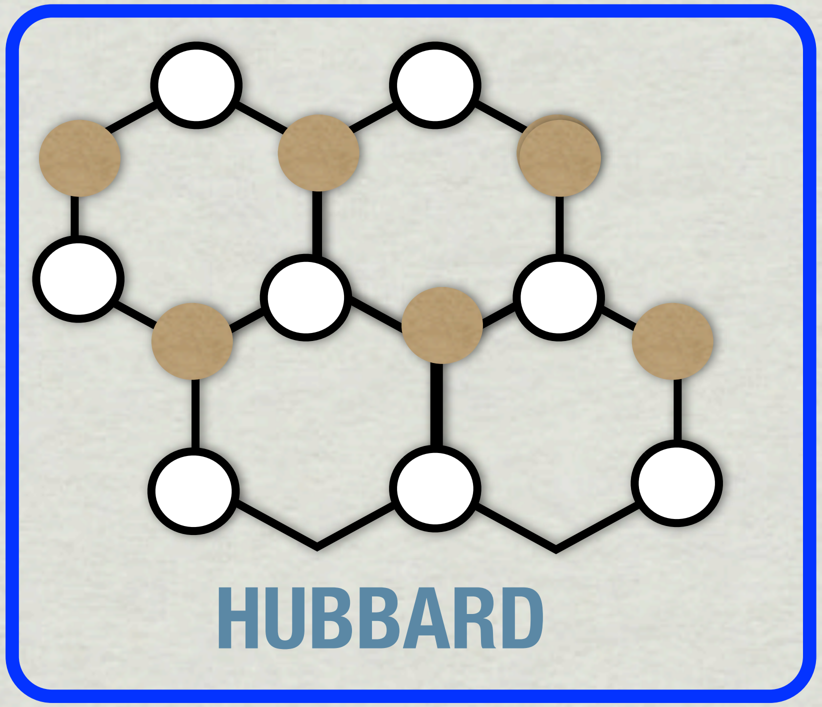












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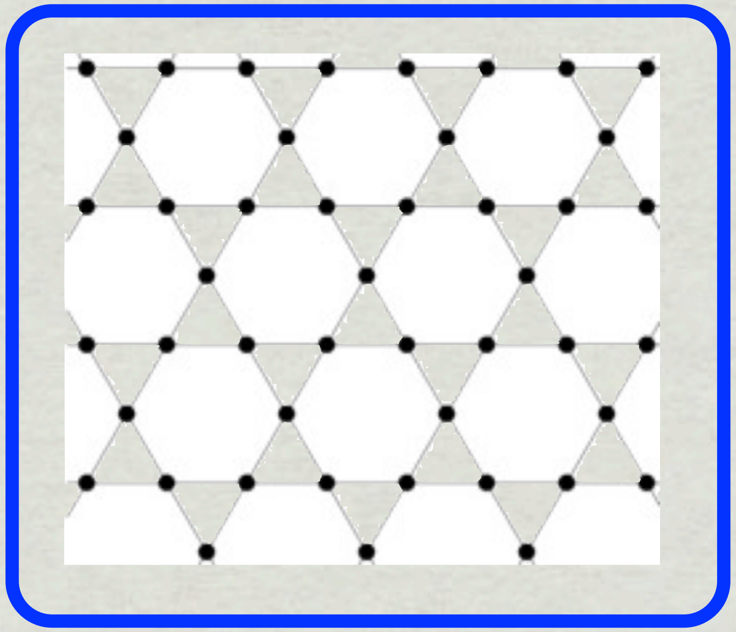

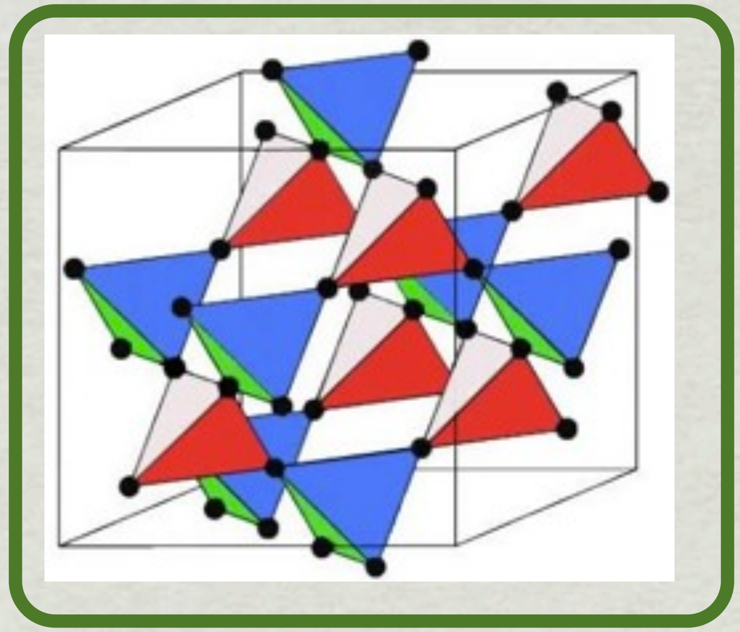

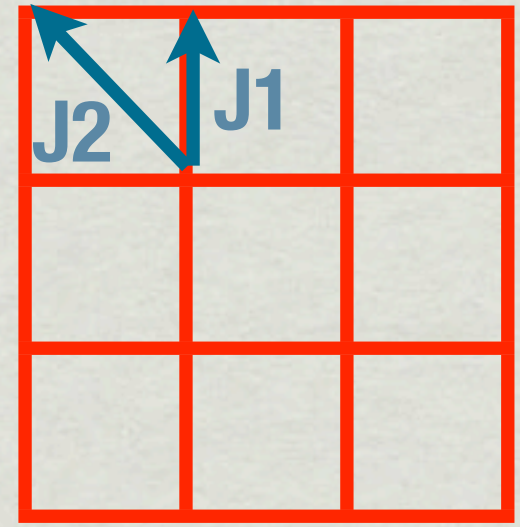

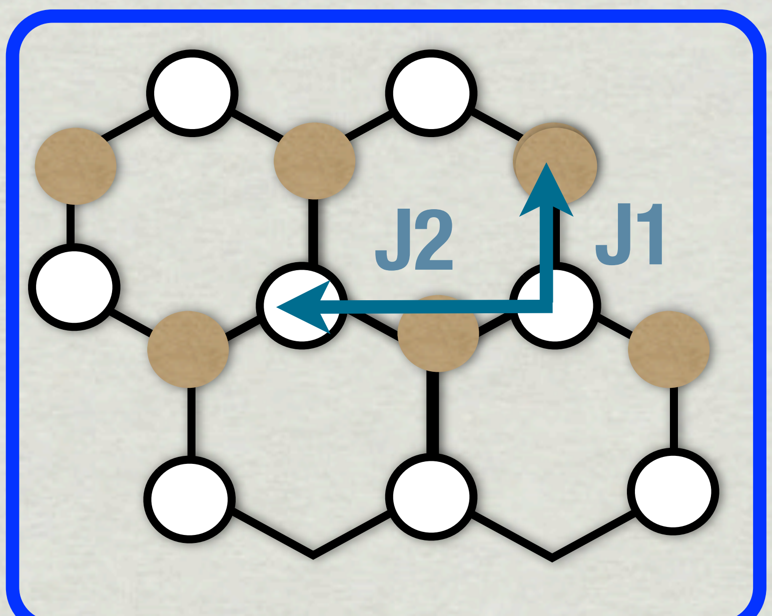

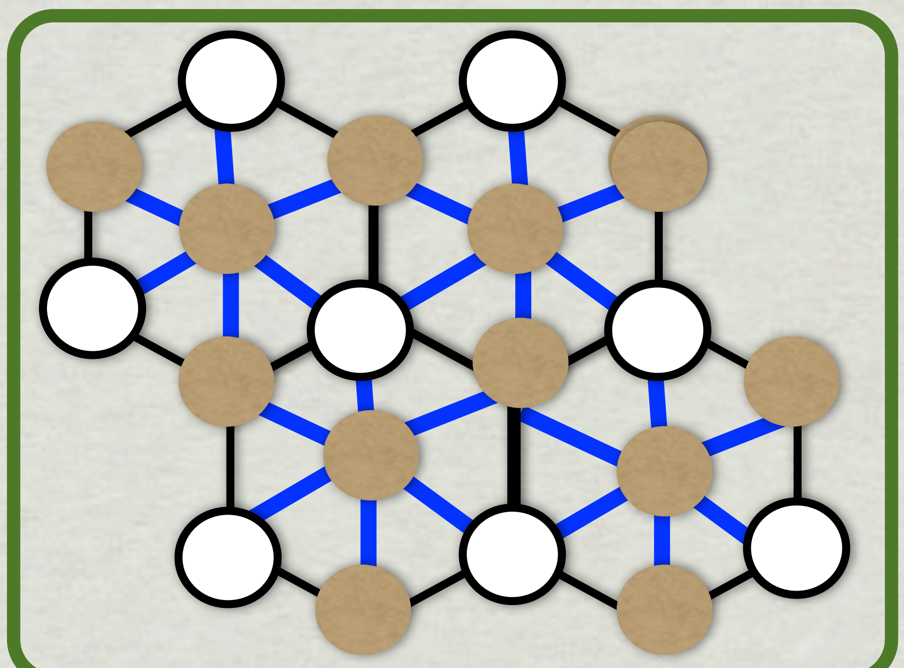

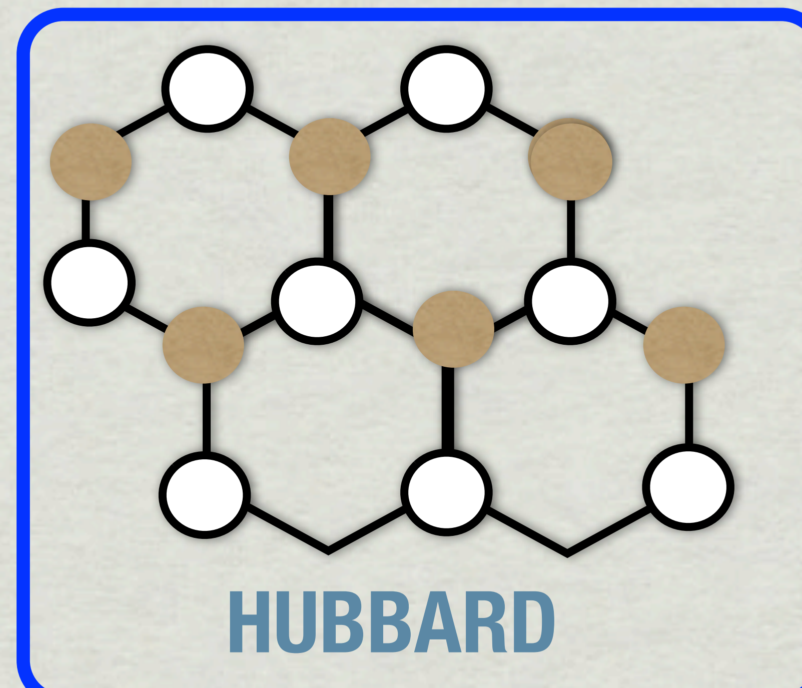

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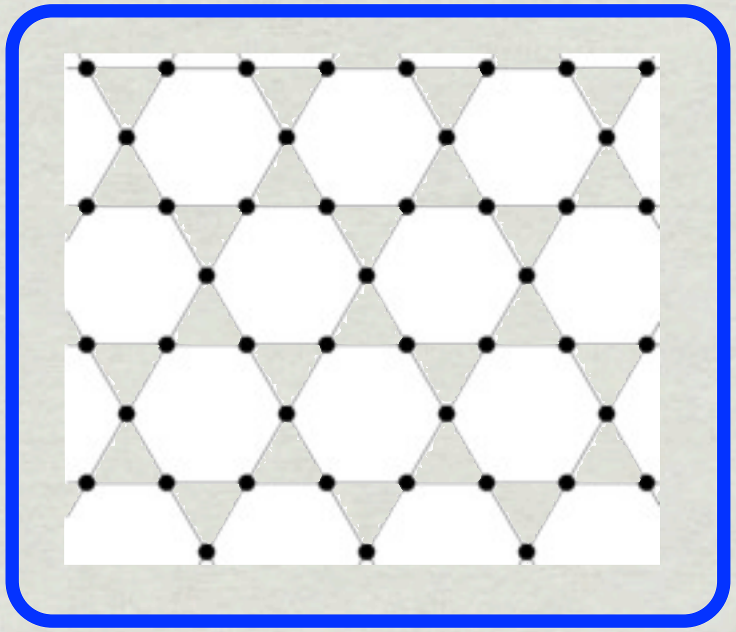
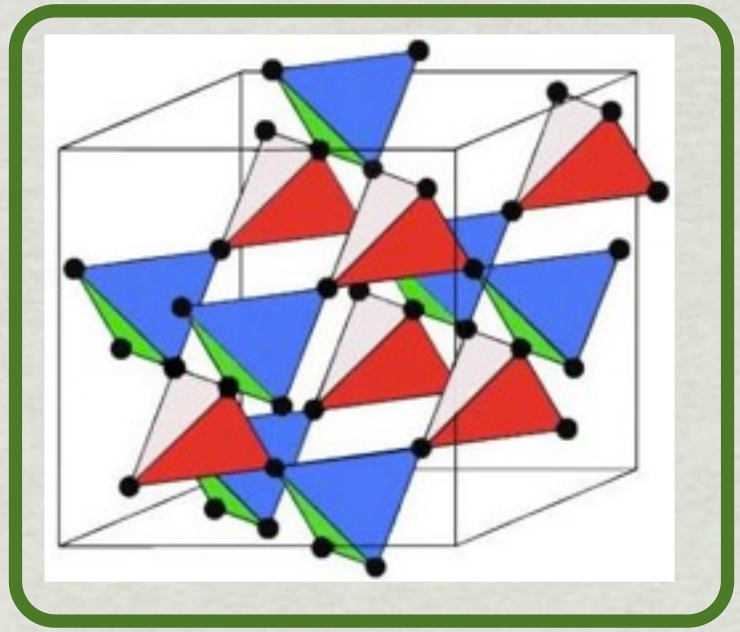
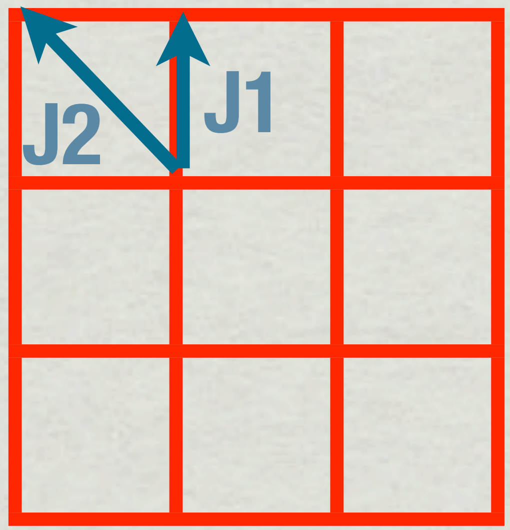
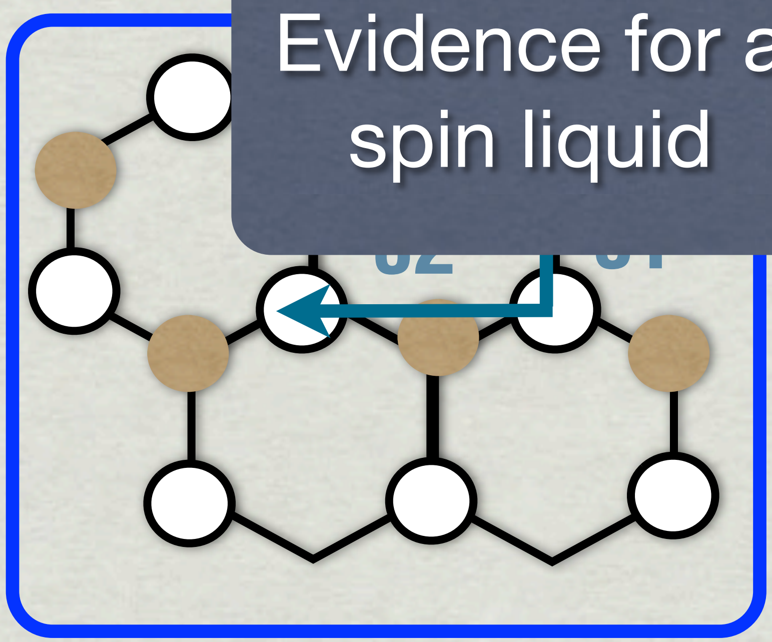
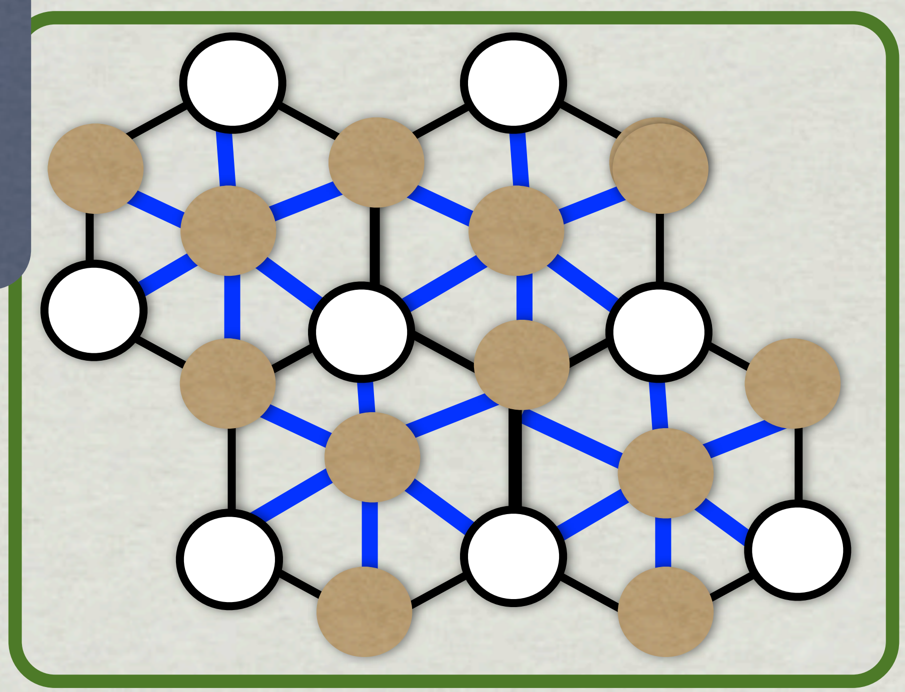


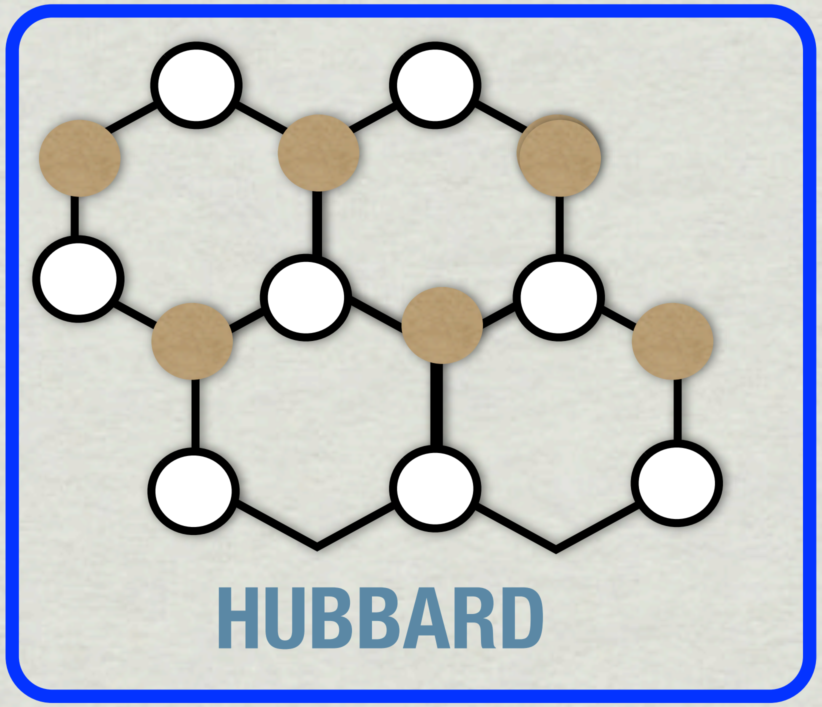






Evidence for a spin liquid





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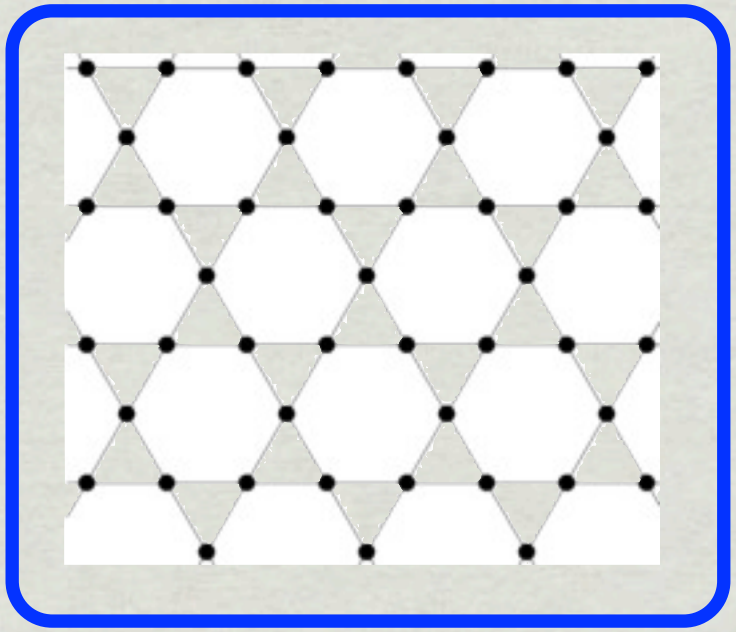

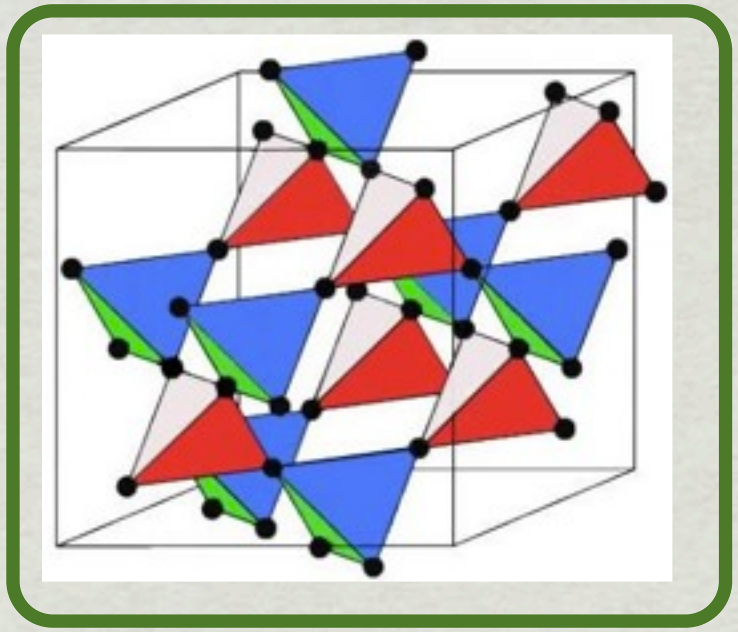

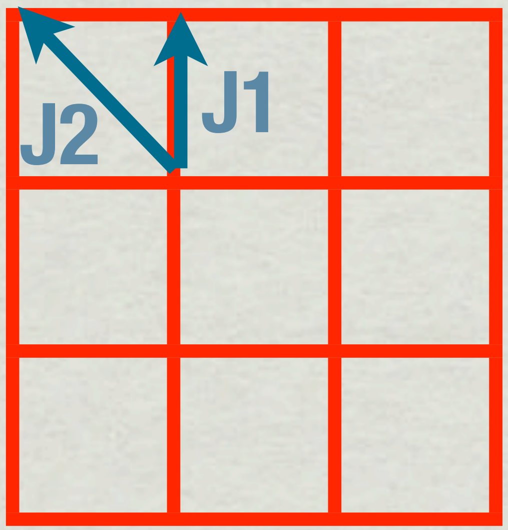

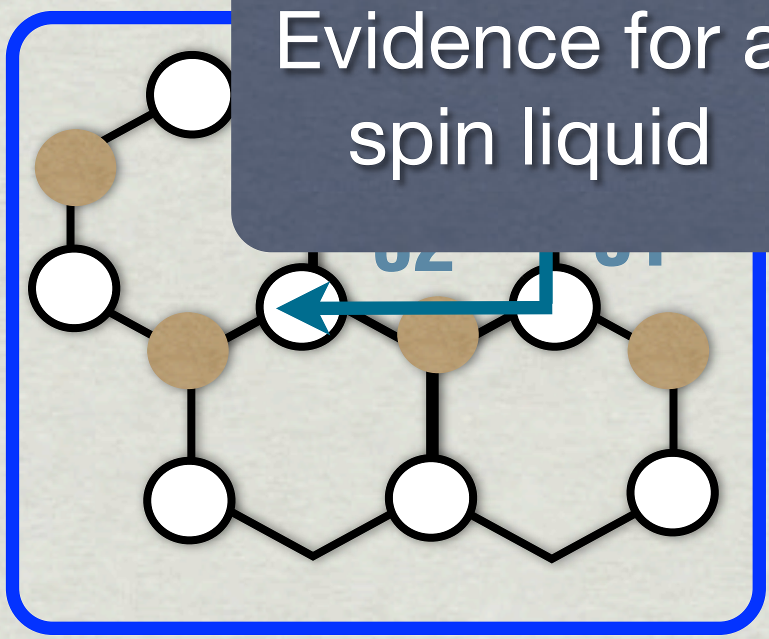

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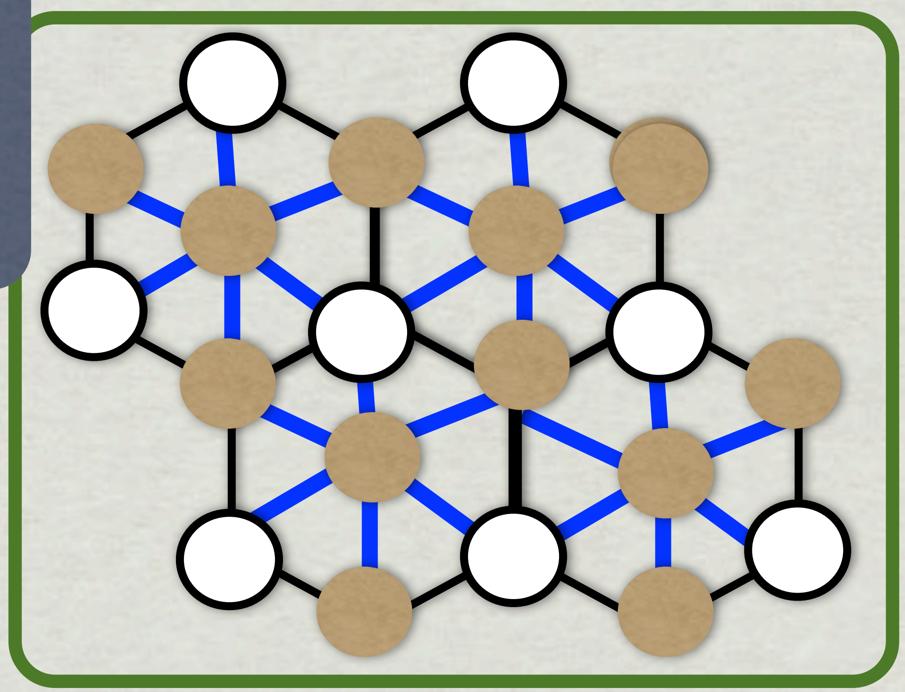

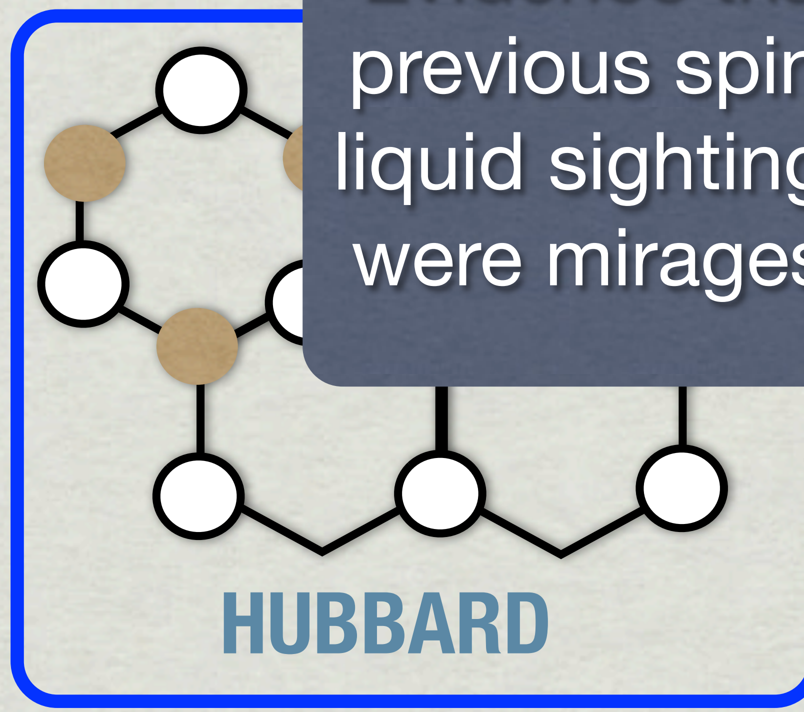

Evidence that previous spin-liquid sightings were mirages.

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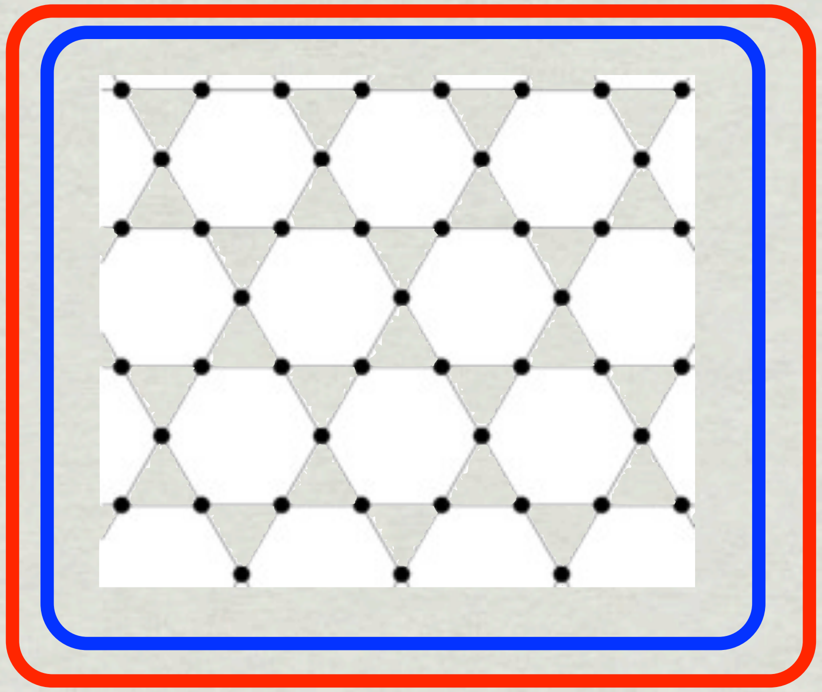

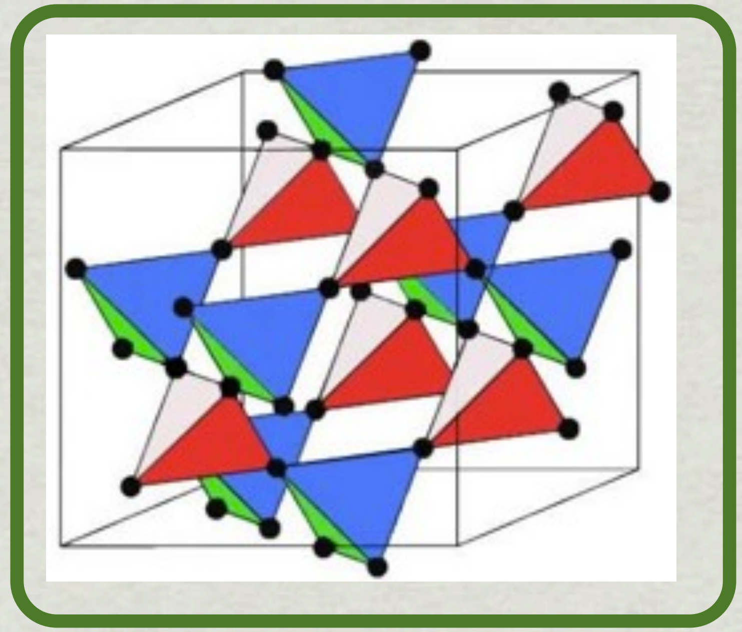

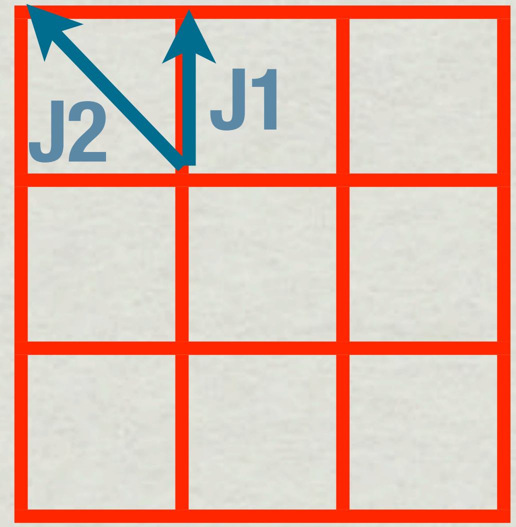

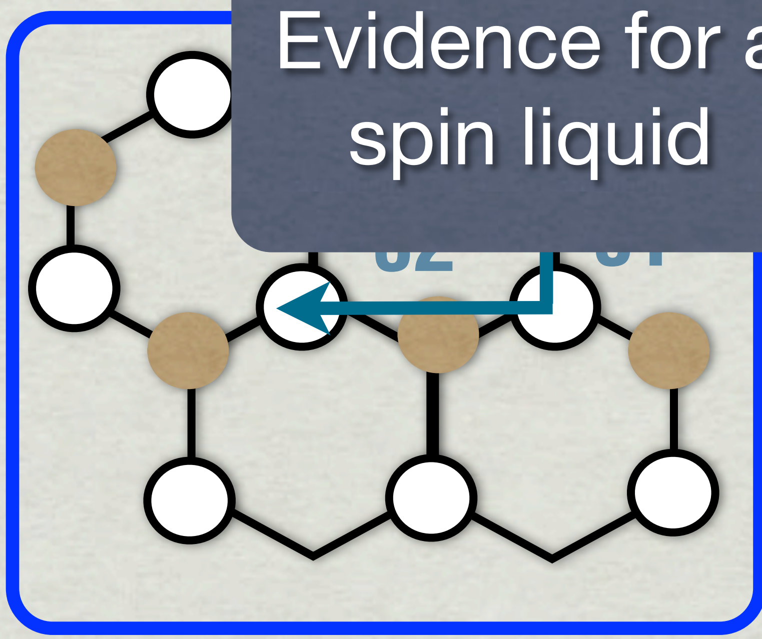

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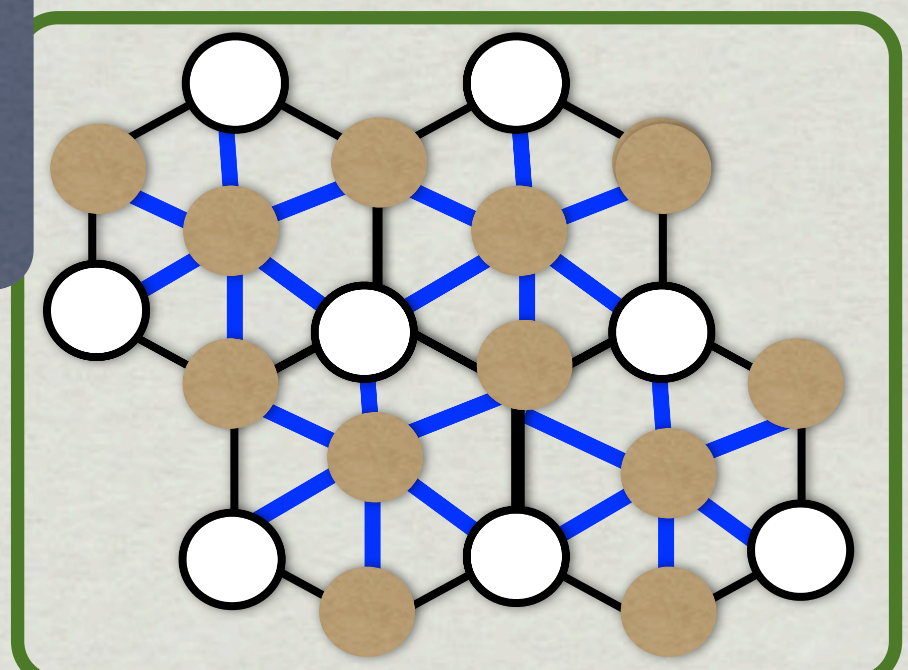
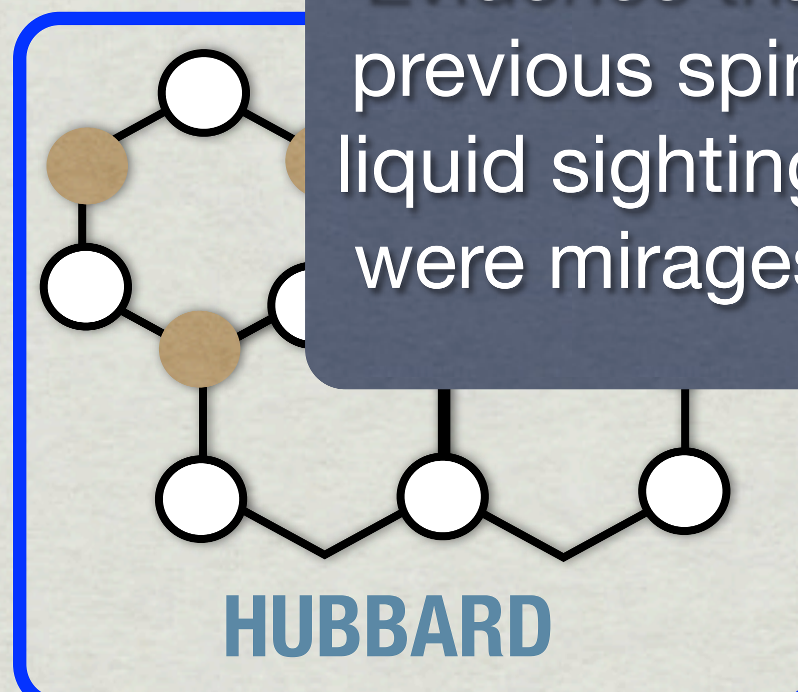
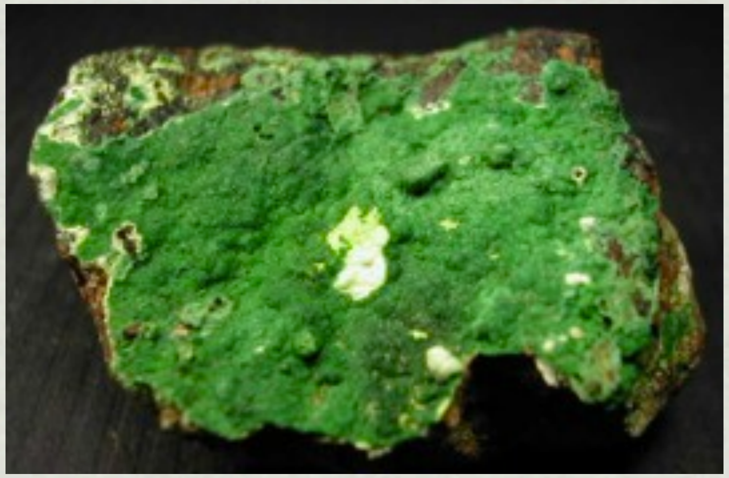




Evidence that previous spin-liquid sightings were mirages.

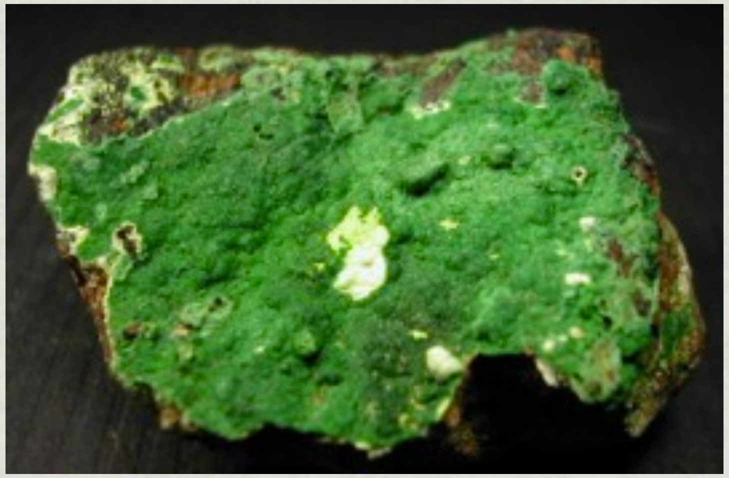
- Herbertsmithite



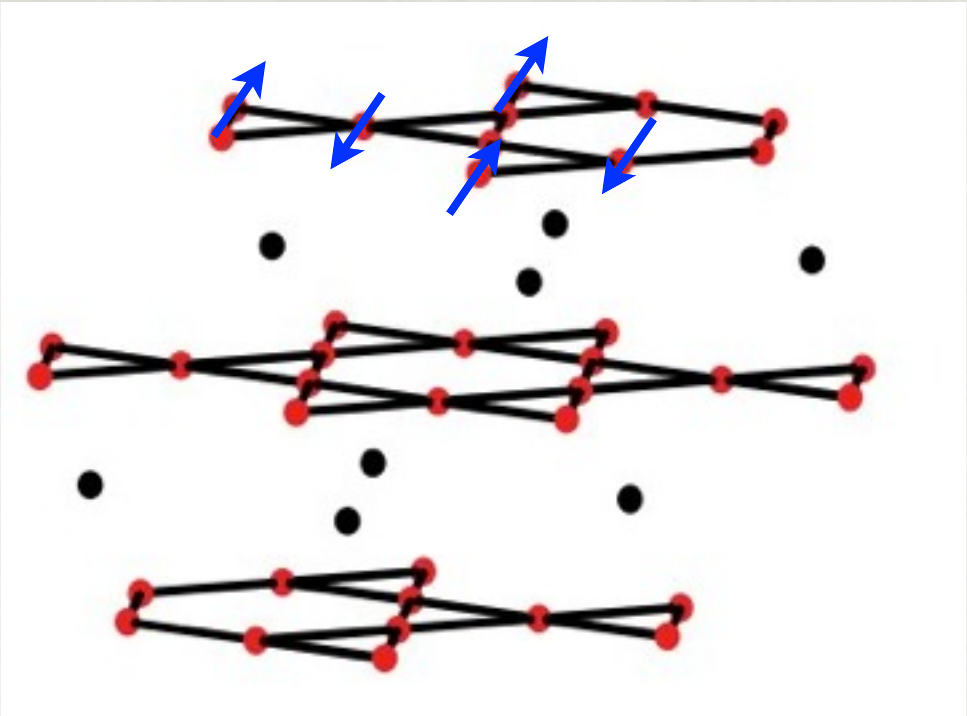
- Zn-Paratacamite (Zn < 1/3)

- Volborthite

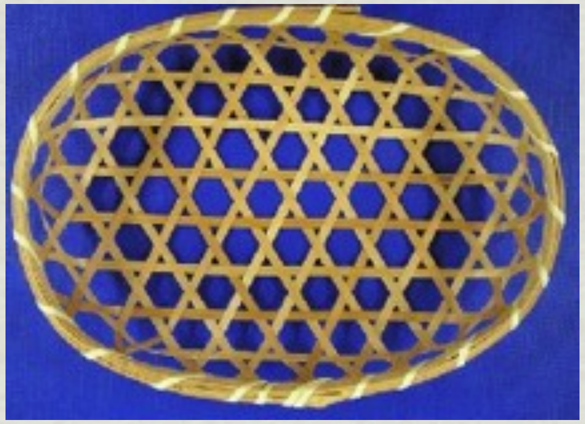
* Herbertsmithite

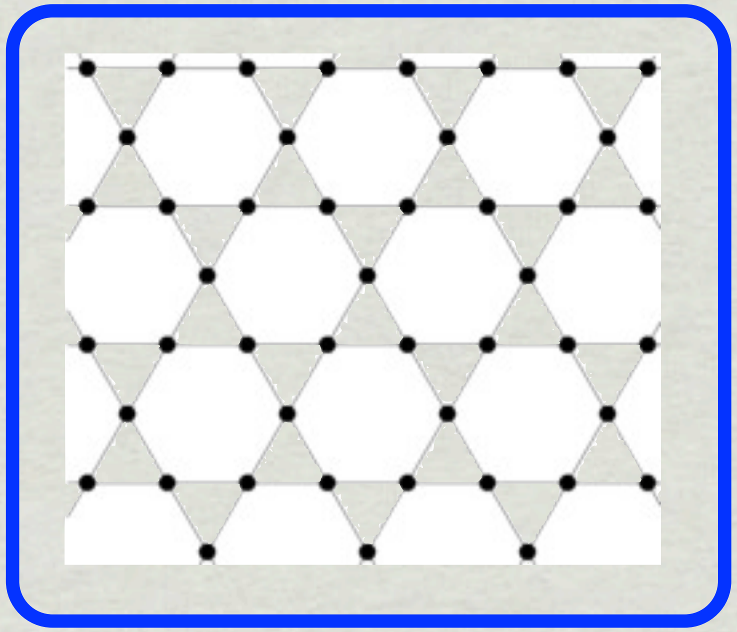


* Zn-Paratacamite (Zn < 1/3)

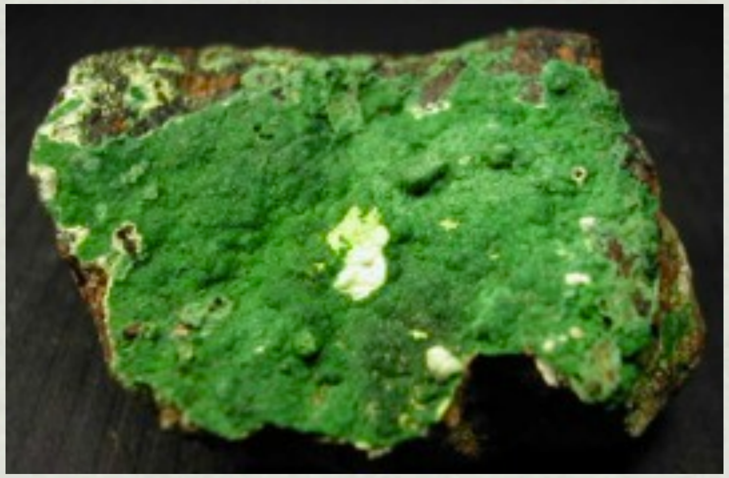


* Volborthite





- Herbertsmithite



$$H = J_1 \sum_{\langle i,j \rangle} \vec{s}_i \cdot \vec{s}_j$$

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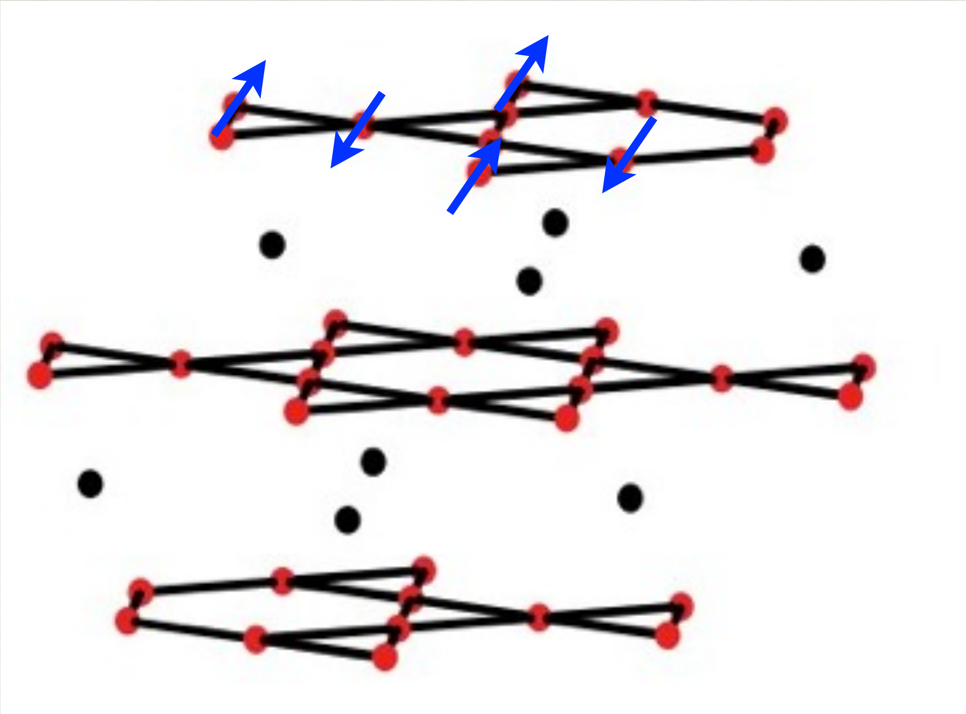
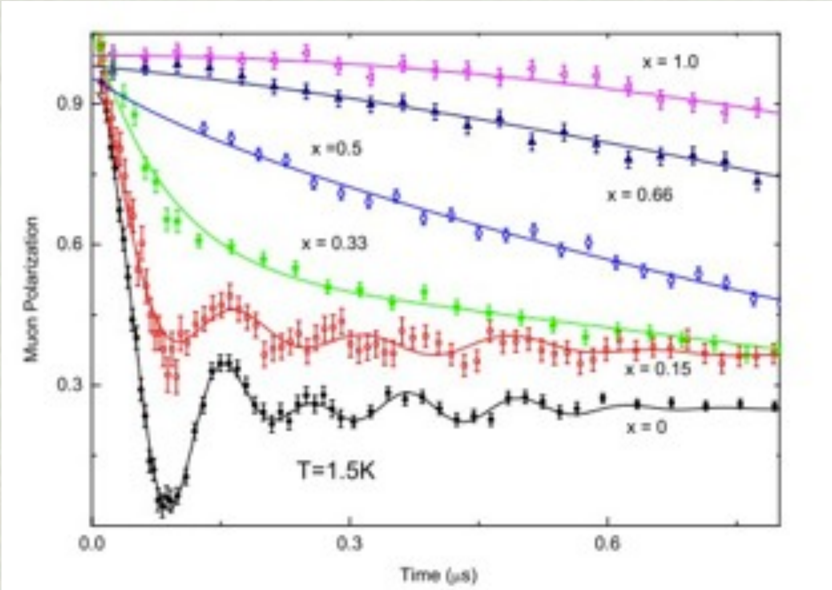
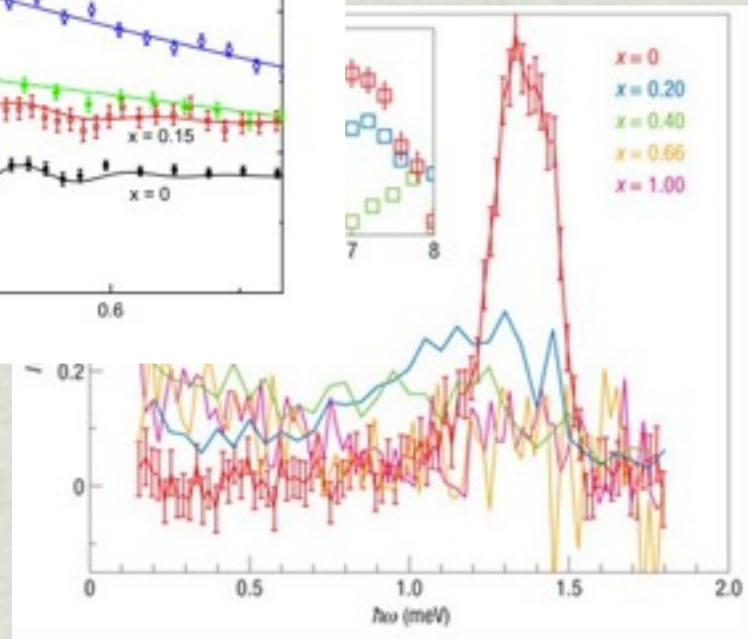


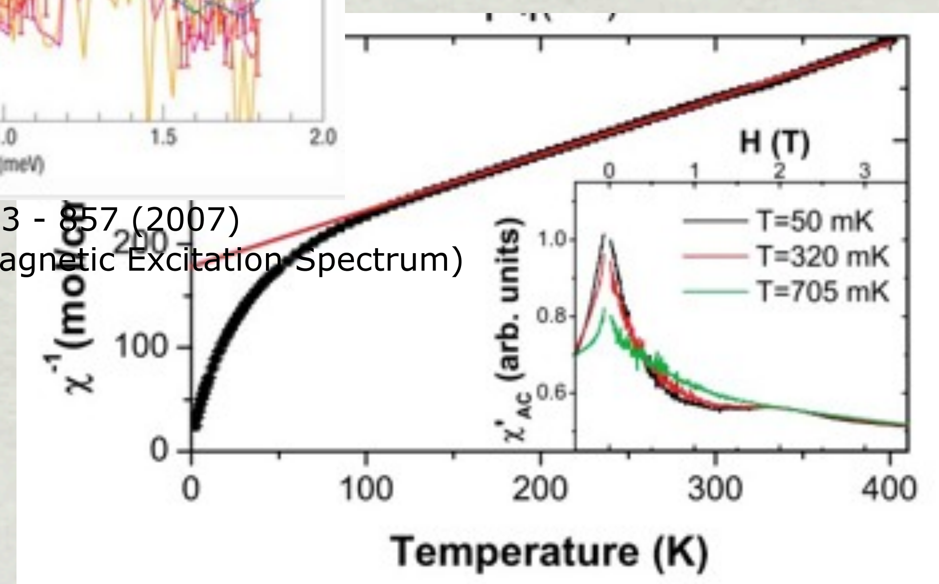
- Volborthite



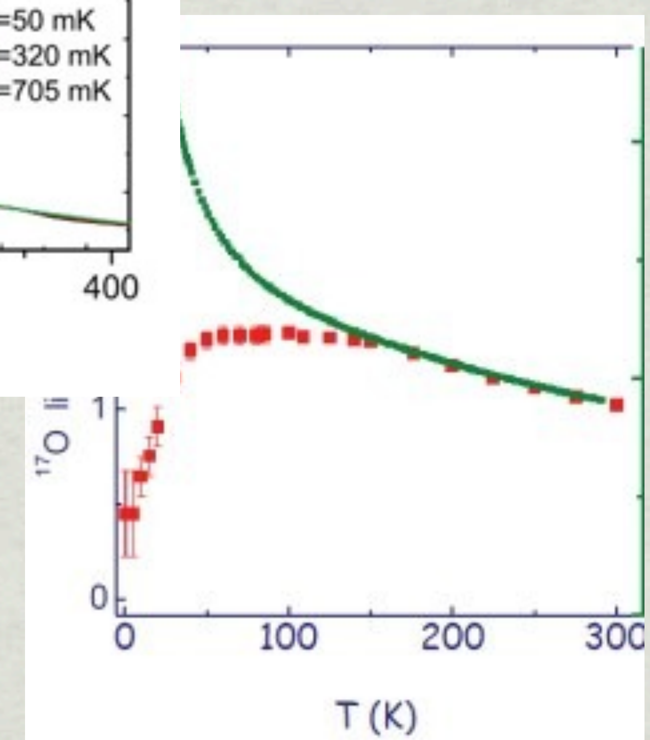
arXiv:1001.0801v1 (mu-sr)



Nature Materials **6**, 853 - 857 (2007)
neutron scattering - Magnetic Excitation Spectrum)



PRL 98, 107204 (magnetic susceptibility)



2011 J. Phys.: Conf. Ser. 320 012004 (nmr)

Experiments suggest no magnetic order

The Variational Approach

Venerable history: BCS Superconductivity

Quantum Hall Effect

Model Wave-functions

Particularly valuable if the wave-function is conceptually simple and connects to analytical theory

---

Question: How do we guess the right wave-function?

HILBERT SPACE IS A BIG PLACE

The Variational Approach

Venerable history: BCS Superconductivity

Quantum Hall Effect

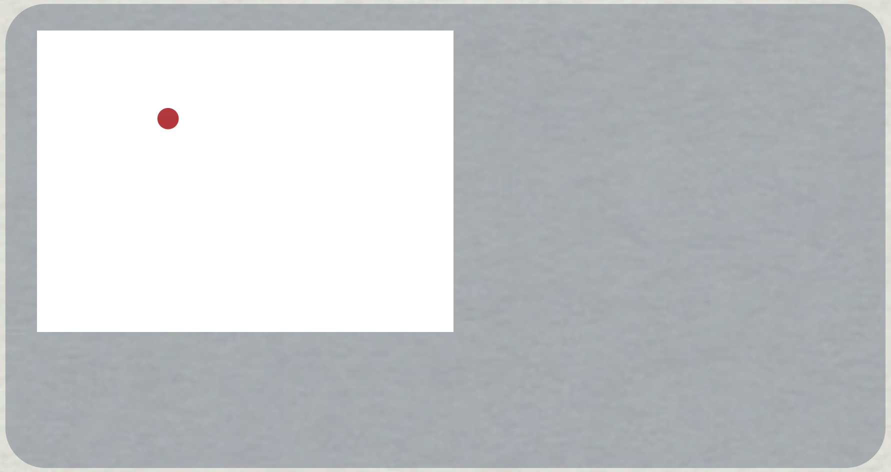
Model Wave-functions

Particularly valuable if the wave-function is conceptually simple and connects to analytical theory

Question: How do we guess the right wave-function?

Carve out a large chunk of Hilbert space.

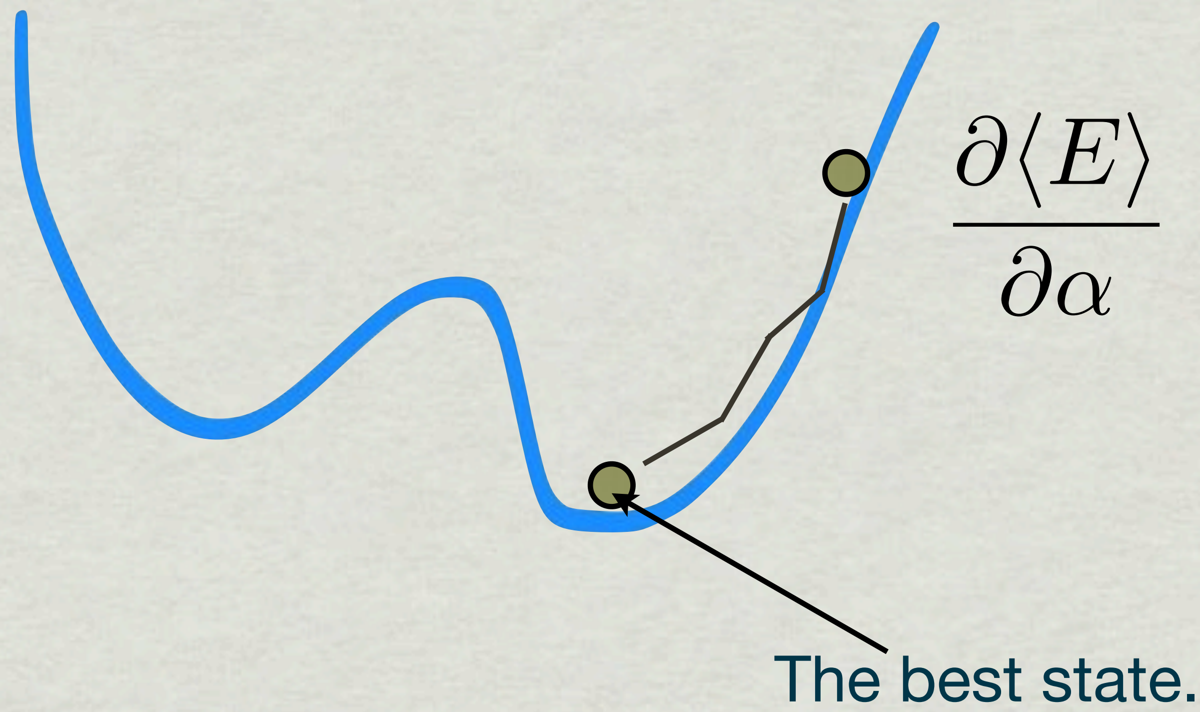
Let the computer find the right wave-function.



HILBERT SPACE IS A BIG PLACE

Variational Monte Carlo

Variational Principle: $E_0 = \langle \Psi_0 | H | \Psi_0 \rangle \leq \langle \Psi_T | H | \Psi_T \rangle$



- Choose set of $\Psi[\vec{\alpha}]$
- Find the best one in set

Highly *nonlinear* optimization with an objective function $\langle E[\Psi[\vec{\alpha}]] \rangle$ and derivatives $\partial \langle E \rangle / \partial \alpha_i$ which can only be evaluated *noisily* and *slowly*.

A short (theoretical) history

1973: RVB proposed for triangular lattice *Anderson*

1987-1990: Quantum Dimer Models *Rokhsar and Kivelson*

Gauge Theories *Fradkin; Kotliar*

Projected Gutzweiller *Anderson; Gros*

Slave Particles *Marston; Affleck; Lee*

2000-2005: Triangular QDM *Sondhi; Moessner*

Large N *Hermele*

Projective Symmetry Group *Wen*

Toric Code *Kitaev*

2012 - : Numerical Evidence

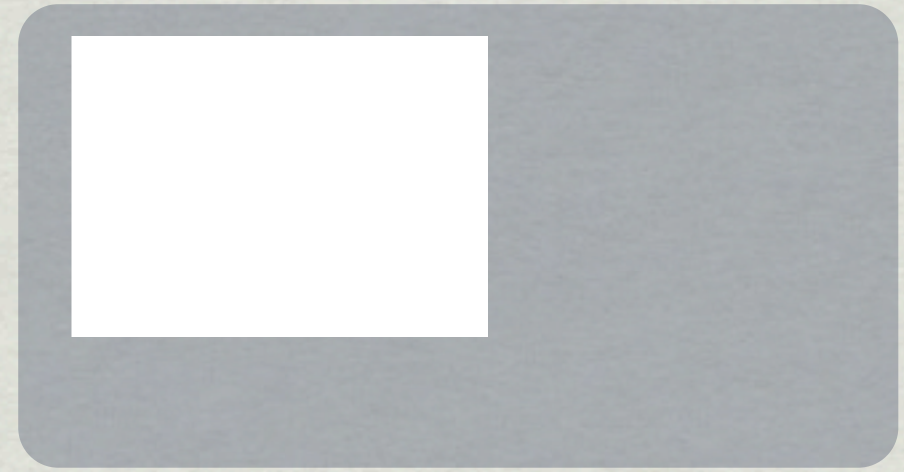
Three Goals

* Theory: Predominately in terms of RVB. Push this approach as hard as one can and see how far we can get.

* Find physically simple and energetically promising wave-functions in a largely unbiased way.

* Connect to experiment.

What chunk of Hilbert space do we pick?



HILBERT SPACE IS A BIG PLACE

Anderson RVB

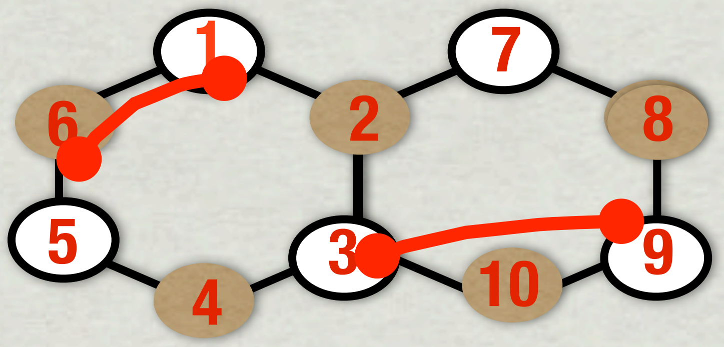
Projected Gutzwiller

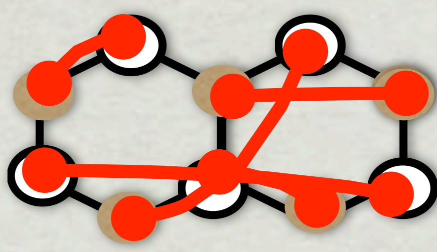
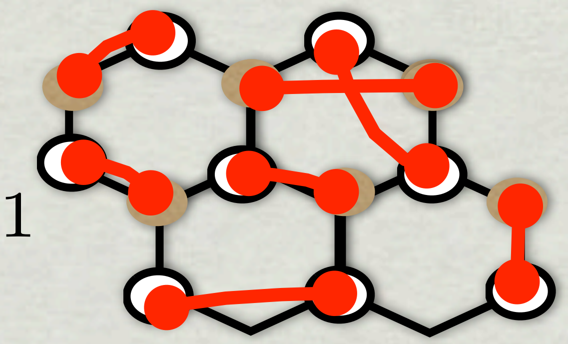
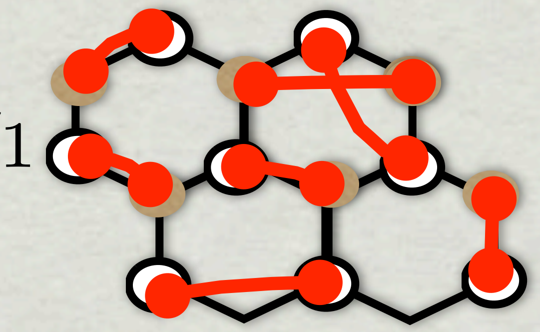
Slave Particles

Anderson RVB

$$|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$$

Each singlet gets a value.



$\Psi = \alpha_1$  $+\beta_1$  $+\gamma_1$  $+ \ldots$

$$\phi(6,1)\phi(2,8)\phi(5,9)\phi(4,7)\phi(3,10)$$

RVB wave functions

$$\Psi = \sum_{dim.covering} \prod_{[ij]} \phi(r_i - r_j)|\uparrow_i\downarrow_j - \uparrow_j\downarrow_i\rangle$$

Technically hard to work with

Projected Gutzwiller

Fermion Hamiltonian:

$$H = \sum_{i,j,\sigma} t_{\sigma ij} c_i^\dagger c_j$$

Solve

$$\Psi_{\text{fermion}}$$

Projection

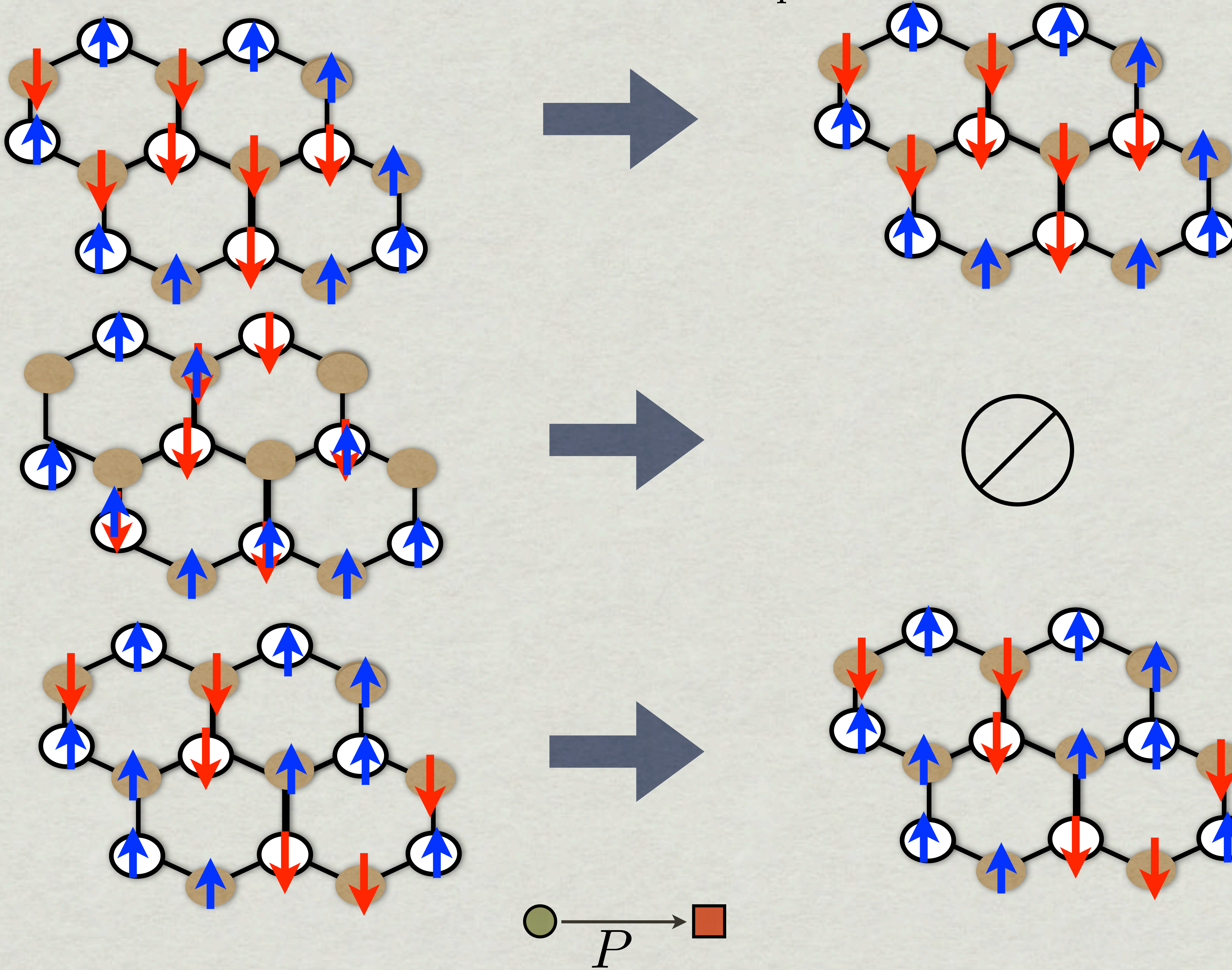
$$\Psi_{\text{spin}}$$

Parameters:
Optimize every hopping

An important trick

ELECTRONS | **SPINS**

$$P\Psi_{\text{electron}} = \Psi_{\text{spin}}$$



Slave Particles

$$H = J_1 \sum_{\langle i,j \rangle} S_i \cdot S_j$$

<u>Another perspective</u>

Slave-Fermion + Mean Field

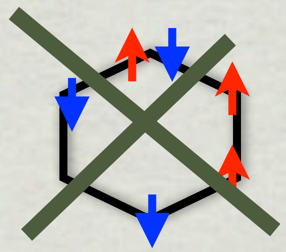
$$S_i = \frac{1}{2} f_{i\alpha} \vec{\sigma}_{\alpha\beta} f_{i\beta} \quad f^\dagger_{i\alpha} f_{i\alpha} = 1 \quad f_{i\alpha} f_{i\beta} \epsilon_{\alpha\beta} = 0$$

$$H_F = -t_{ij} \sum_{\langle i,j \rangle, s} f^\dagger_{is} f_{js} + \sum_{ij} \Delta_{ij} (f^\dagger_{i\uparrow} f^\dagger_{j\downarrow} - f^\dagger_{i\downarrow} f^\dagger_{j\uparrow}) + h.c.$$

Solve mean field Hamiltonian and implement constraint by projection.

$$\Psi_{PBCS} = P \prod_k (u_k + v_k c^\dagger_{k,\uparrow} c^\dagger_{-k,\downarrow}) |0\rangle$$

Project out double and zero occupancy.



$$\langle R | \Psi_{PBCS} \rangle = \det M$$

$$M_{ij} = \phi(\vec{r}_{\uparrow,i} - \vec{r}_{\downarrow,j}) \equiv \phi(\vec{r}_{ij})$$

Slave Particles

$$H = J_1 \sum_{\langle i,j \rangle} S_i \cdot S_j$$

Another perspective

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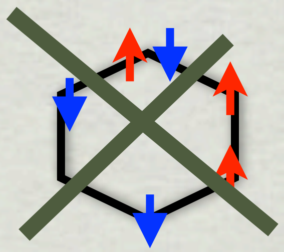

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RVB wave functions

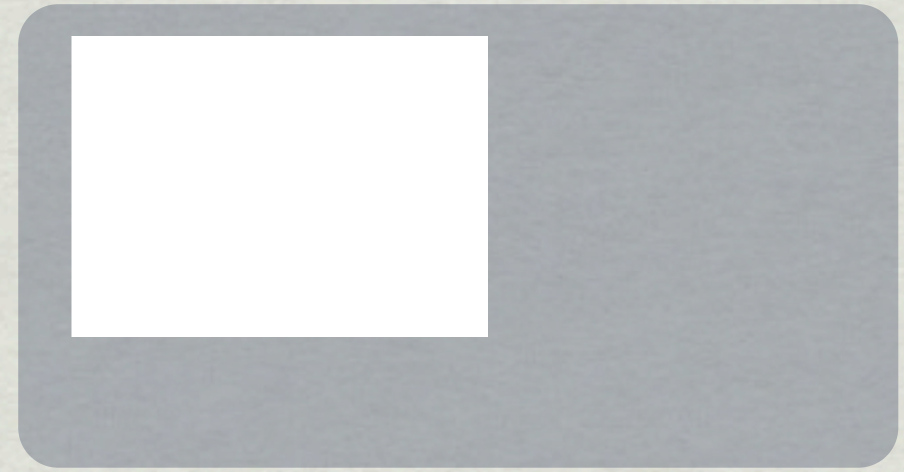
$$\Psi = \sum_{dim.covering} \prod_{[ij]} \phi(r_i - r_j) | \uparrow_i \downarrow_j - \uparrow_j \downarrow_i \rangle$$

These are (almost) the same.

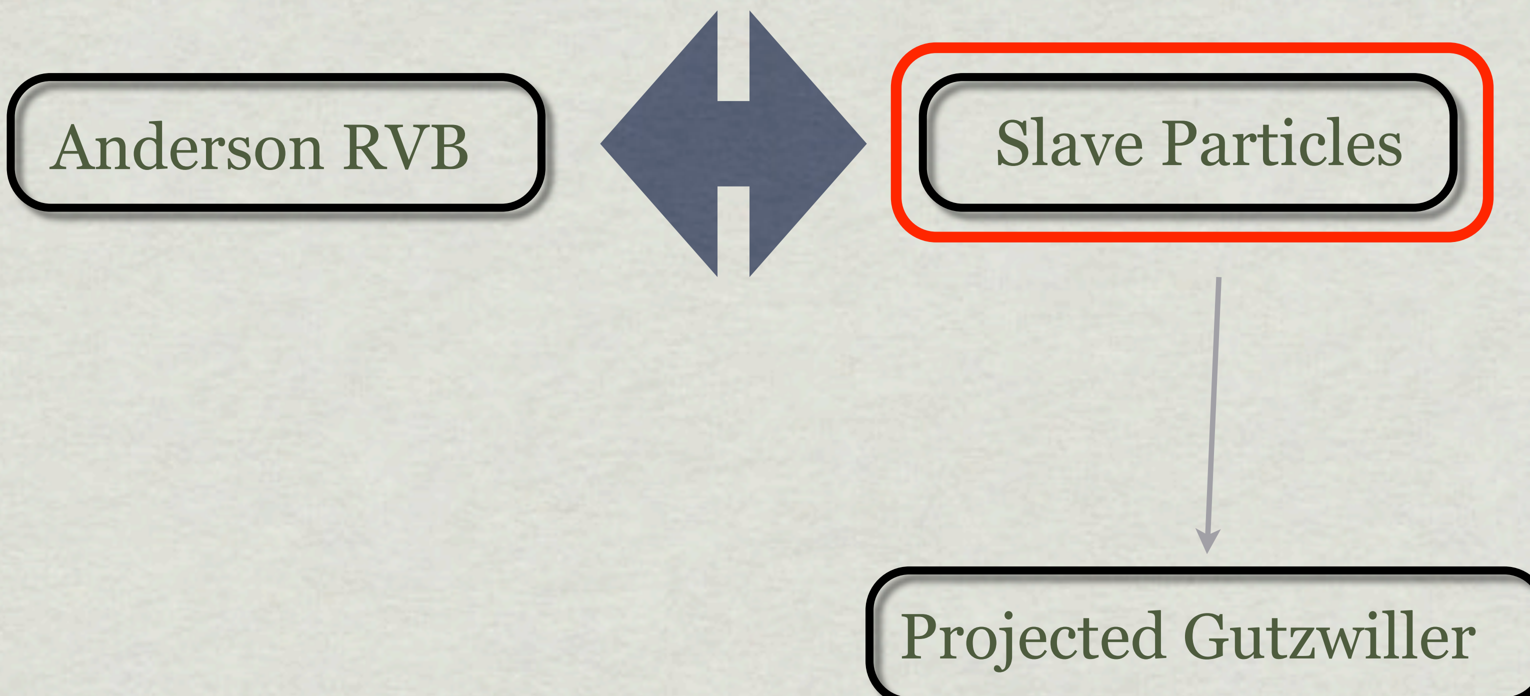
(up to a sign we can often gauge away)

Sunday, March 10, 13

What chunk of Hilbert space do we pick?



HILBERT SPACE IS A BIG PLACE



Goes under the name of Projected BCS

Projected BCS: The de-facto standard

2004 (ICM): Becca, Sorella; *J1-J2 square*

2004 (PRL): Yunoki, Sorella; *Triangle, square*

2006 (PRB): Sorella; *Anisotropic Triangular*

2006: Ran, Hermele, Lee, Wen; *Kagome*

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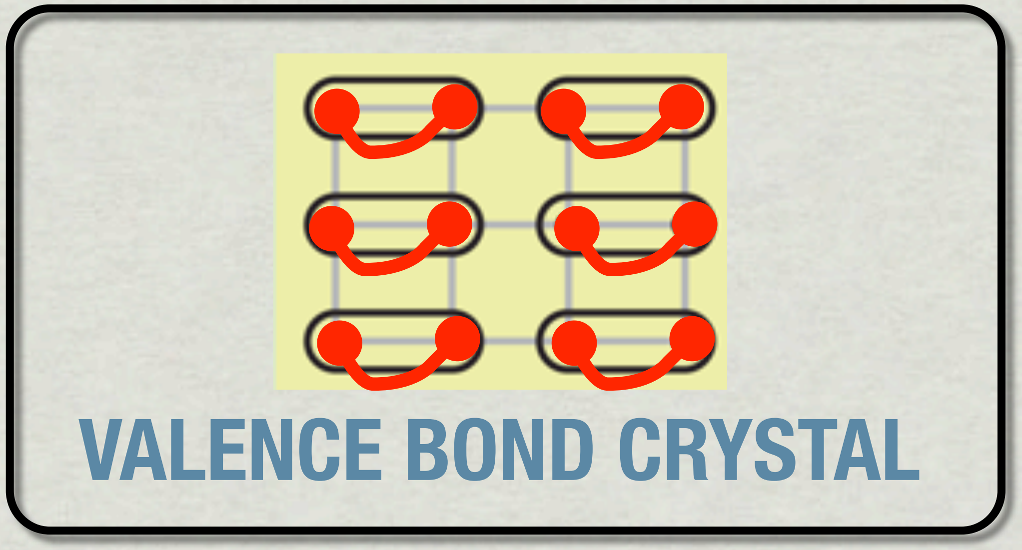
What states can Projected BCS give you?

One possibility: A valence bond crystal

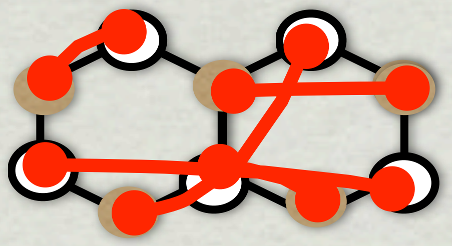
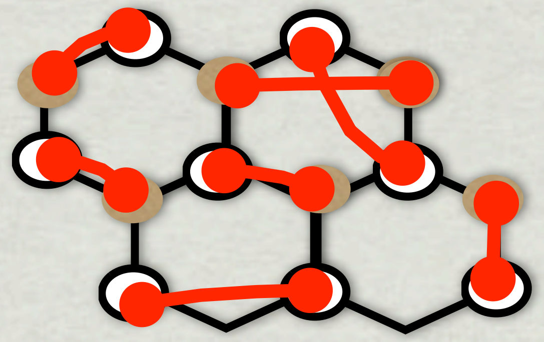
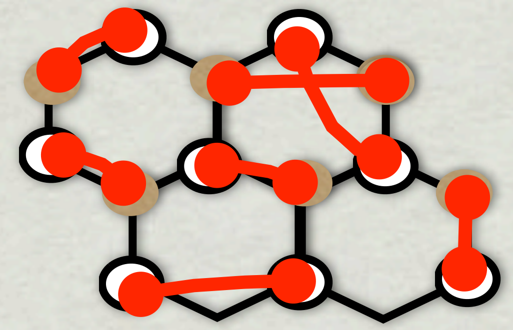


Monogamous pairs

Gapped

What states can Projected BCS give you?

One possibility: A spin liquid

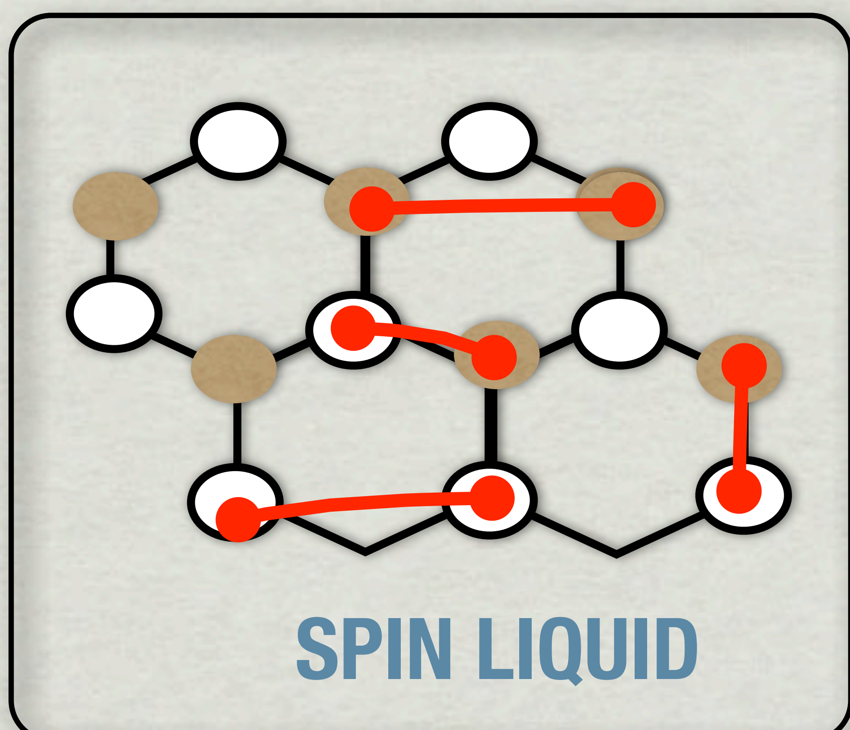
$\Psi =$  $+$  $+$ 

We can see that it is ....

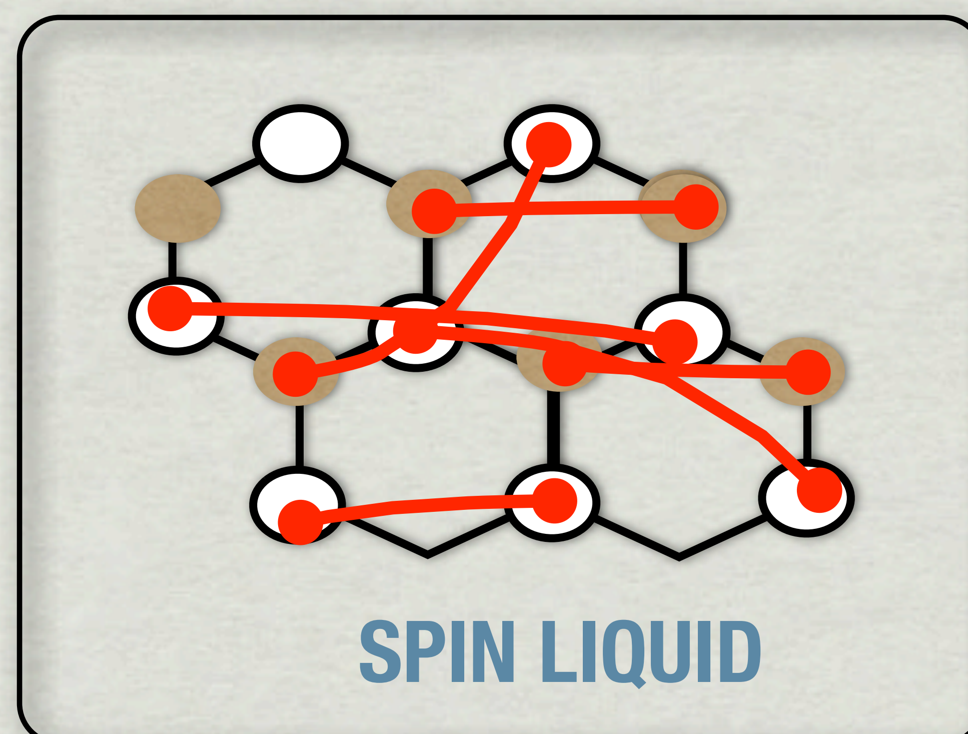
featureless

fractionalized excitations

long range entangled



Gapped

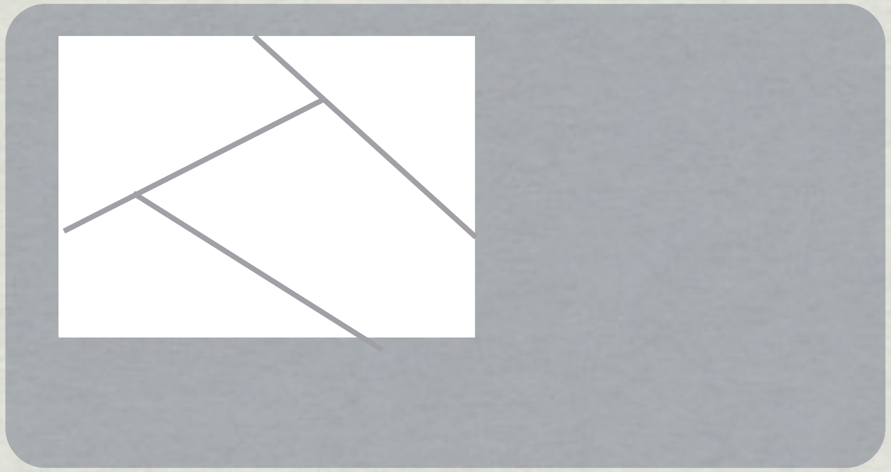


Gapless

What states can Projected BCS give you?

One possibility: A spin liquid

The projective symmetry group carves up the spin liquids.



The Variational Approach

Venerable history: BCS Superconductivity

Quantum Hall Effect

Model Wave-functions

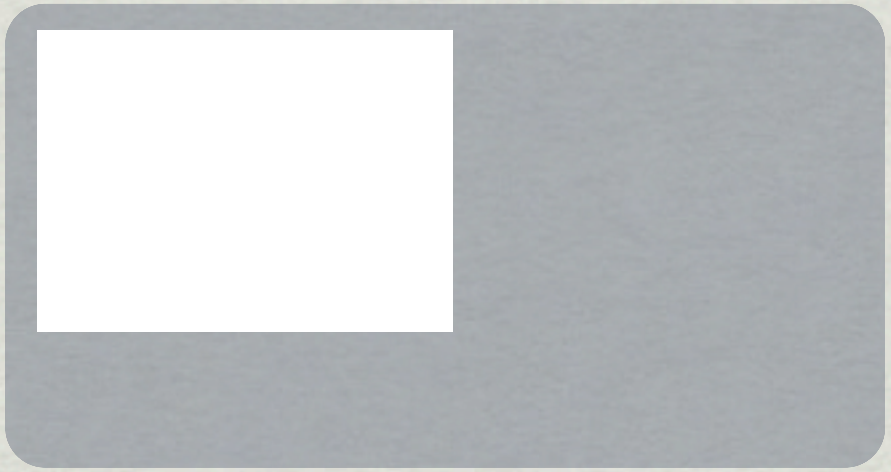
Particularly valuable if the wave-function is conceptually simple and connects to analytical theory

The perennial complaint about variational approach:

Biased - You get out what you put in.

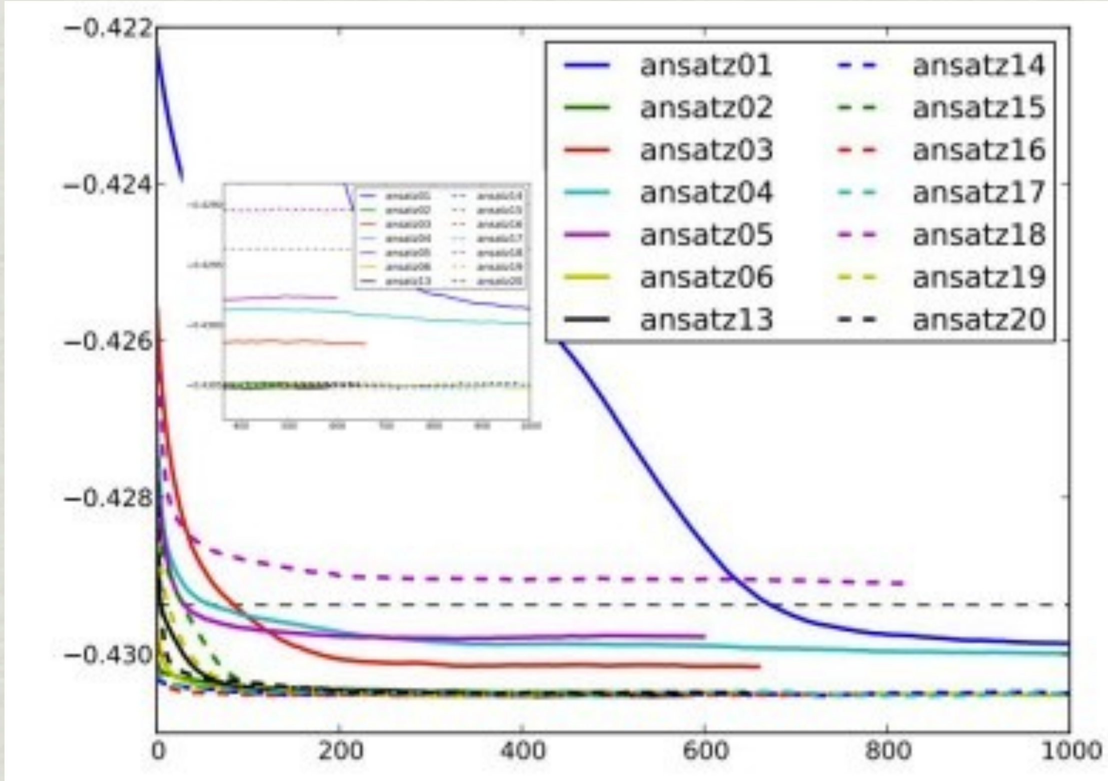
Often true ... We will minimize that bias by taking a huge number of parameters.
~1000 - 10,000 parameters

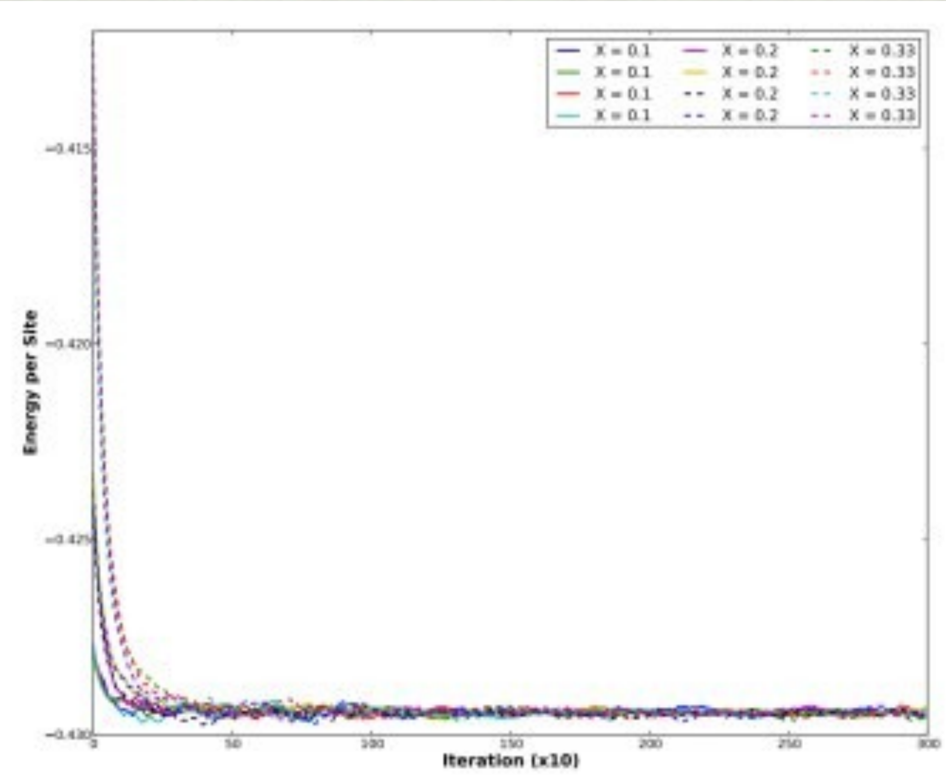
We take the idea of Projected BCS seriously and span the *entire* space of projected BCS. This is the first time this has been done in frustrated magnetism (lattice models at all).



HILBERT SPACE IS A BIG PLACE

OPTIMIZATION





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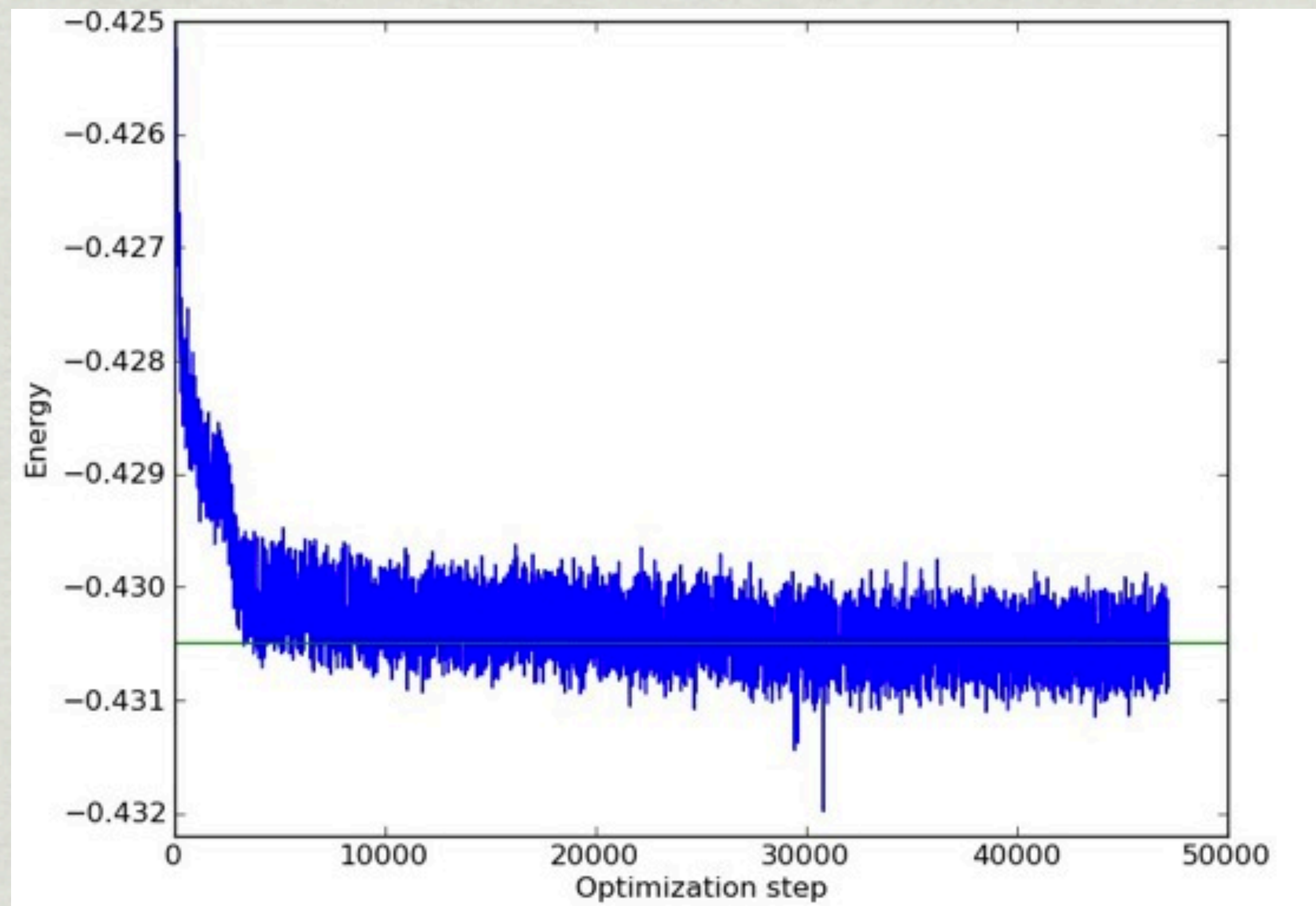
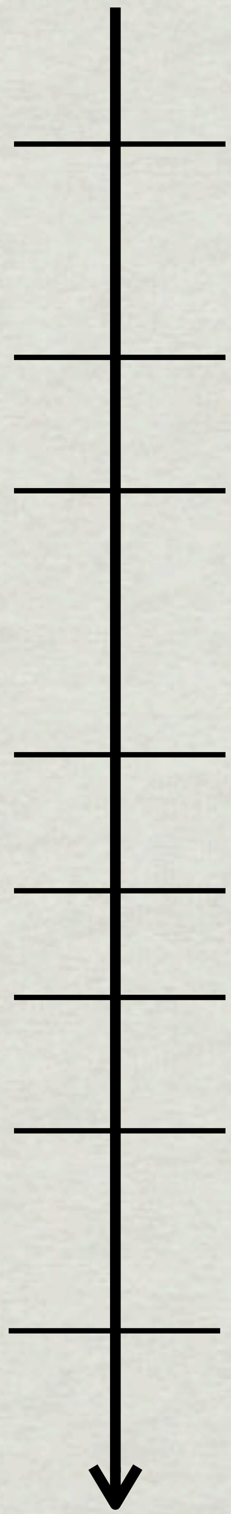
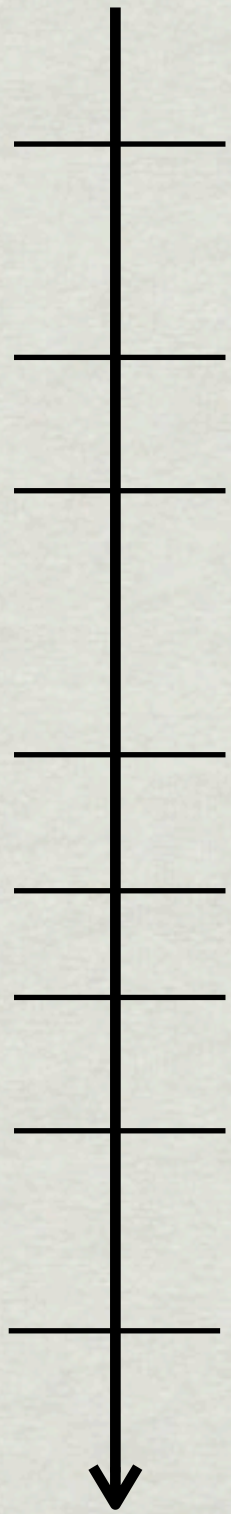


Energies



-0.429 Dirac Spin Liquid (Ran, Hermele , Lee, Wen; Poiblanc, et al)

Energies



-0.409 Nearest neighbor Anderson RVB (BKC)

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Energies

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-0.4305 VMC on PBCS (BKC, Kinder, Neuscamann, Chan, Lawler)

-0.433 DMC on PBCS (BKC, Kinder, Neuscamann, Chan, Lawler)

Another nearby spin liquid?

Metric for spin liquid-ness:

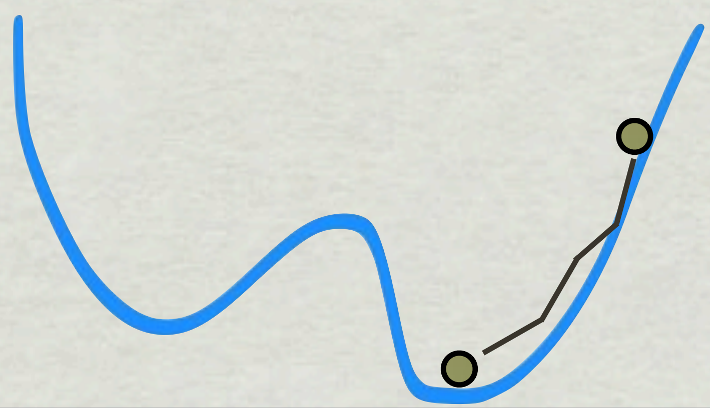
Assymetry in pre-projected $\vec{s_i} \cdot \vec{s_j}$

Search for a low-energy spin liquid:

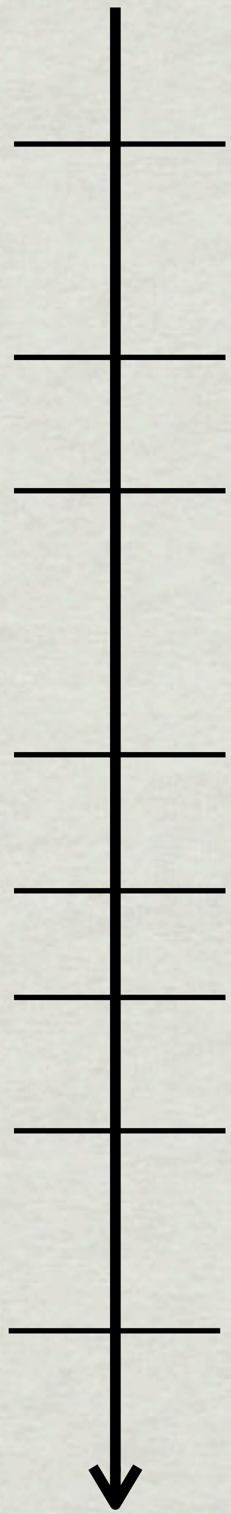
- Start with the striped spin-liquid crystal
- Take a random step in Hamiltonian space.
- Accept this step if you become more "featureless."

Walks uphill in energy to the Dirac spin liquid!

Dirac spin liquid is closest state.



Energies



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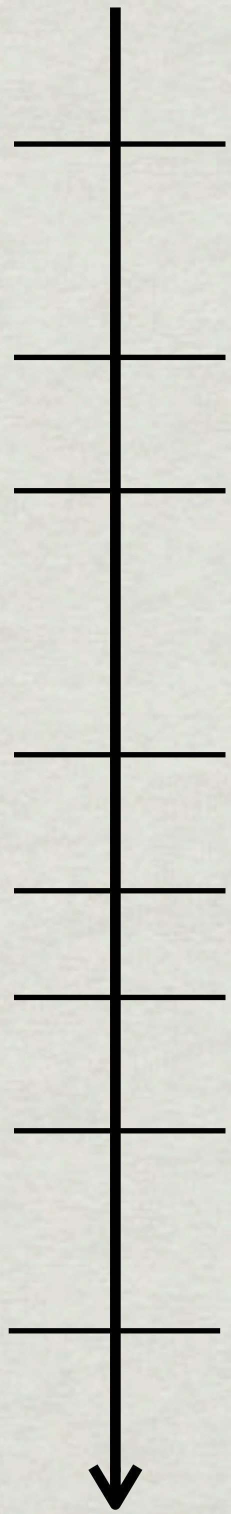

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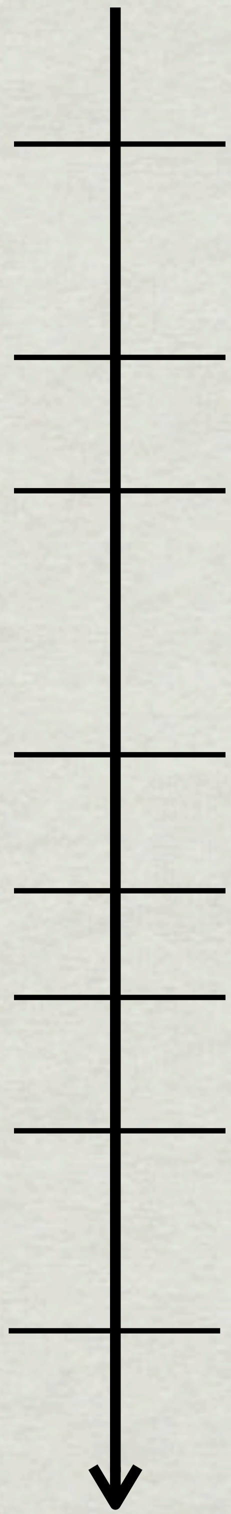

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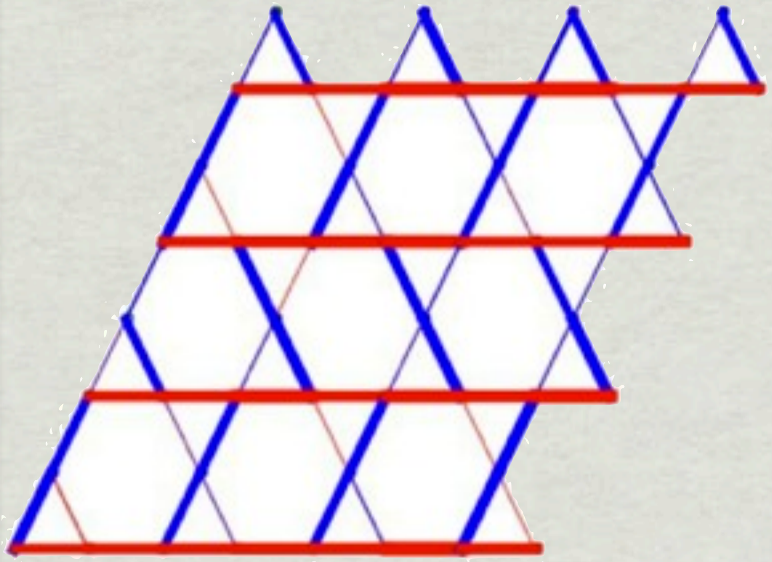
Something new!

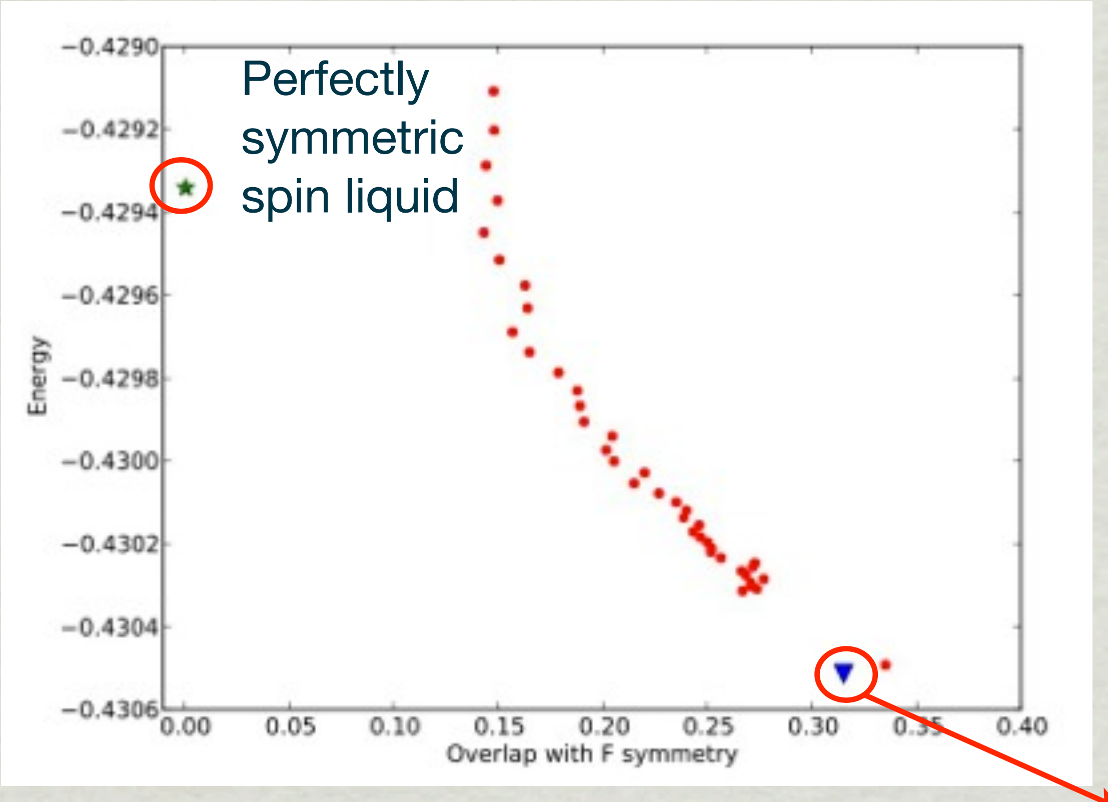


The typical viewpoint (for spin liquids): Featureless

Our new state: Doubles unit cell. Makes stripes.
Not a spin liquid.

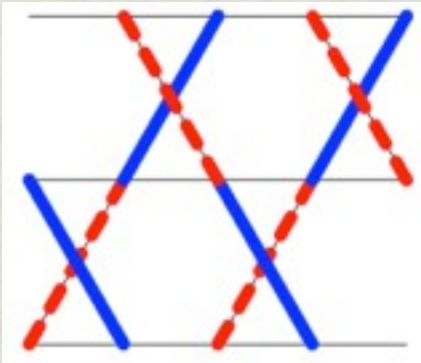
But: Almost as symmetric as a spin liquid
Energy variance: 10^{-3}
Not a valence bond solid!

Breaks F symmetry



"F Assymetry"

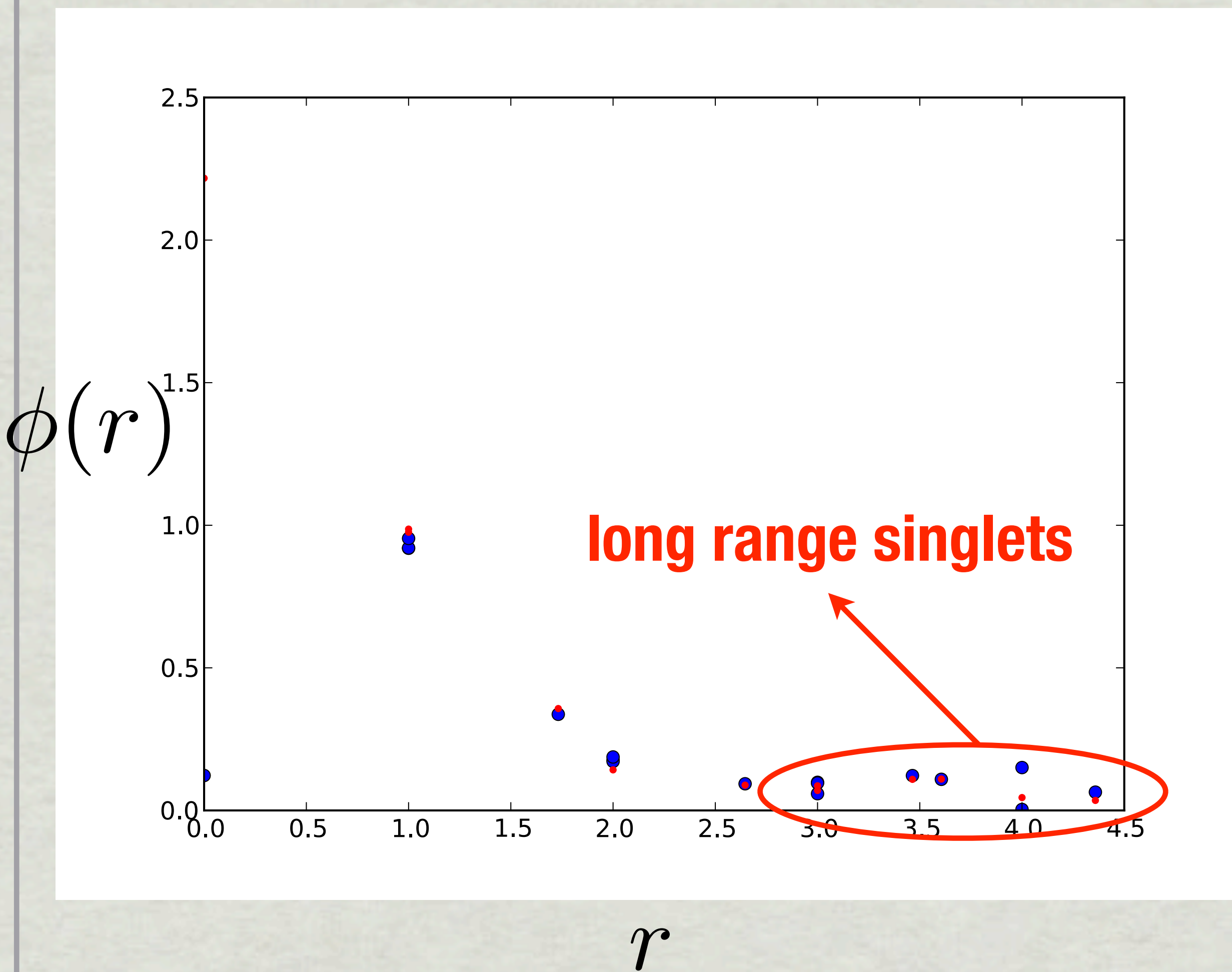
Sufficiently unbiased that we've found a totally new phase out of a variational study.



Broken symmetry

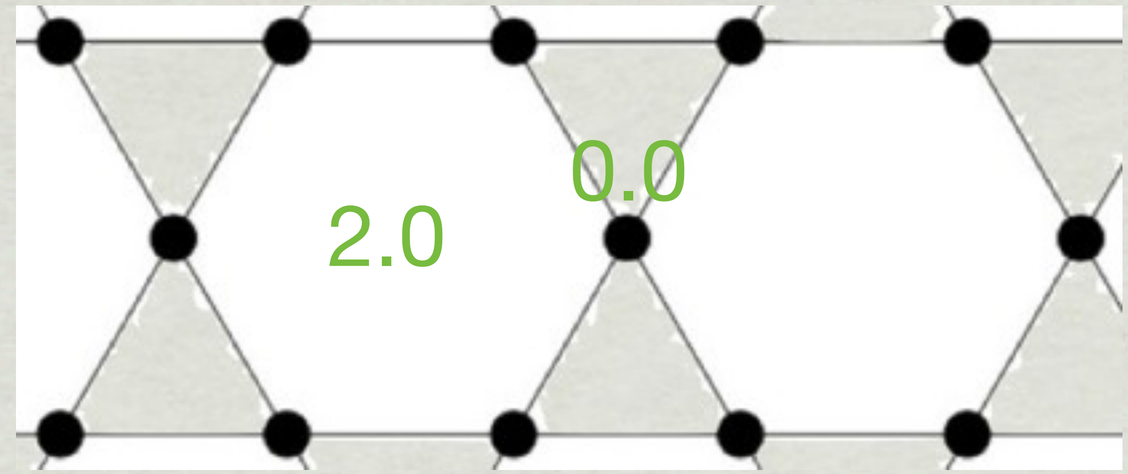
What am I?

Gapped or Gapless?



Gapless

Long Range Entangled?



Climbs uphill to the dirac state.

Almost uniform

Long range entangled

Long Range Entangled

Like a spin liquid, but symmetry broken.

There has been a huge amount of work understanding and classifying “spin-liquid” phases recently and broken symmetry phases previously. We now have a concrete example of something simultaneously both. Many open theoretical questions!

Projected BCS: The de-facto standard

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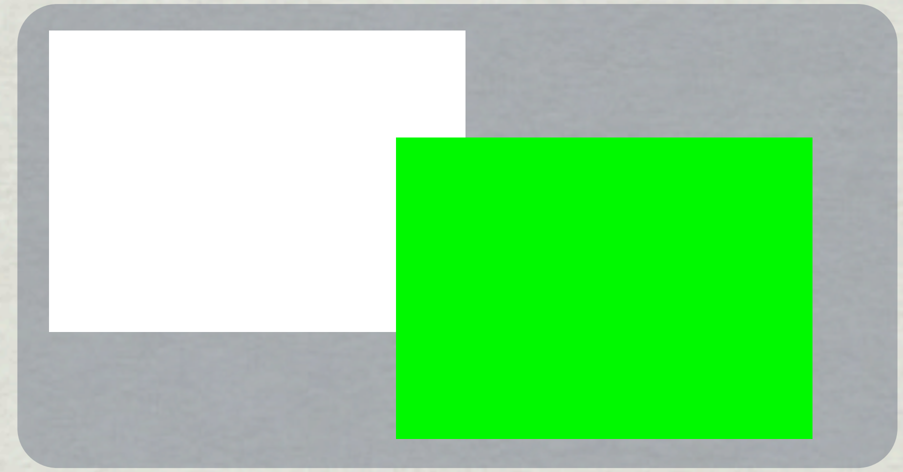
2012 (Nature): Jiang, Block, Mishmash, ..., Motrunich, Fisher; *Ring Exchange*

Projected BCS: The de-facto standard



HILBERT SPACE IS A BIG PLACE

2004 (ICM): Becca, Sorella; *J1-J2 square*

2004 (PRL): Yunoki, Sorella; *Triangle, square*

2006 (PRB): Sorella; *Anisotropic Triangular*

2006: Ran, Hermele, Lee, Wen; *Kagome*

2009 (PRB): Gros, Becca; *Anisotropic Triangular*

2009 (PRB): Iqbal, Becca, Poilblanc; *Kagome*

2010 (Nature): Yan, White, Huse; *Kagome*

2010: Iqbal, Becca, Poilblanc; *Kagome*

2010 (PRB): Grover, Trivedi, Senthil, Lee; *Triangular + Ring Exchange*

2011: Iqbal, Becca, Poilblanc; *Kagome*

2011: Tay, Motrunich; *Kagome* (Schwinger-Boson)

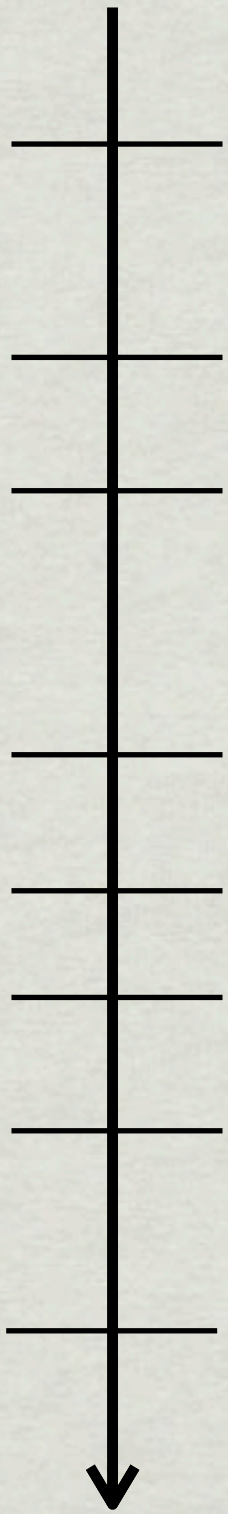
2012: Iqbal, Becca, Poilblanc; *Kagome*

2012 (Nature): Jiang, Block, Mishmash, ..., Motrunich, Fisher; *Ring Exchange*

2013: Evenbly and Vidal; *Kagome* (MERA)

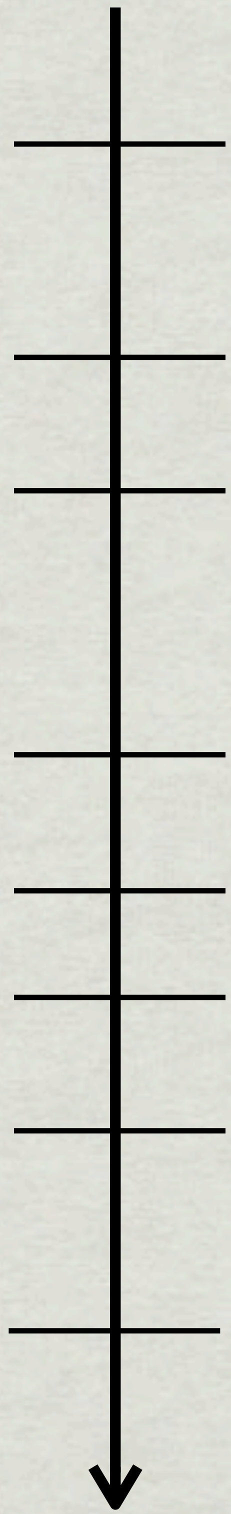
2013: Poiblanc and Schuch; *Kagome* (PEPS)

Energies



-0.429 Dirac Spin Liquid (Ran, Hermele , Lee, Wen; Poiblanc, et al)

Energies



-0.409 Nearest neighbor Anderson RVB (BKC)

-0.429 Dirac Spin Liquid (Ran, Hermele , Lee, Wen; Poiblanc, et al)

Energies

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-0.4305 VMC on PBCS (BKC, Kinder, Neuscamann, Chan, Lawler)

-0.433 DMC on PBCS (BKC, Kinder, Neuscamann, Chan, Lawler)

Energies

- **-0.409** Nearest neighbor Anderson RVB (BKC)
- **-0.418** PEPS (Poiblanc and Schuch)
- **-0.42** Schwinger Boson (Tay and Motrunich)
- **-0.429** Dirac Spin Liquid (Ran, Hermele , Lee, Wen; Poiblanc, et al)
- **-0.4305** VMC on PBCS (BKC, Kinder, Neuscamann, Chan, Lawler)
- **-0.432** MERA gives Valence Bond Solid (Vidal)
- **-0.433** DMC on PBCS (BKC, Kinder, Neuscamann, Chan, Lawler)
- **-0.438** DMRG (White and Huse)

Materials

- **Herbertsmithite**

✓ Gapless

✓ No magnetic order

We have proposed a state that is gapless and has no magnetic order in agreement with experiment.

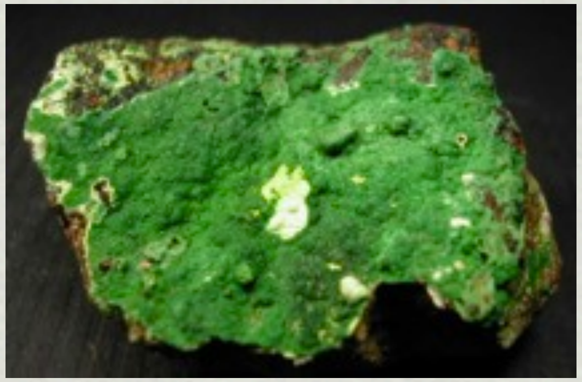
One concern:

Symmetry breaking should couple to lattice and have artifacts in neutron scattering.

Maybe symmetry restored in Herbertsmithite?

- **Volborthite**

- **Zn-Paratacamite (Zn < 1/3)**



Neel state at T=0

Interesting finite temperature transition into distorted kagome lattice *in the F pattern.*

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Tantalizing possibility:

Striped spin liquid crystal → Distorted Kagome

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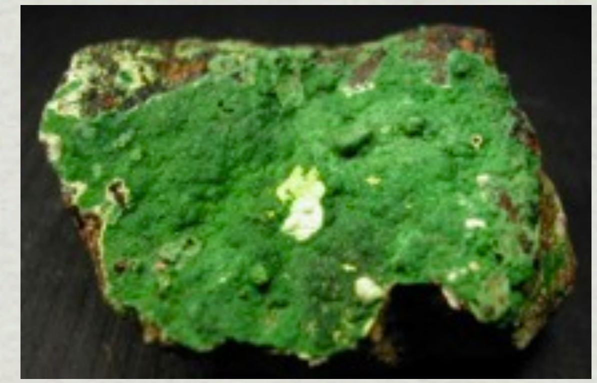

Neel state at T=0

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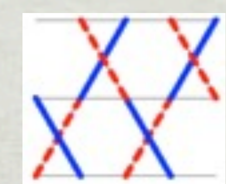


Interesting finite temperature transition into distorted kagome lattice *in the F pattern.*

Tantalizing possibility:

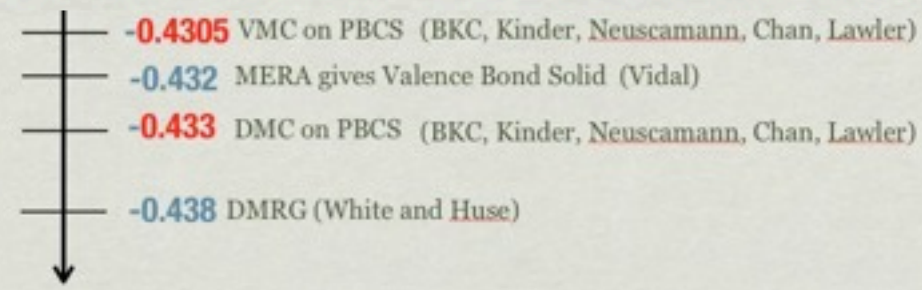
Striped spin liquid crystal ⇄ Distorted Kagome

Even if kagome distorts for other structural reasons, makes good candidate for striped spin liquid crystal.

Conclusions 1

- Theory: Predominately in terms of RVB. Push this approach as hard as one can and see how far we can get.

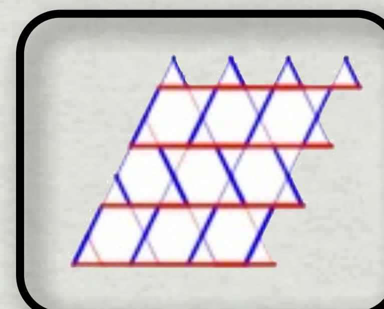
Reasonable low energy state.
Better then tensor product state (MERA,PEPS)
A bit worse (on quasi-1D ladders then DMRG)



...maybe different physics. Not clear how to reconcile?

- Find physically simple and energetically promising wave-functions in a largely unbiased way.

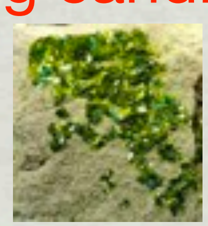
A new phase (in the language of RVB singlets)



- Connection to experiment.

Matches much of the experimental data for Herbertsmithite:

Strong candidate for finite temperature phase of Volborthite; Zn paratacamite.



Nonequilibrium dynamics

Mott Insulating Bosons in a Tilted Lattice

$$H = P\left[-\sum_i \sigma_i^x + \delta(t)\sum_i \frac{1}{2}(\sigma_i^z + 1)\right]P$$

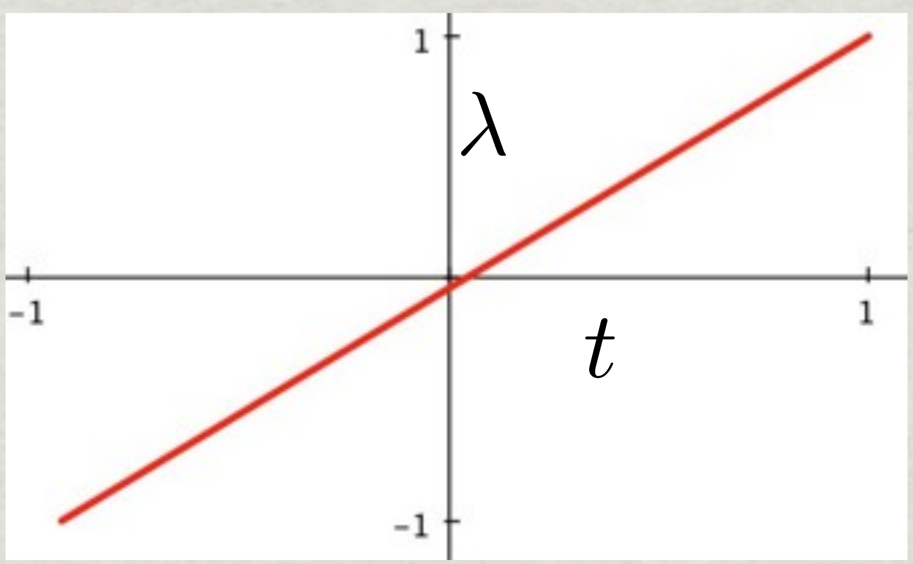
Projects out ↑↑

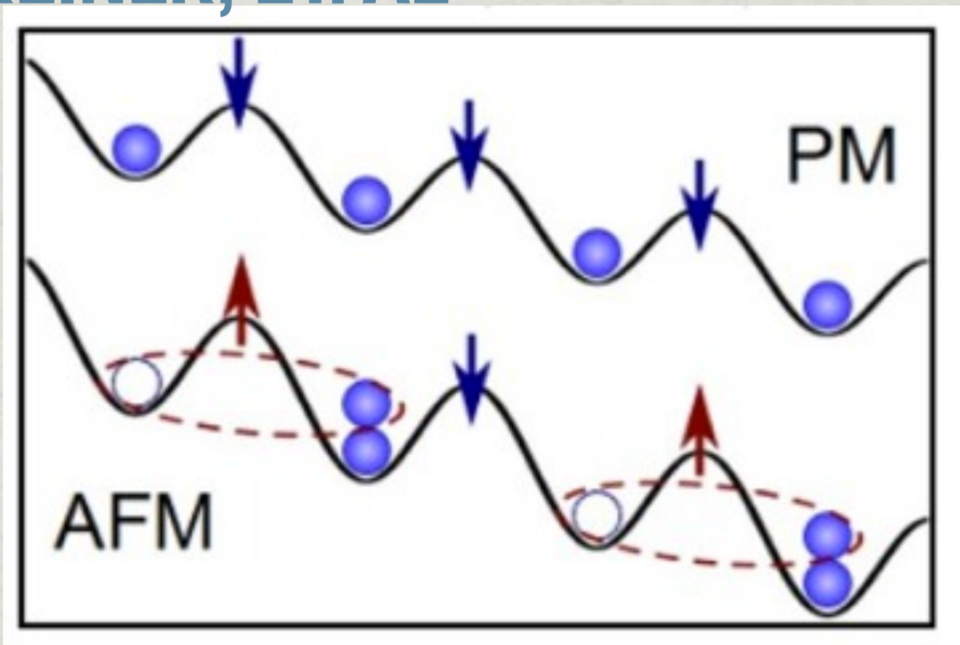
$$H[\lambda] = -\frac{1}{2}\sum_j \left[s_j^z s_{j+1}^z + (1-\lambda)s_j^x\right]$$

← PARAMAGNET 0 FERROMAGNET → λ

GREINER, ET. AL

Quantum critical point as you tune the ramp.





Time Evolution

1. Start with $\Psi_{\mathrm{MPS}} = \sum_{\sigma_i} Tr[M_1^{\sigma_1} M_2^{\sigma_2} \ldots M_k^{\sigma_k}] | \sigma_1 \sigma_2 \ldots \sigma_k \rangle$

   for ferromagnet ground state.

   $\left(\quad \right)$ k x k matrix.

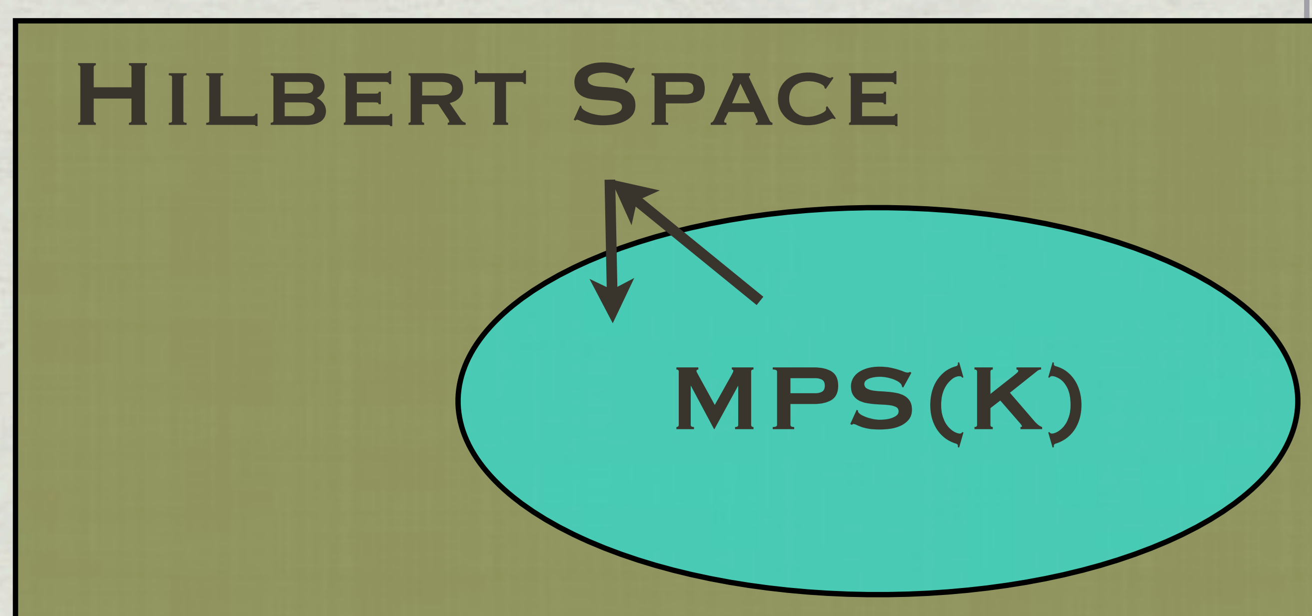
2. Apply $\exp\left[-it \left(-\sum_i \sigma_i^x + \delta(t) \sum_i \frac{1}{2}(\sigma_i^z + 1) \right) \right]$ exactly. This

   increases the bond dimension to something too large.

   $\left(\quad \right)$ 4k x 4k matrix.

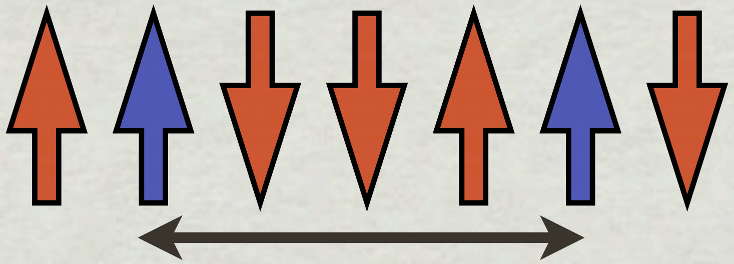
3. Project back to bond

   dimension of size k.

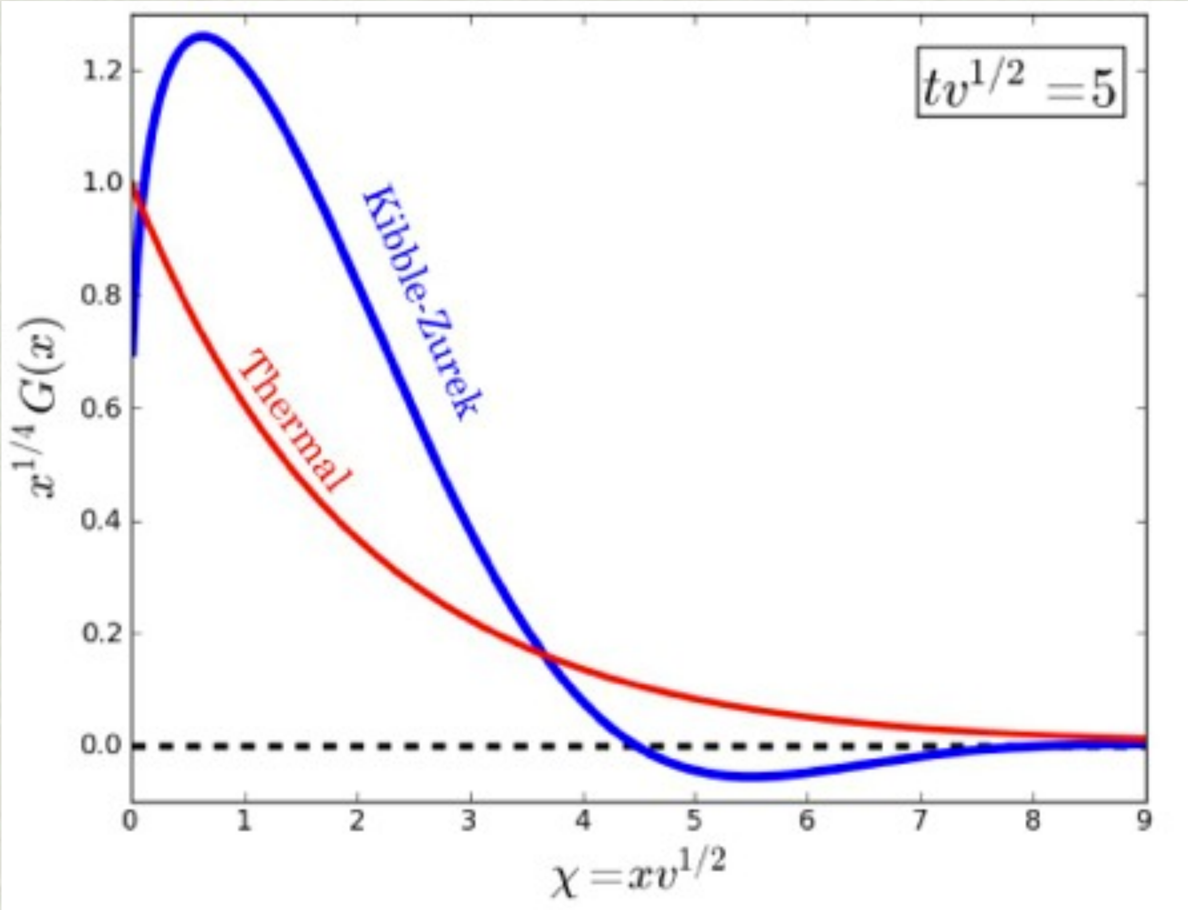


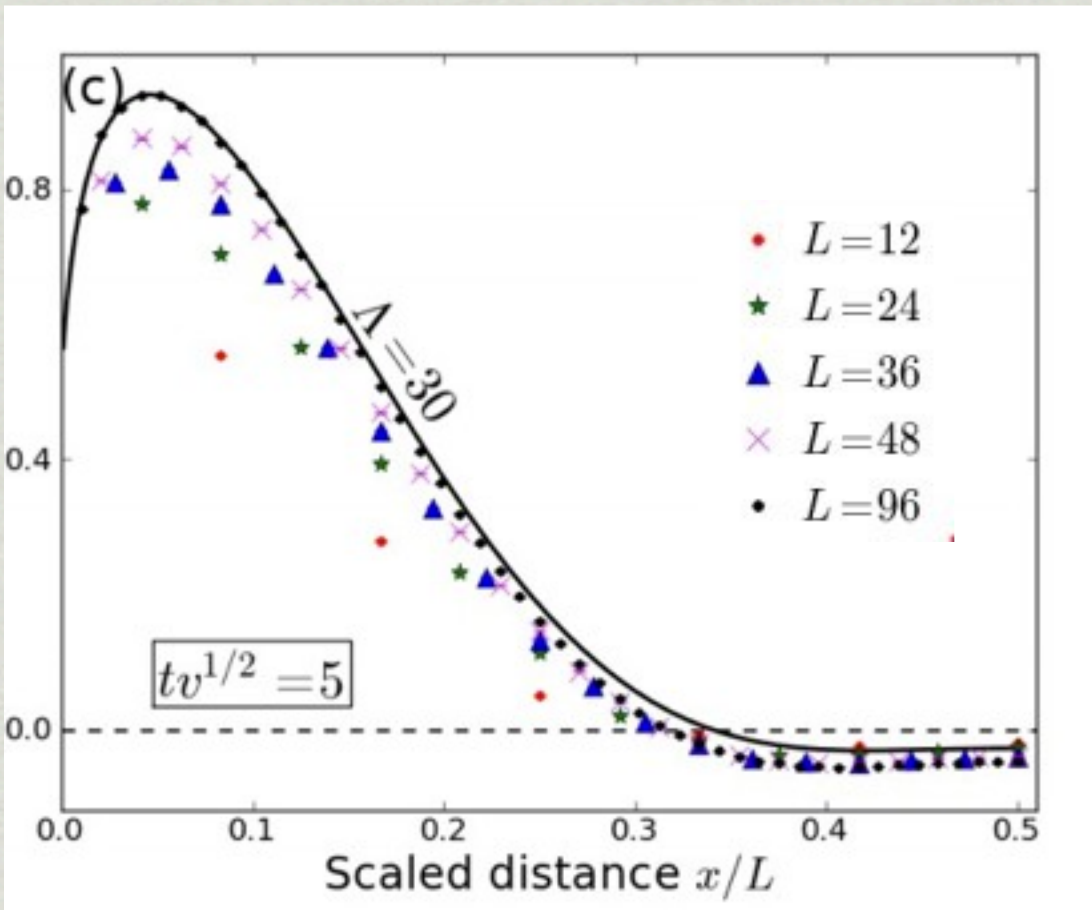
Q: Can Ramps Produce interesting states?

Thermal States

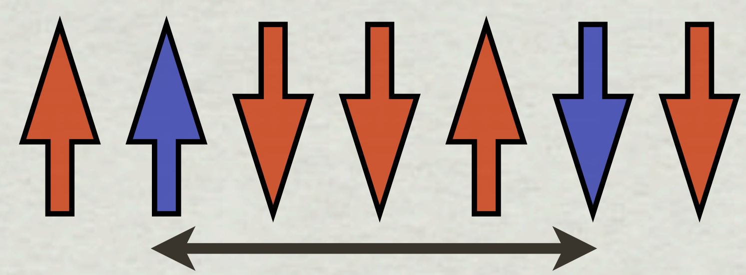


If I'm up, then you're probably up as well.





Athermal States

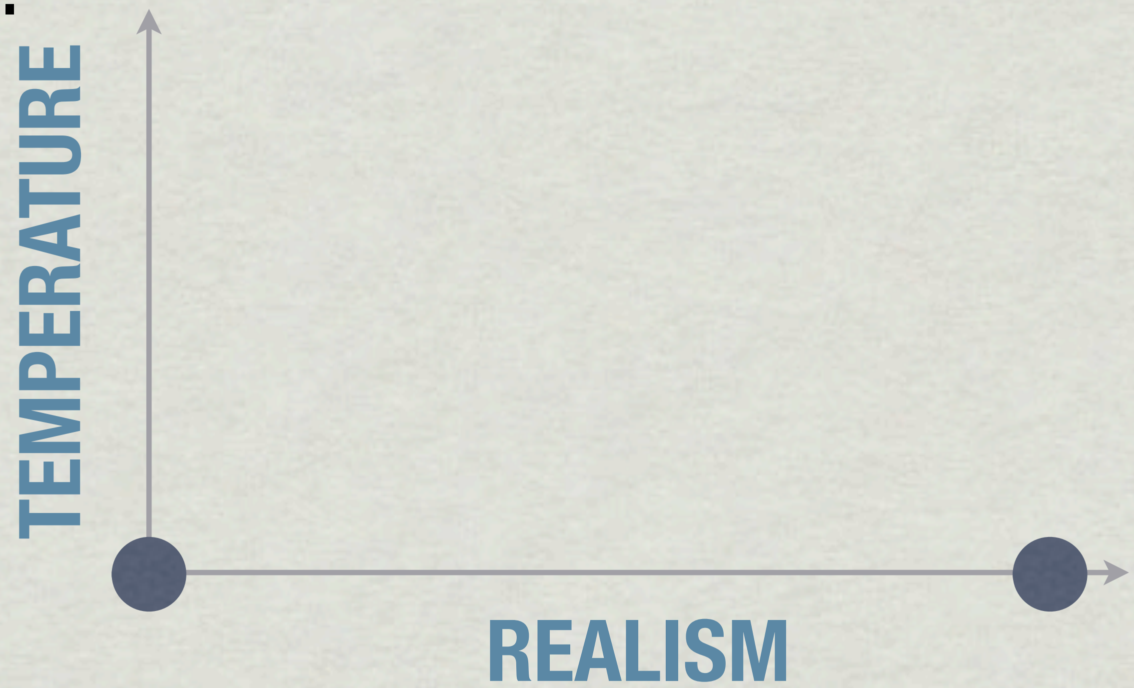


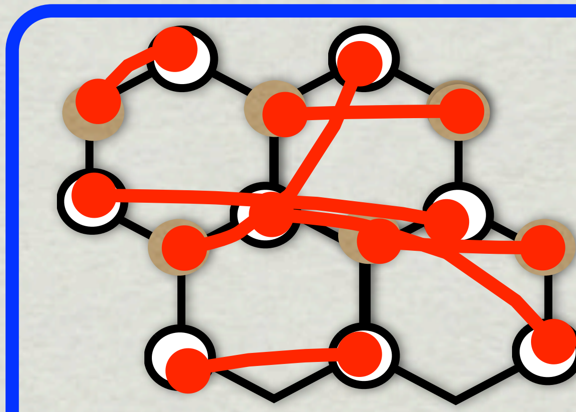
If I'm up, then you're probably down.

!!!

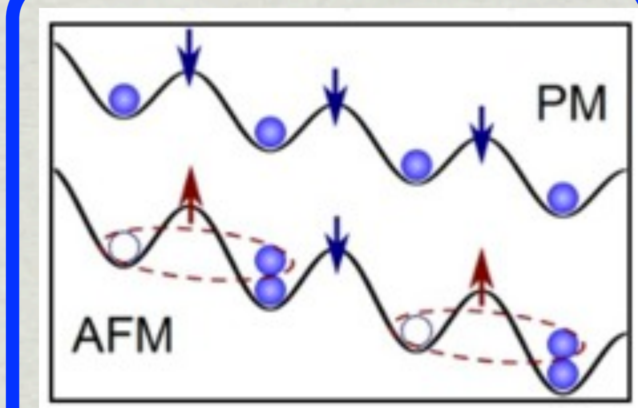
Conclusions 2

Optimistic about the future of computational condensed matter to make progress on many of the hardest problems in physics.

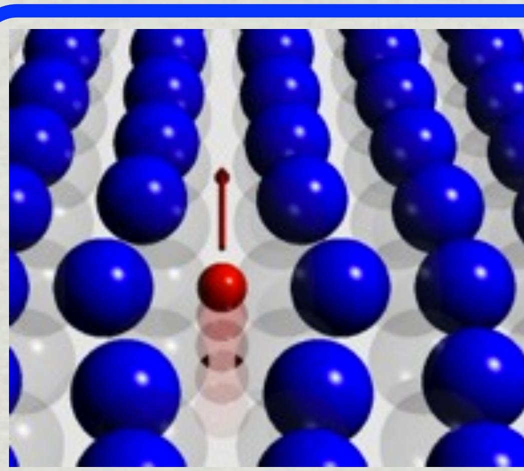




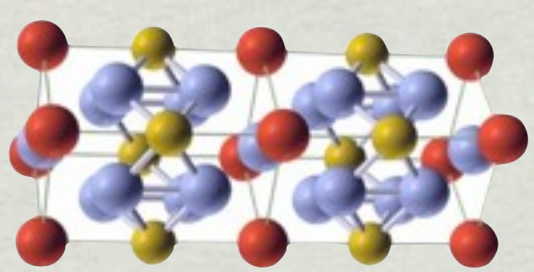
Frustrated Magnetism



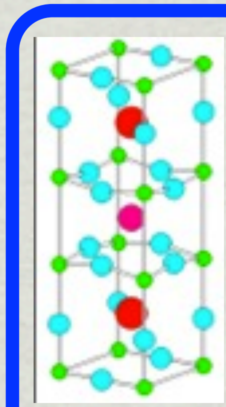
Non-equilibrium



Cold Atoms

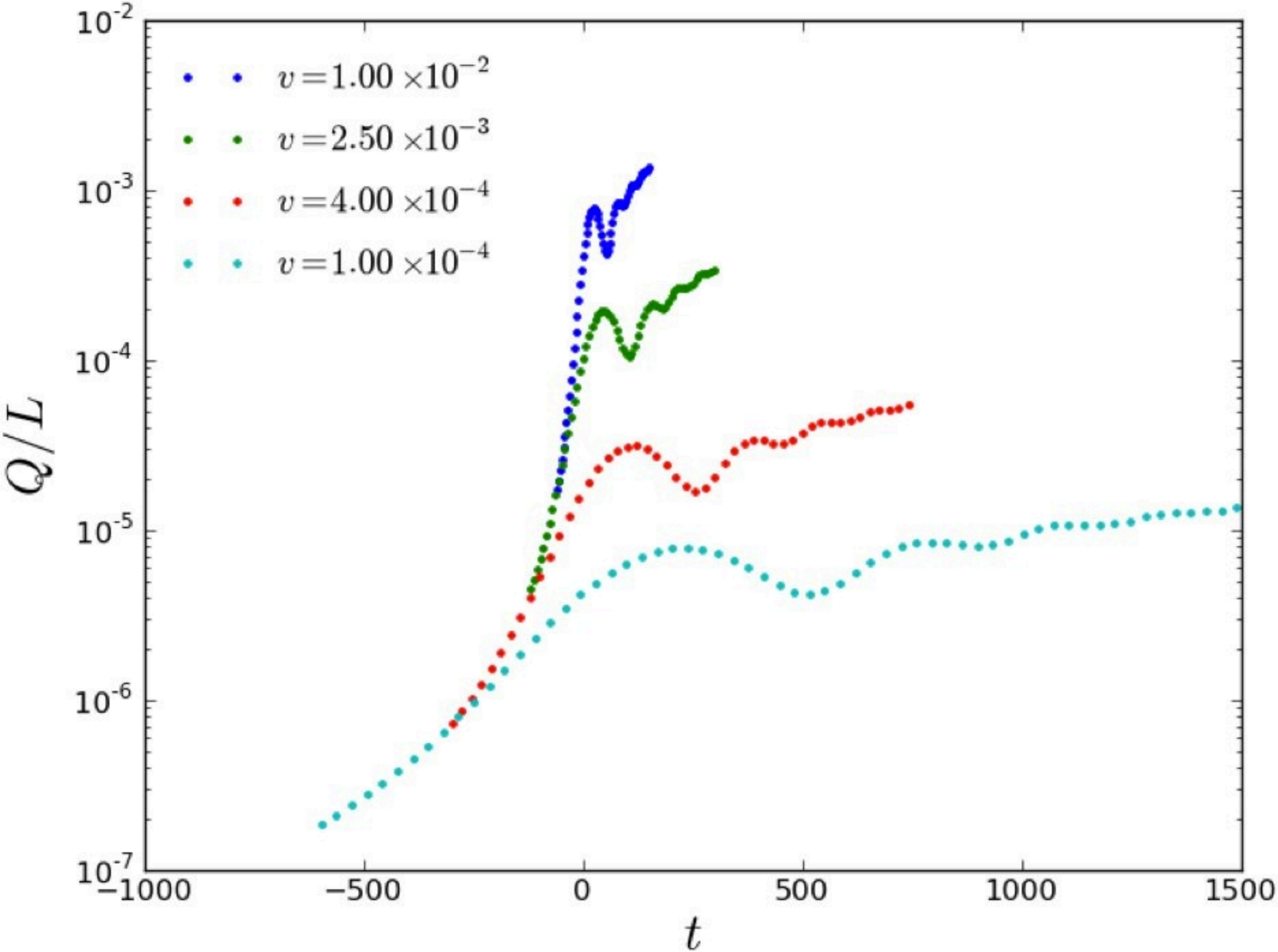


Heavy Fermions

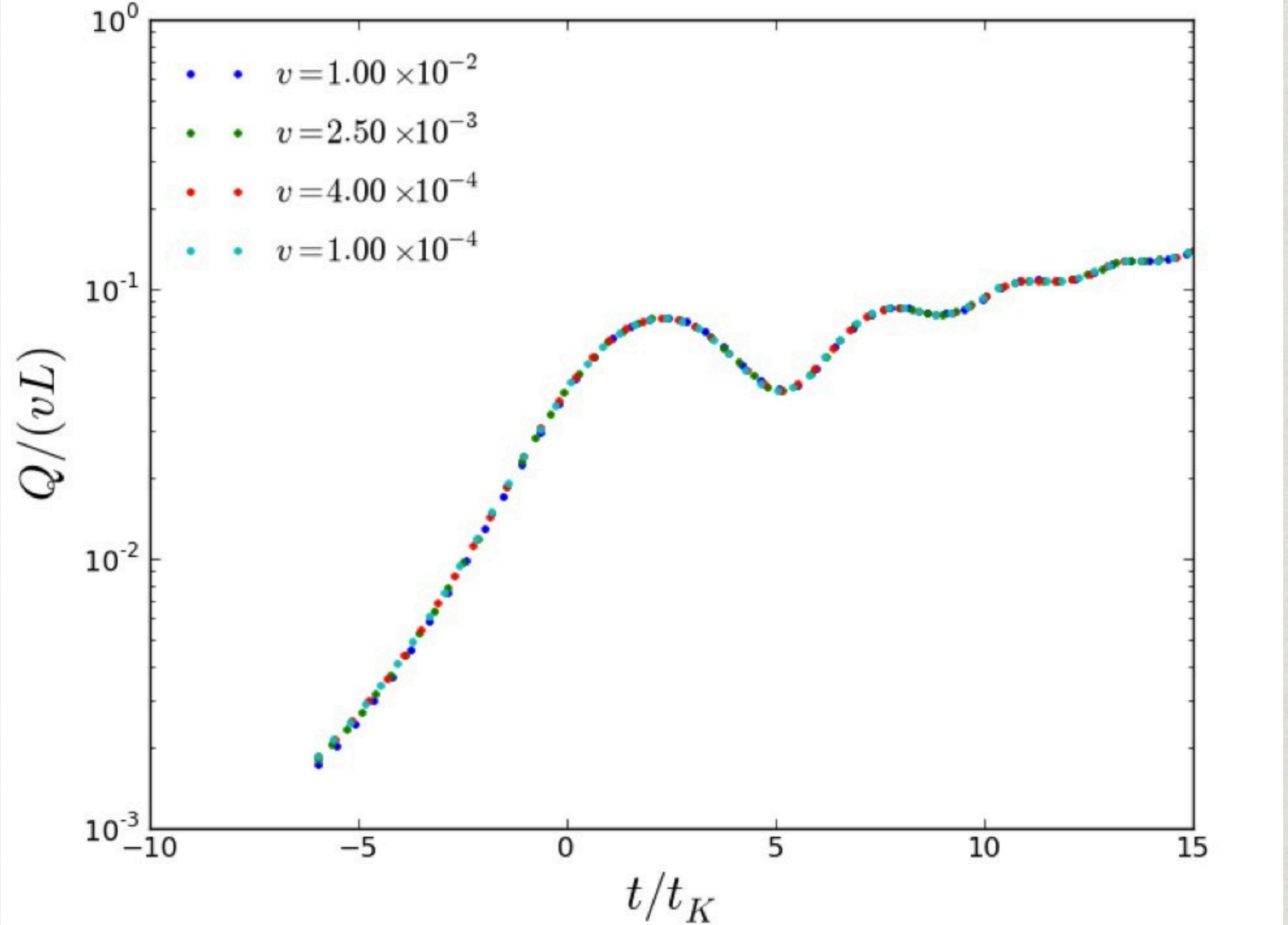


High Tc

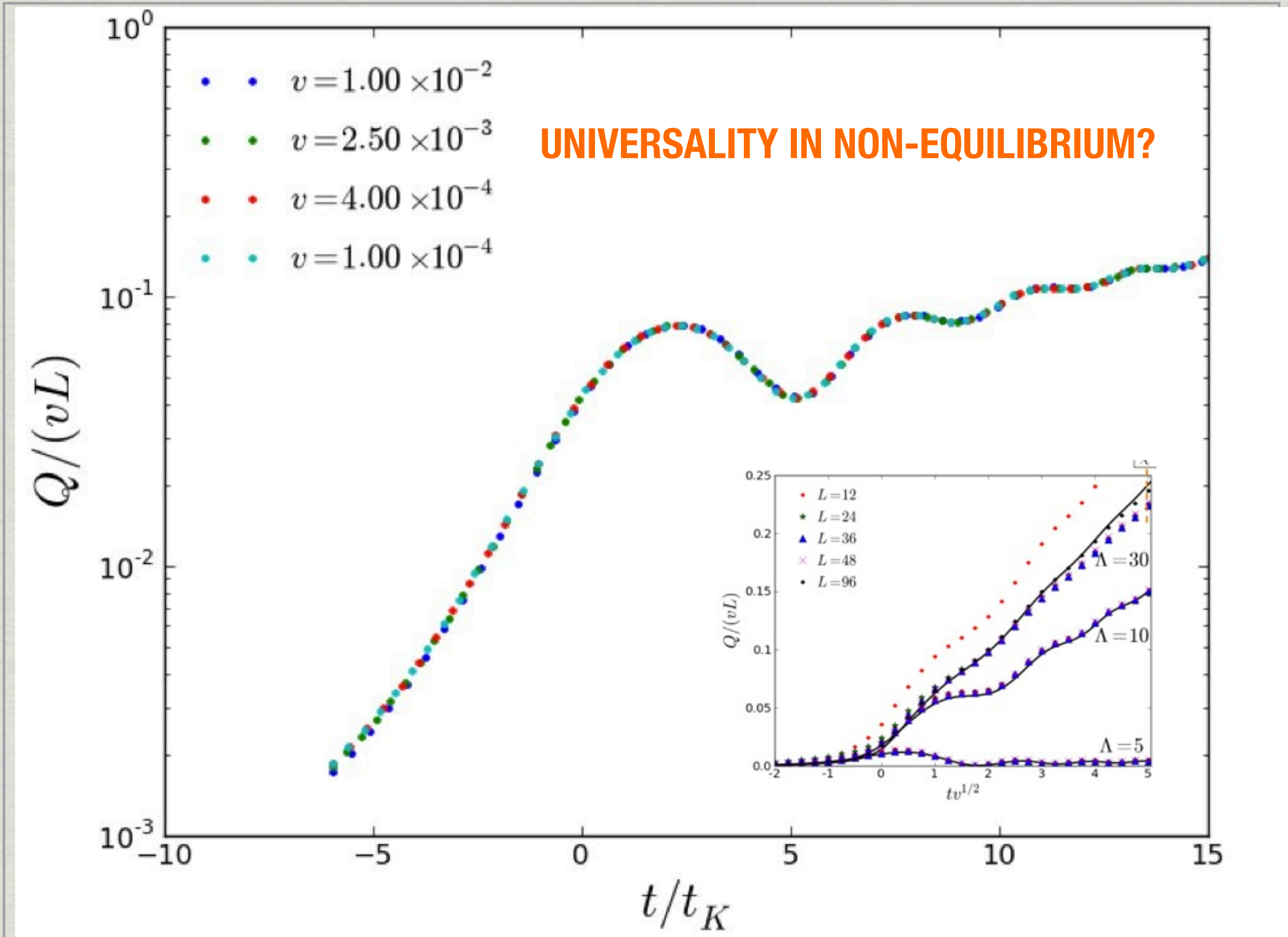
Non-fermi liquid



Sunday, March 10, 13



$v = 1.00 \times 10^{-2}$
$v = 2.50 \times 10^{-3}$
$v = 4.00 \times 10^{-4}$
$v = 1.00 \times 10^{-4}$
10^{0}
10^{-1}
10^{-2}
10^{-3}
$Q/(vL)$
−10
−5
0
5
10
15
t/t_K


UNIVERSALITY IN NON-EQUILIBRIUM?
$v = 1.00 \times 10^{-2}$
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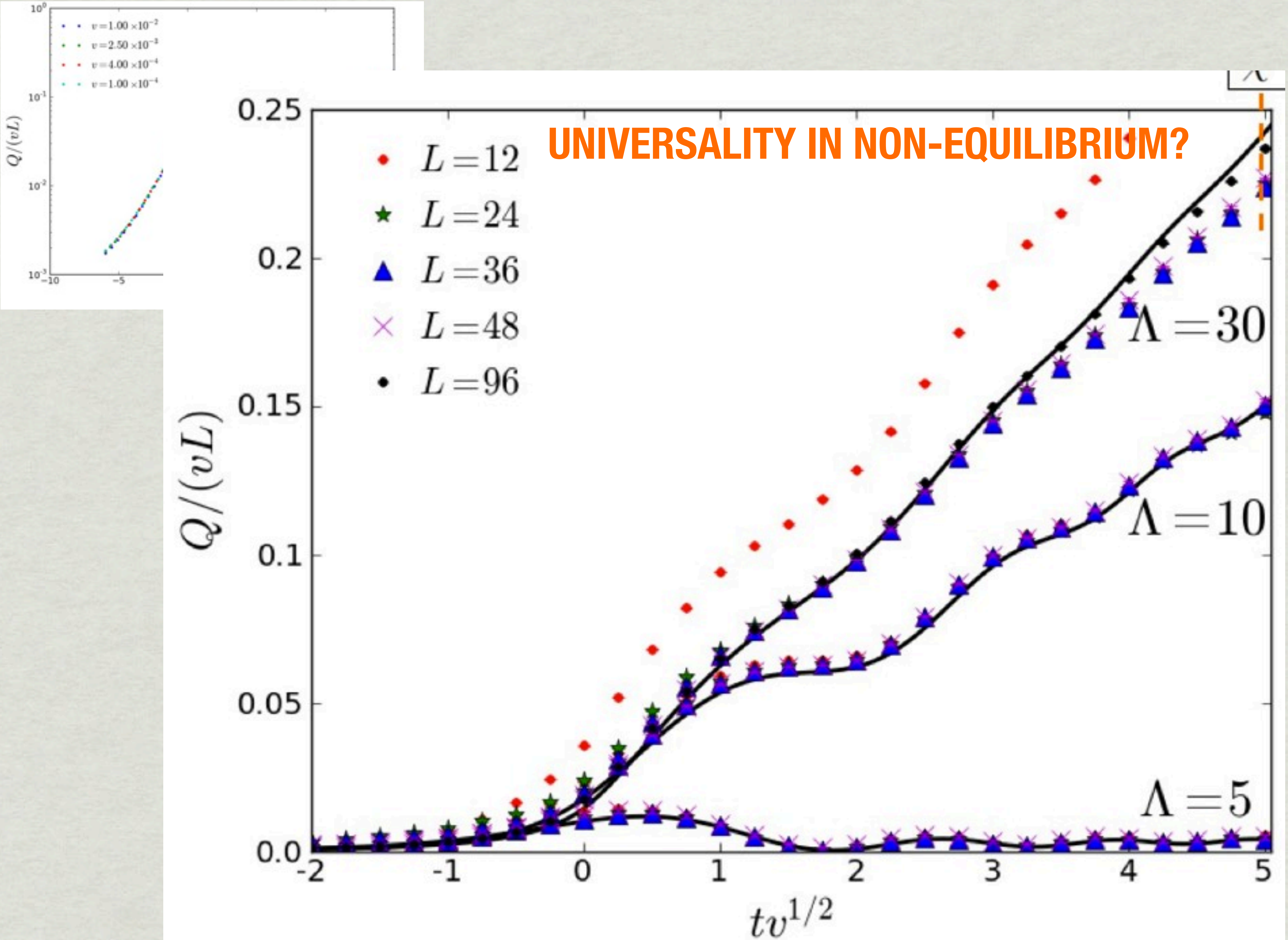
$Q/(vL)$
t/t_K
$L = 12$
$L = 24$
$L = 36$
$L = 48$
$L = 96$
$\Lambda = 30$
$\Lambda = 10$
$\Lambda = 5$
$tv^{1/2}$

UNIVERSALITY IN NON-EQUILIBRIUM?



Ramps

Ground States: $H[\lambda]|\Psi_0[\lambda]\rangle = E_0[\lambda]|\Psi_0[\lambda]\rangle$

Time Evolution: $|\Psi(t)\rangle = \exp[iH[\lambda]t]|\Psi(0)\rangle$

Adiabatic Theorem: Slow ramps stay in the instantaneous ground state.

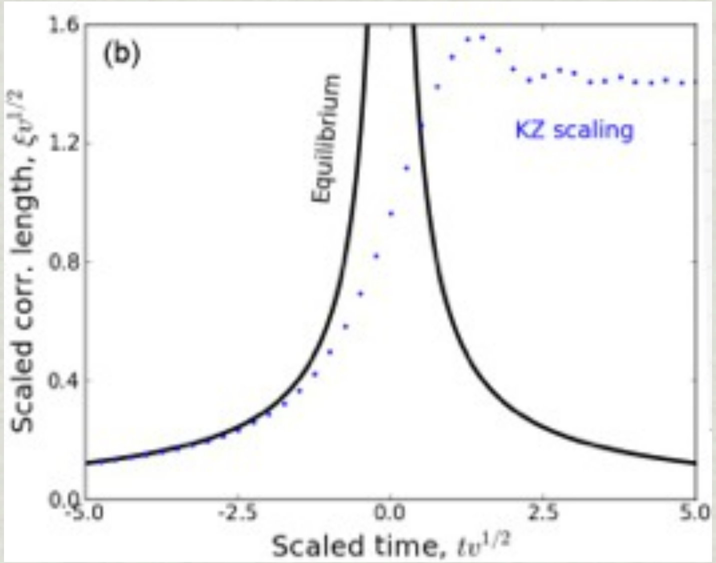
For linear ramps: $T \gtrsim \frac{||H_{\rm final} - H_{\rm init}||}{\Delta^2}$

Gap

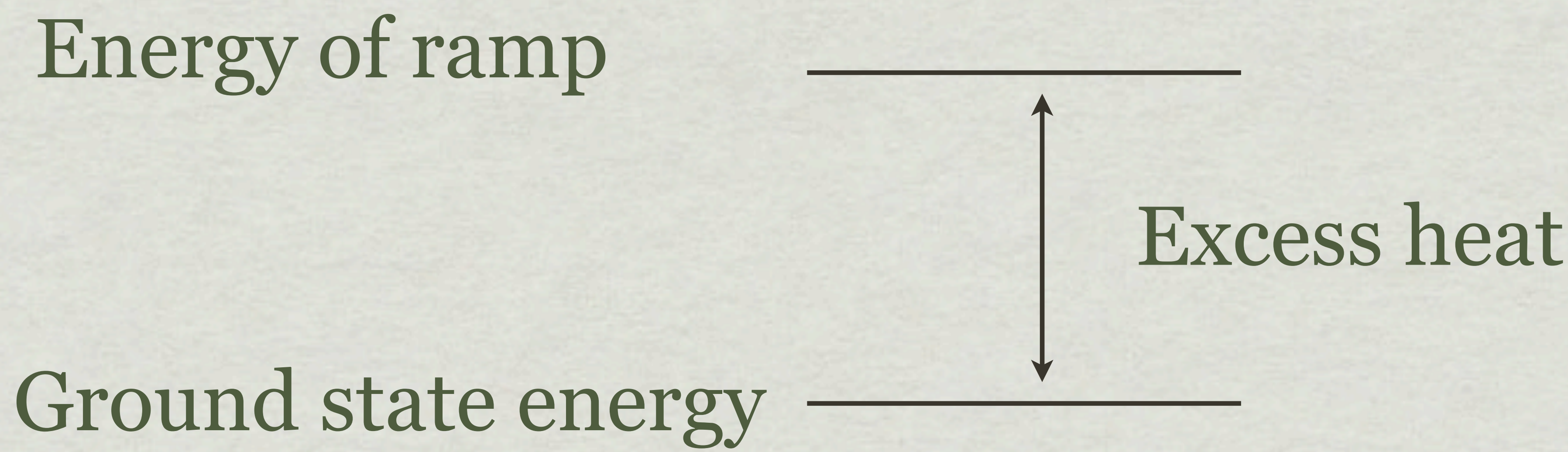
At a QCP, $\Delta \to 0$

All ramps eventually fall out of the ground state!

Physically: Correlation length grows faster than time spent in region.



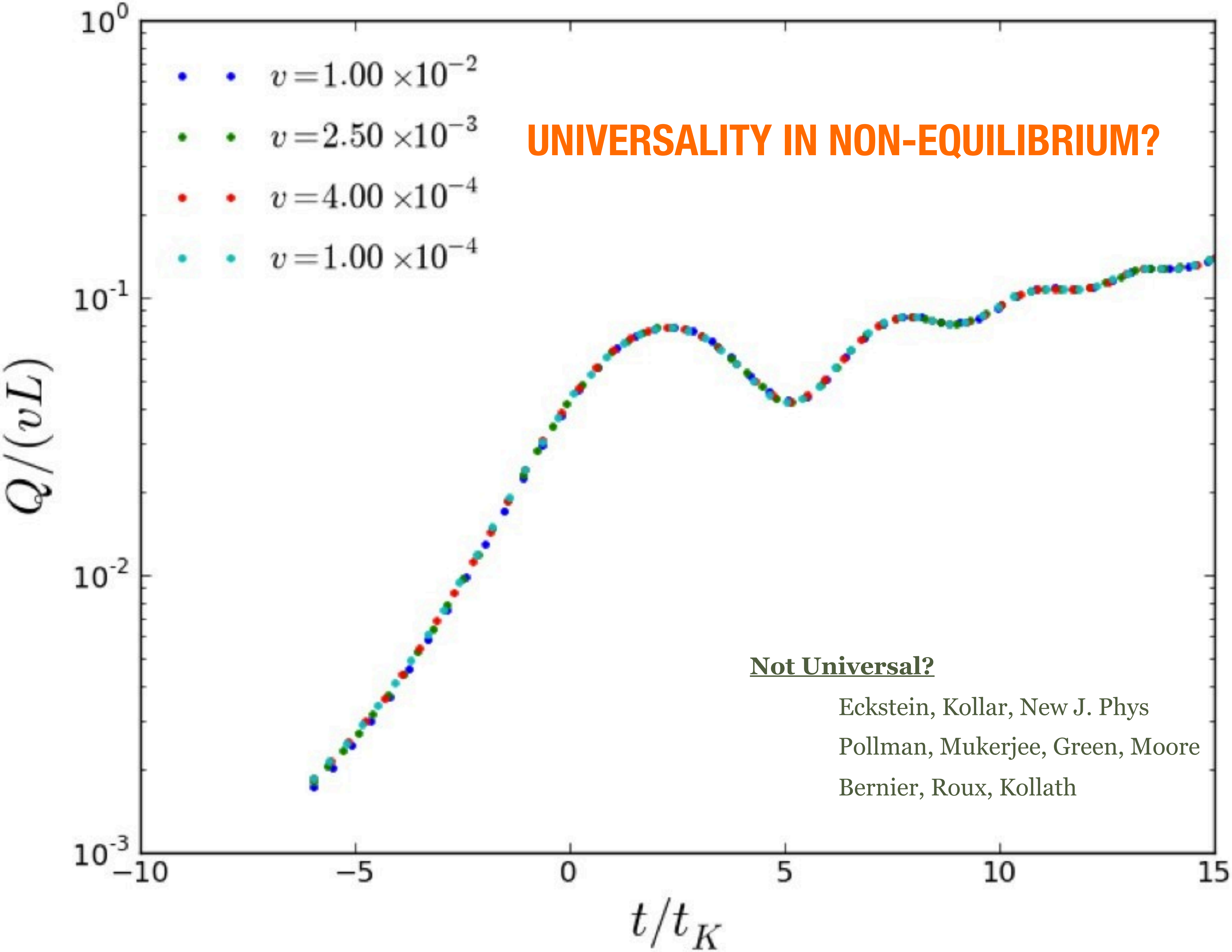
What to measure



Excess Heat: $$Q = \langle \Psi(t)|H(t)|\Psi(t)\rangle - \langle \Psi_0|H(t)|\Psi_0\rangle$$

$$\frac{Qt_k}{L/l_k} = \frac{Q}{vL} = q(\tau, \Lambda)$$

UNIVERSALITY IN NON-EQUILIBRIUM?



Not Universal?

Eckstein, Kollar, New J. Phys

Pollman, Mukerjee, Green, Moore

Bernier, Roux, Kollath