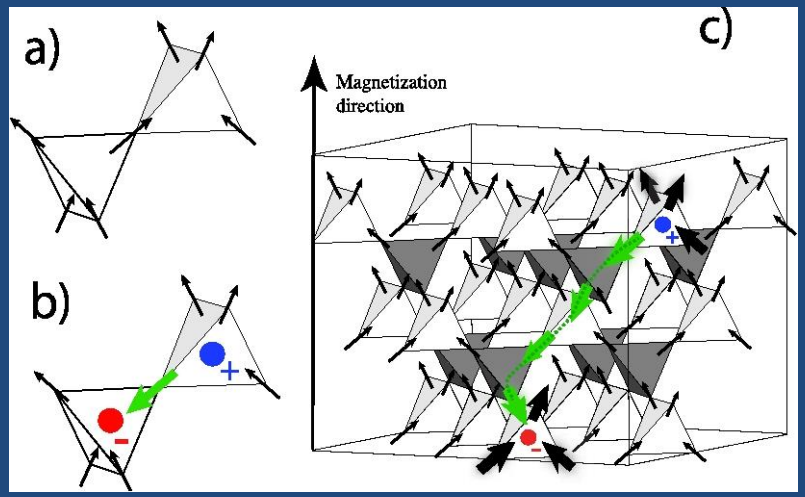
Local Entanglement and Confinement Transitions in Random Quantum Spin Ice Models



R. R. P. S. + A. Menon (UC Davis)
T. Pardini + S Hau-Reige Livermore Lab

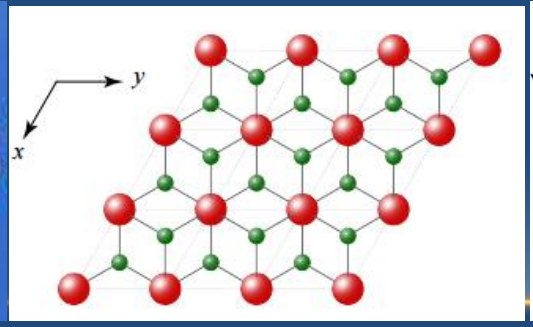
OUTLINE

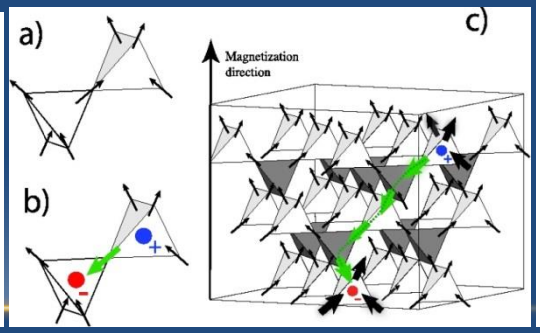
- Introduction to Quantum Spin Liquids/ Spin Ice
- Ising Model on Pyrochlore Lattice in random transverse field
- Ground State Phases and Properties
- Relevance to rare-earth pyrochlore magnets
- Summary and Future Directions

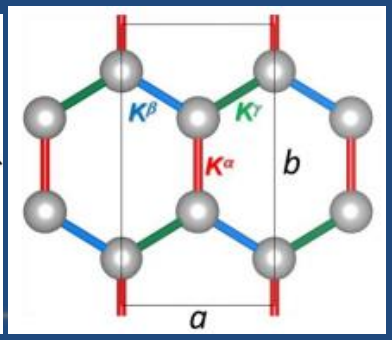
QUANTUM SPIN LIQUID PHASES OF MATTER

Highly entangled phases --- new paradigms of emergence in Quantum Matter

A number of materials systems are being explored yet convincing demonstration is still missing— one of the reasons is quenched impurities



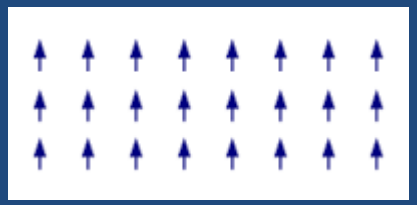


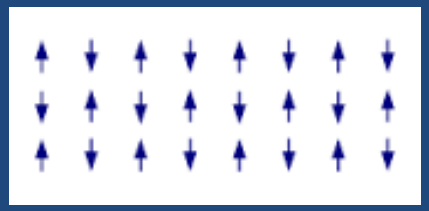


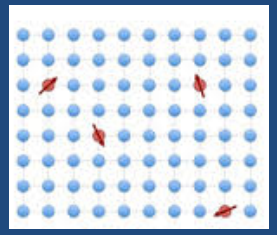
What is a Quantum SPIN LIQUID?

Consider a (periodic) solid: atoms (fixed position) with unpaired spins
Fluidity of spin-orientation

Exchange Interactions: $\sum J_{ij}\, S_i S_j$







Spins `**solidify**' at low temperatures in
crystalline (super)-structures (FM/AFM)

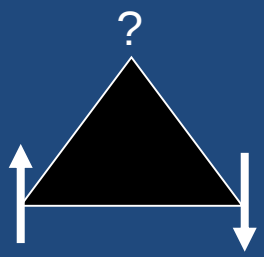
And fluctuate independently like
a spin-**gas** in a paramagnet at high-T

T

How can they form a quantum spin-liquid?

Inertness+ Lightness :: Geometric Frustration + Low spin

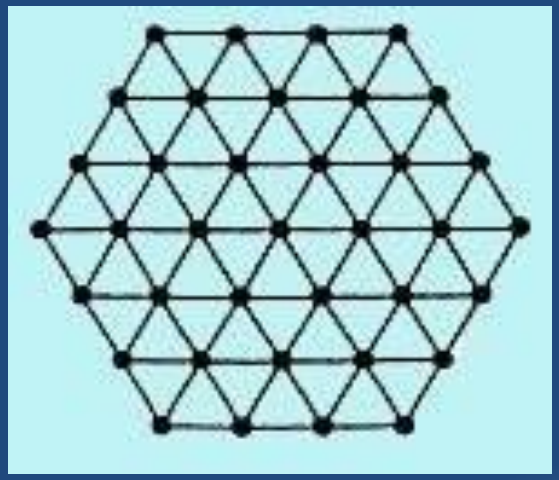
Antiferromagnetic
Ising Model



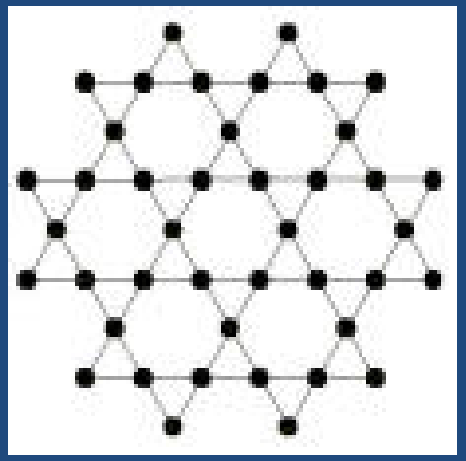
6 of 8 spin configurations have lowest energy

uud udu duu udd dud ddu

Lattices with Triangles and Tetrahedra can have low energy manifold with residual entropy : A classical spin liquid



Triangular-Lattice : Wannier



Kagome Lattice

Degeneracy + QM : should lead to release of entropy, emergence of a ground state

Ising Model + small Transverse Fields / Transverse exchange

$$\sum J_{ij} S^z{}_j S^z{}_j + \sum h_i S_i{}^x \sum \lambda J_{ij} S^x{}_j S^x{}_j$$

Generically one of two things can happen:

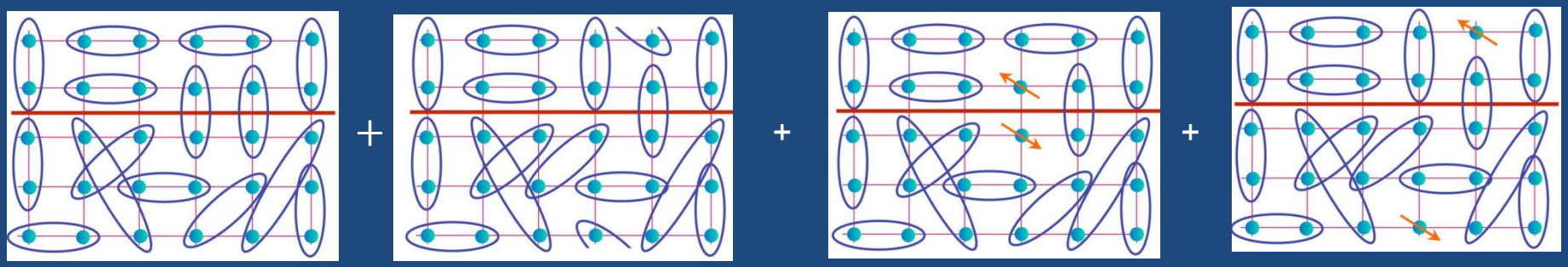
1. New ground state is a linear superposition of the many degenerate configurations: highly resonating entangled state of matter: A QSL
2. Selection of a specific configuration as the global ground state Order by Disorder

High degree of entanglement is a hallmark of QSLs

QUANTUM SPIN LIQUID must have Global Entanglement

Resonating Valence Bonds — Anderson 1973

High-Tc superconductivity — Baskaran,…. Affleck,… Kivelson, … Sachdev, ...



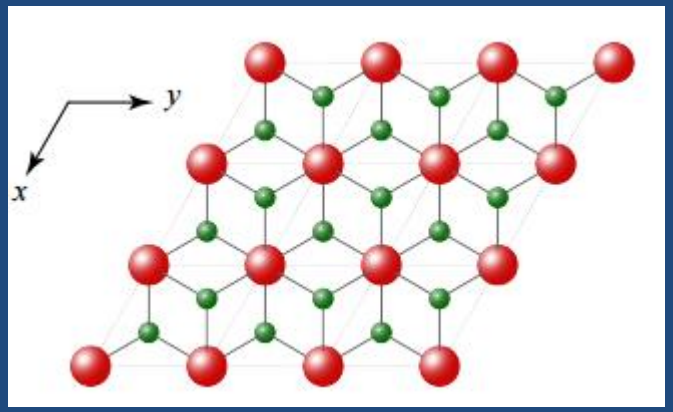
It is important that entanglement is not limited to cluster of spins (VBC)

High degree of global entanglement and resonance leads to new degrees of freedom

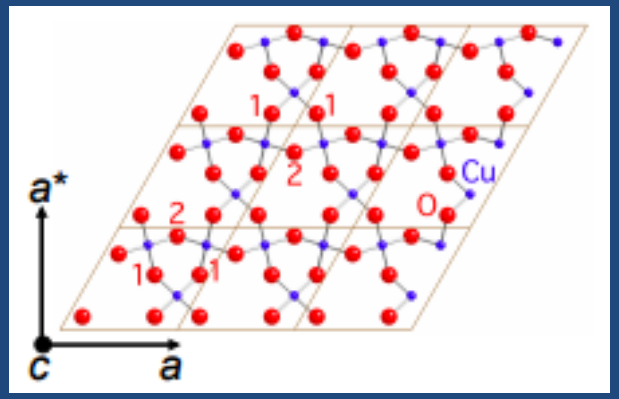
- Fractionalization (deconfined spinons) $c_\sigma = b f_\sigma$
- Emergent Gauge Fields

Quest for QSL is a search for new degrees of freedom and emergent gauge-fields in real materials

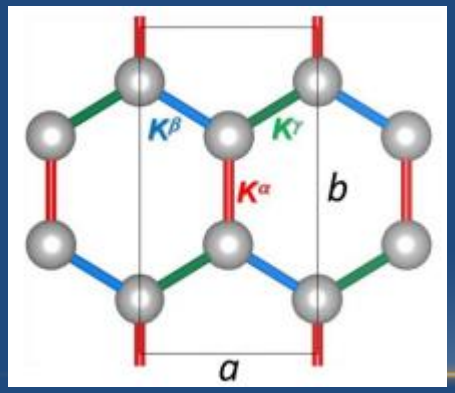
Material candidates for realizing a quantum spin-liquid



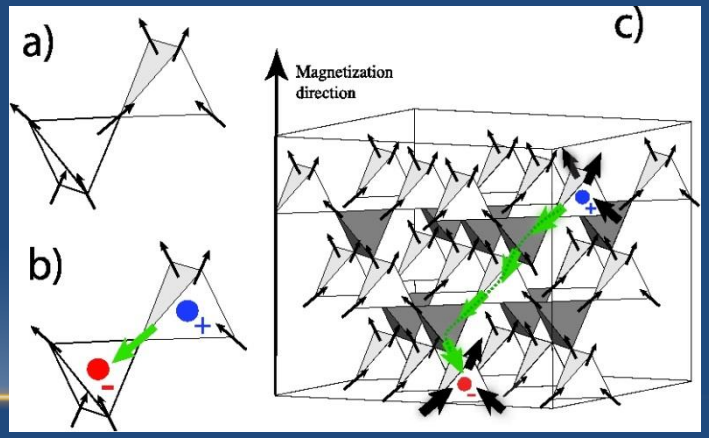
Growing list of Triangular AFM
$Yb\ Mg\ Ga\ O_4$ / Organics



Kagome Materials
Herbertsmithites (Nocera)



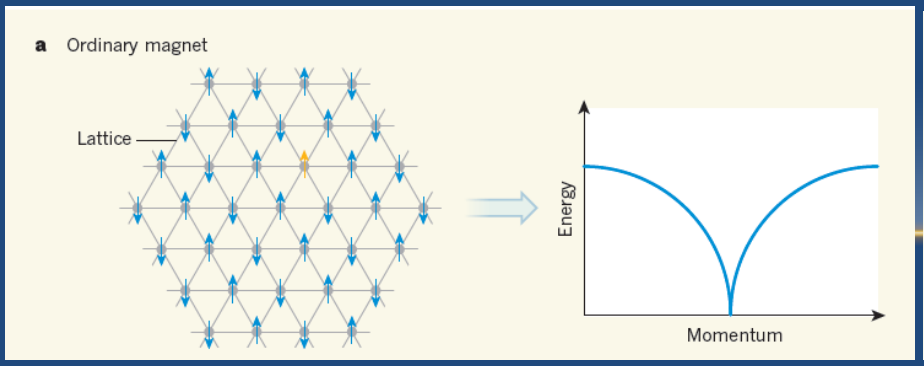
Kitaev-Jackeli-Khalliulin materials $RuCl_3$
Arnab Banerjee, … Nagler et al

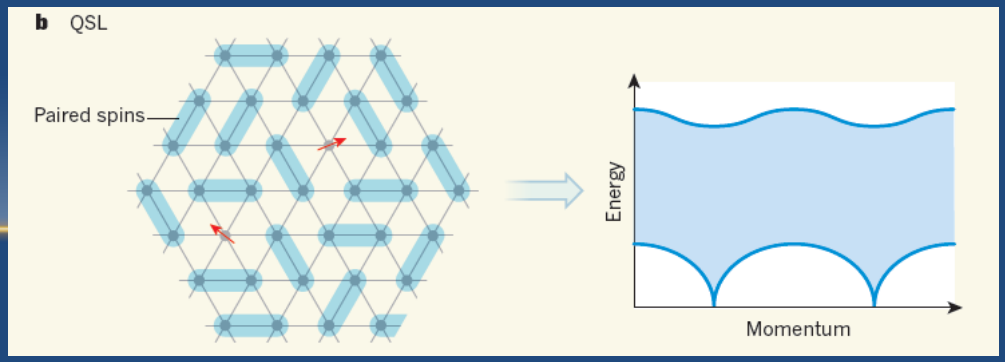


Rare-earth pyrochlores: $Yb_2\ Ti_2 O_7$
Quantum spin-ice

Challenges in establishing a true QSL

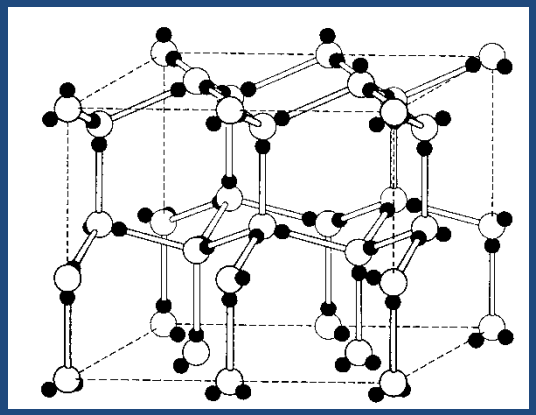
- Direct measurement of entanglement is very difficult –Cold Atoms - probably not scalable
- Fractional/emergent degrees of freedom do not directly couple to external probes (Continuum in scattering remains one of the most important probes)
- Power-laws in **heat capacity, susceptibility, thermal conductivity, …** can it be corrupted by extraneous effects? ……disorder can mask or mimic many signatures
- In this talk focus on role of disorder in a specific context of spin-ice systems

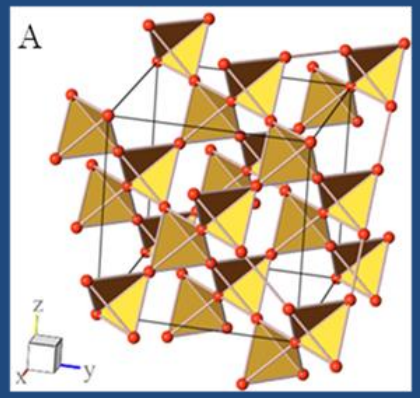


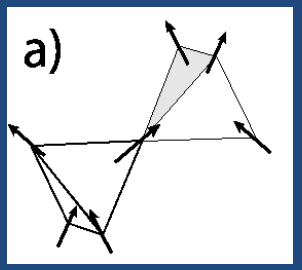


Balents

ICE RULES AND SPIN ICE



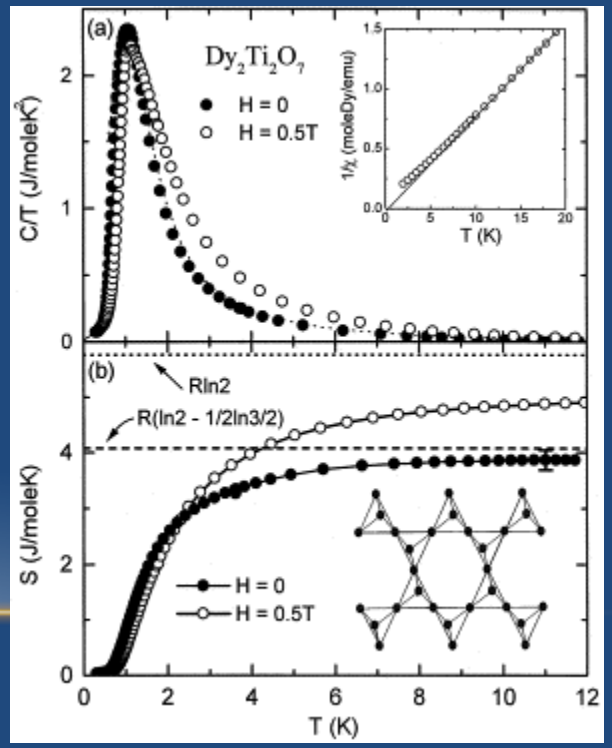




Ordinary ice has a high residual entropy (Pauling)
Exponentially Large Degenerate Configurations

Spins (on Pyrochlore lattice) are analogs of ice
with the same residual entropy (Anderson)
Ramirez et al Dy2Ti2O7 Nature 1999

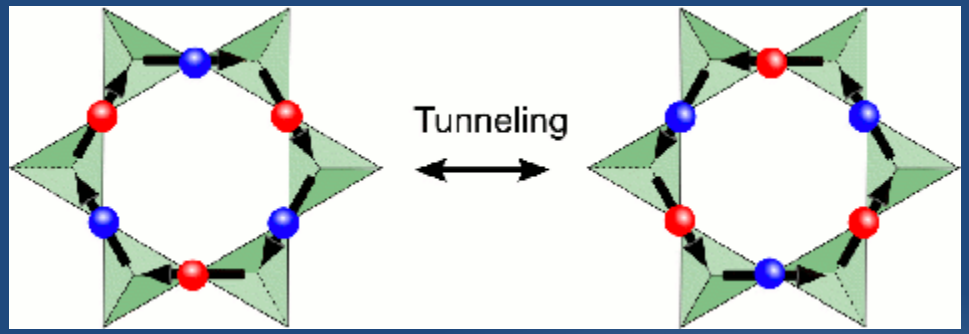
Classical Spin Liquid with Monopoles/Spinons
Classical Gauge Fields
Castelnovo et al

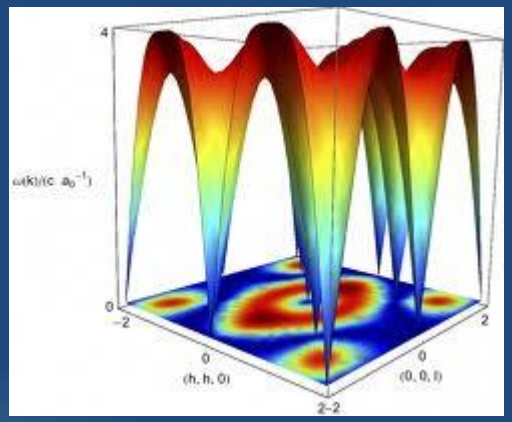


ADDING QUANTUM FLUCTUATIONS TO SPIN ICE
QUANTUM SPIN ICE

XXZ Model: Quantum Spin Liquid (Hermele, Fisher, Balents)
(Weak quantum fluctuations on top of a highly degenerate subspace)

Out of an ensemble of spins can EMERGE – a novel phase with Charges, Monopoles & Photons– a full fledged fictitious Quantum Electrodynamics





Search for QSI is search for emergent QED in spin-ice materials (dynamical photons)
Nic Shannon et al

Spin ice materials provide a lot of variety: $R_2M_2O_7$
Varying amounts of quantum fluctuations and anisotropy

Group → / ↓ Period	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1 H																	2 He
2	3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
3	11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba	*	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra	**	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Uut	114 Uuq	115 Uup	116 Uuh	117 Uus	118 Uuo
* Lanthanides				57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
** Actinides				89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

Kramers vs non-Kramers

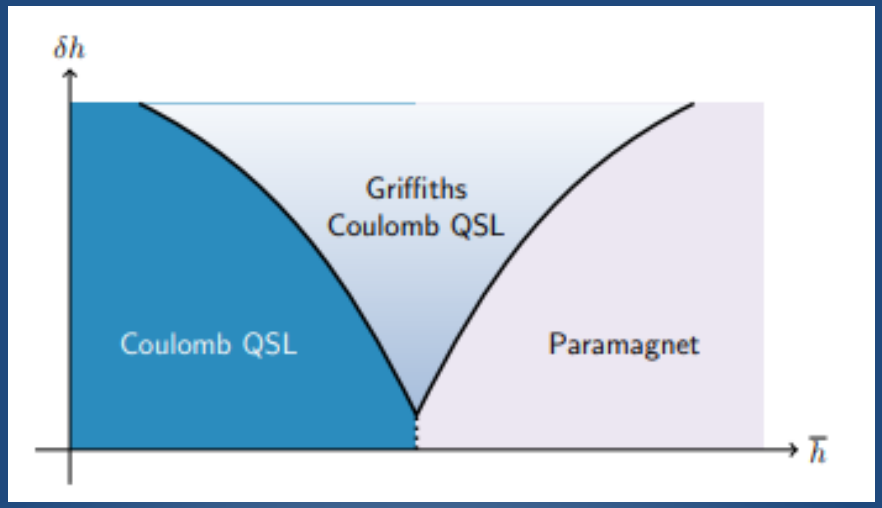
Disorder-induced entanglement in spin ice pyrochlores

Lucile Savary[1,*] and Leon Balents[2]

Disorder: Splitting of doublet --- transverse-field

Random Transverse Field Ising Model

$$\mathcal{H} = J \sum_{<i,j>} \sigma_i^z \sigma_j^z - \sum_i h_i \sigma_i^x ,$$



Interesting dynamics including relevance to MBL (only starting to study)

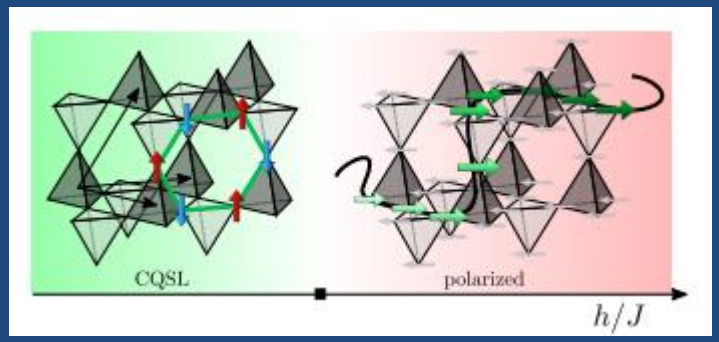
Non-random system

Series expansion in h and 1/h

$$\mathcal{H} = J \sum_{<i,j>} \sigma_i^z \sigma_j^z - \sum_i h_i \sigma_i^x,$$

Spin liquid and quantum phase transition without symmetry breaking in a frustrated three-dimensional Ising model

Julia Röchner,[1] Leon Balents,[2] and Kai Phillip Schmidt[3]



Polarized along x on one side

Ring exchange QSL on other

Weakly first order transition

Random Transverse Field Ising Hamiltonian

$$\mathcal{H} = J \sum_{<i,j>} \sigma_i^z \sigma_j^z - \sum_i h_i \sigma_i^x ,$$

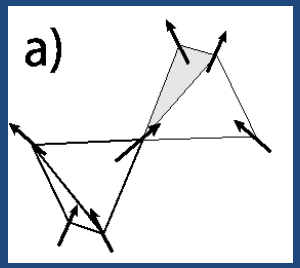
Properties we study by ED (PBC), NLC and Perturbation Theory

Average moment along the field (PM)

$$m_x = [\frac{1}{N} \sum_i | < \sigma_i^x > |].$$

Entanglement for a single tetrahedron of spins (QSL)

$$S_A = S_B = -\operatorname{Tr} \rho_A \ln \rho_A .$$



Ising SG Correlation sum (ISG)

$$C_{zz} = [\frac{1}{N^2} \sum_{i,j} | < \sigma_i^z \sigma_j^z > |],$$

NLC has the accuracy of series expansion when they are convergent
Can be easily extended to random system and include non-perturbative local effects

NUMERICAL LINKED CLUSTER EXPANSION

Combines Linked Cluster + ED (Rigol, Bryant, RRPS PRL)

An extensive property can be expressed as

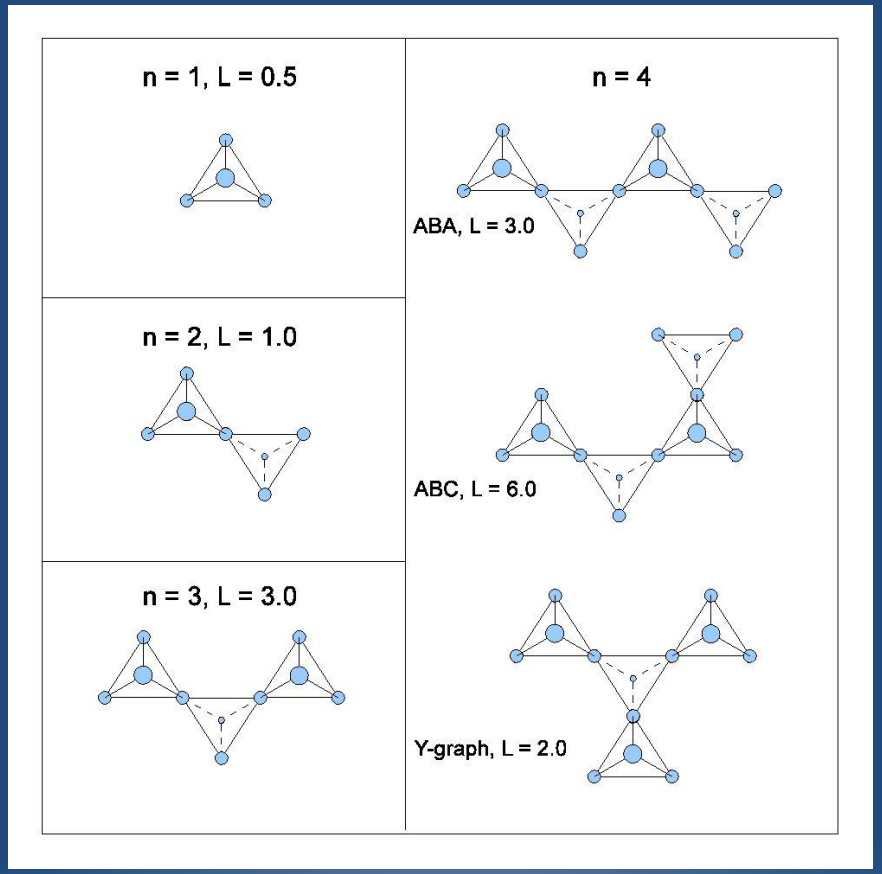
$$P/N = \Sigma_c \;\; L(c) \times W(c)$$

$L(c)$: is a count of the cluster on a lattice
$W(c)$: contribution of the cluster obtained by ED
and the *Principle of Inclusion and Exclusion*

$$W(c) = P(c) - \sum_{s \subset c} W(s)$$

Obtained for any set of parameters (T, h, J, ……)
Numerically exact at high T (builds in HTE)
Numerically exact at high fields (builds in HFE)
Correct short distance Physics
Ideal for Spin-Ice to use tetrahedral clusters

GROUND STATE NLC TO 5TH ORDER (LANCZOS)



NLC FOR T=0 ENTROPY (CLASSICAL ISING MODEL)

P = $\sum L(c) * W(c)$ (Lattice Constant L, Weight W)

Order 0: Single Site: S(0) = ln(2); W(0) = ln(2); L(0)=1;

S/N=ln(2)

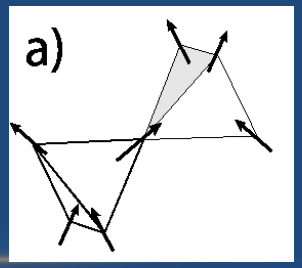
Order 1: One tetrahedron: S(1) =ln(6); W(1)=ln(6)-4ln(2)= ln(6/16); L(1)=1/2;

S/N=ln(2) + (1/2) ln(6/16)= (1/2) ln(3/2) (Pauling)

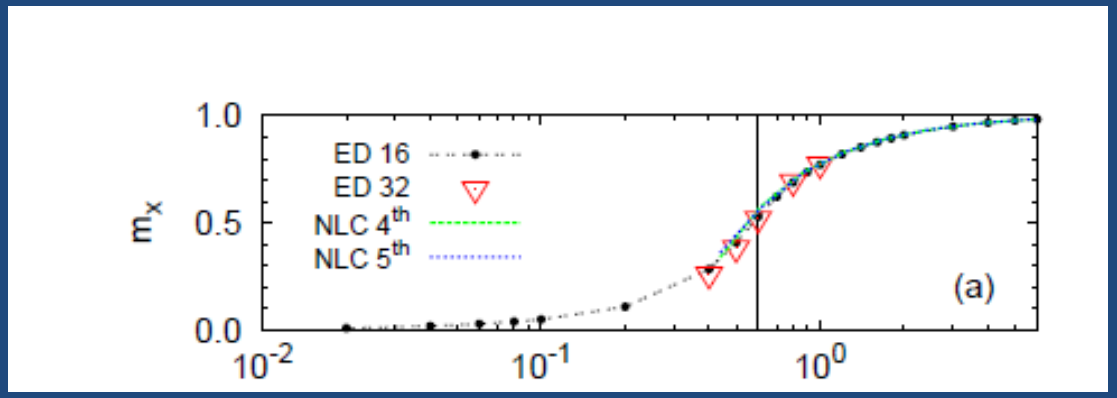
Ist Order NLC: Corresponds to Pauling Approx.

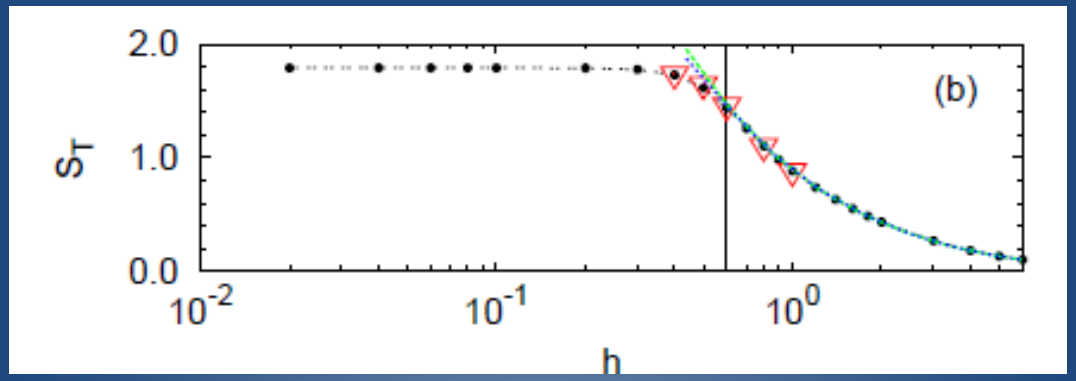
Accurate to a few percent down to T=0 for S, C, χ

RRPS and J. Oitmaa PRB 2012



Results for uniform (non-random) system (ED+NLC)

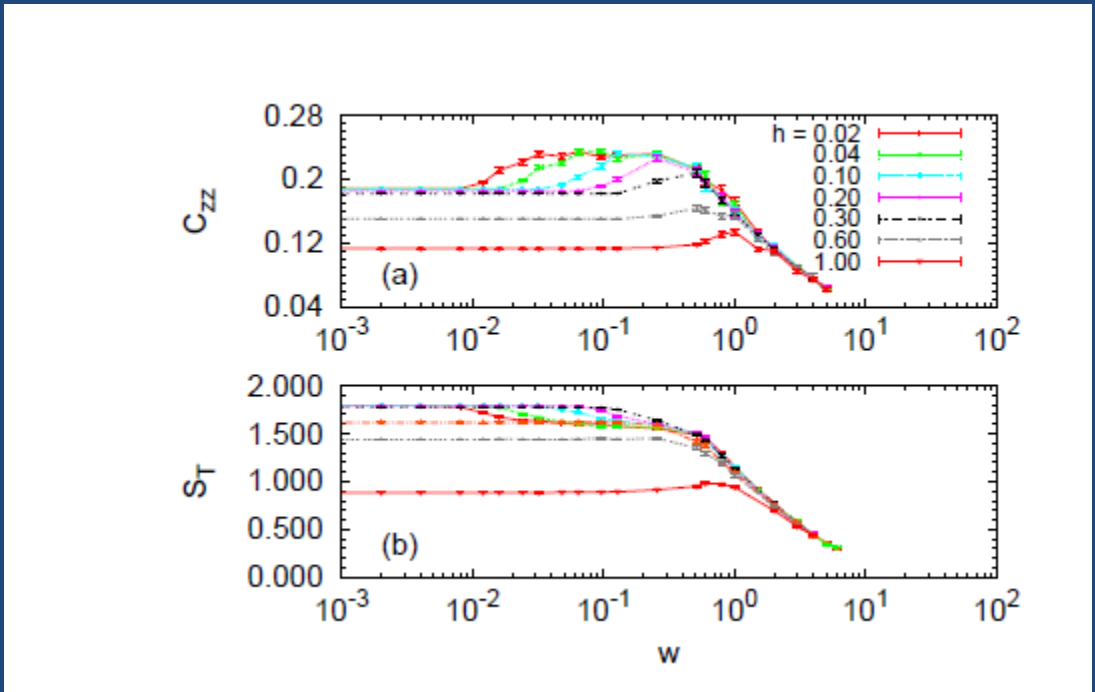




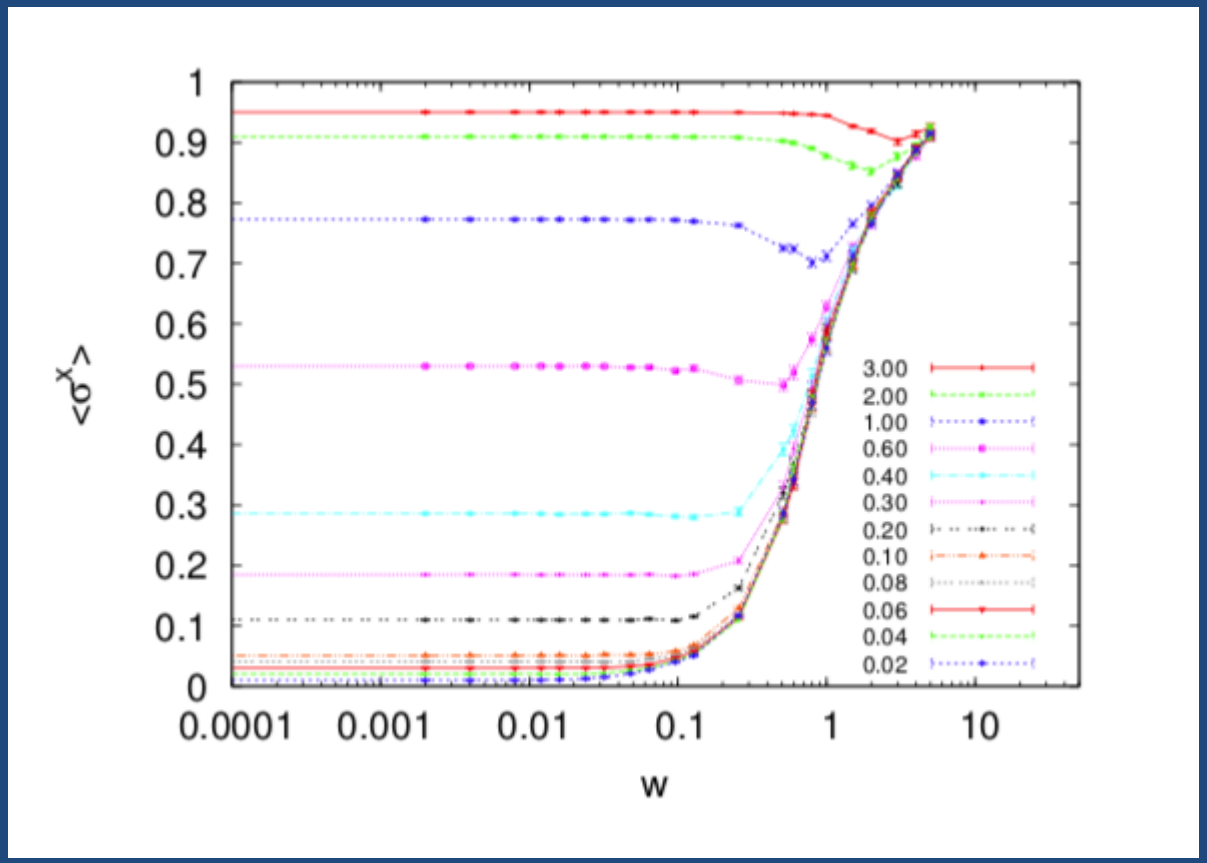
Very little finite size effect in PM phase (compare ED with NLC)

QSL: Tetrahedron entropy ln(6)

Random System ED (16 sites PBC)

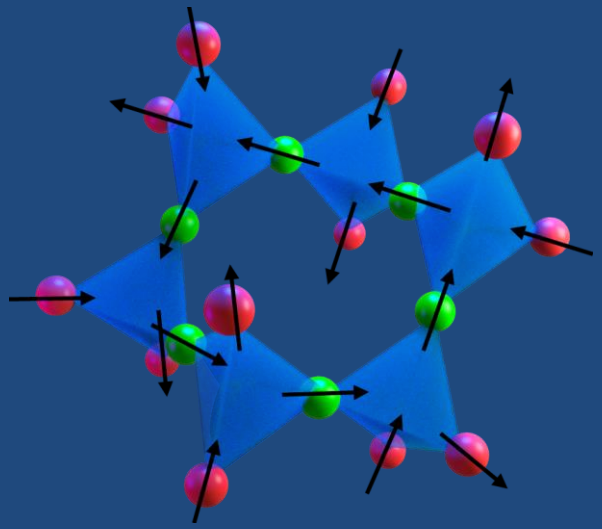


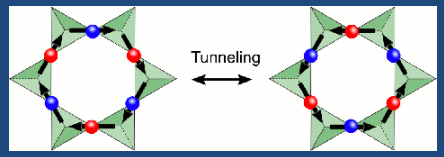
Sudden increase in Ising correlation + decrease in entanglement entropy



No signature of anything happening in the polarization
Changes are within the ice manifold

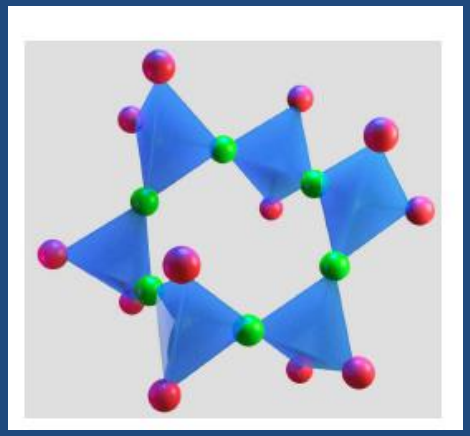
Naïve NLC does not converge in the QSL phase
Need to embed clusters inside spin-ice
Maps on to the ring exchange model
First cluster for any substantial contribution: 6 tetrehedra

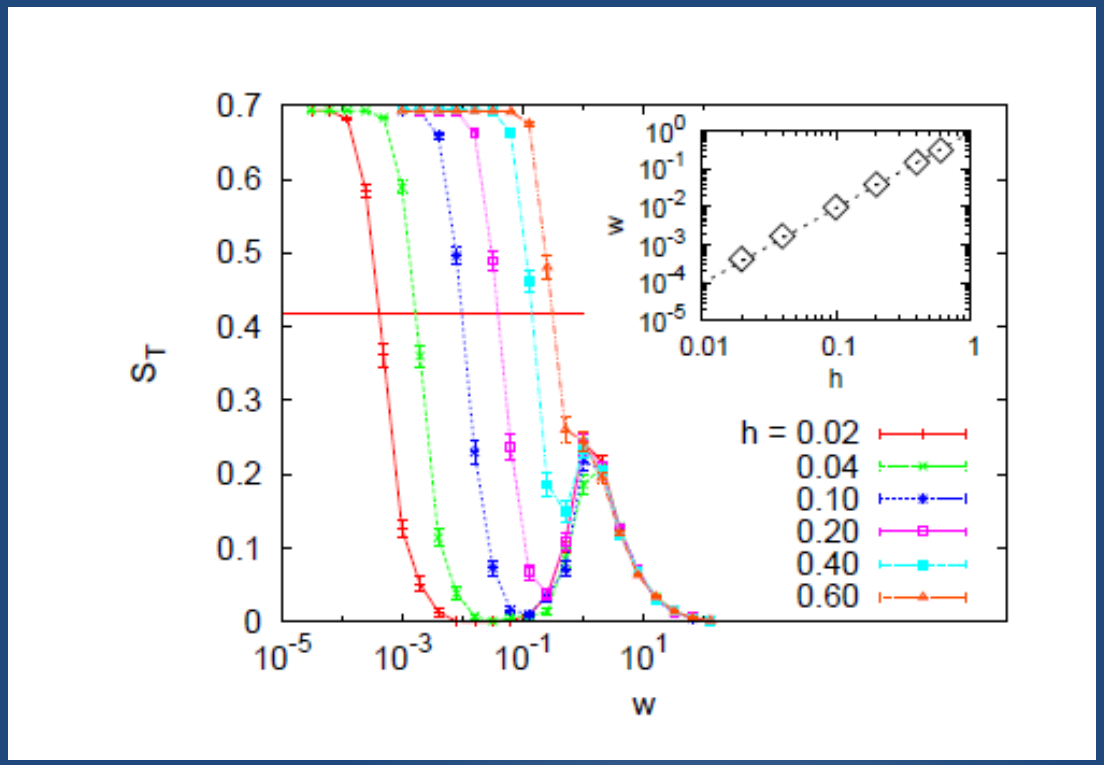




In the QSL phase all the entanglement comes from ring exchanges and how often configurations arise that allow ring exchanges

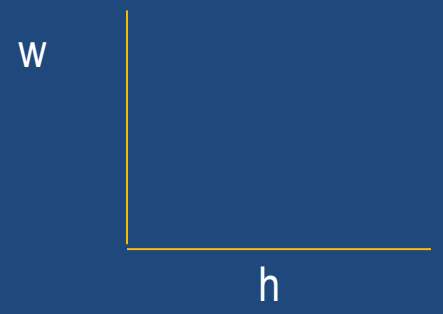
NLC for random system





Randomness causes freezing of hexagonal resonance

What kind of phase results from freezing of resonance? Confinement



Increasing h : --- leave ice space --- polarize along field
Confinement with X correlations of spins : spinon condensation

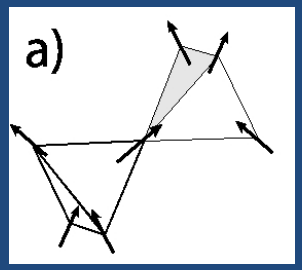
Increasing disorder: Confinement within ice space ---- Selection of Ising or Z correlations: monopole condensation

Spinglass order? How much entanglement/fluctuations remains?

How much disorder can a QSL tolerate?

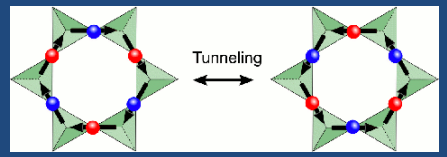
ED for original model is very limited in size

Must study an effective model obtained from perturbation theory



Random ring exchange + Ising model (ED up to N=64)

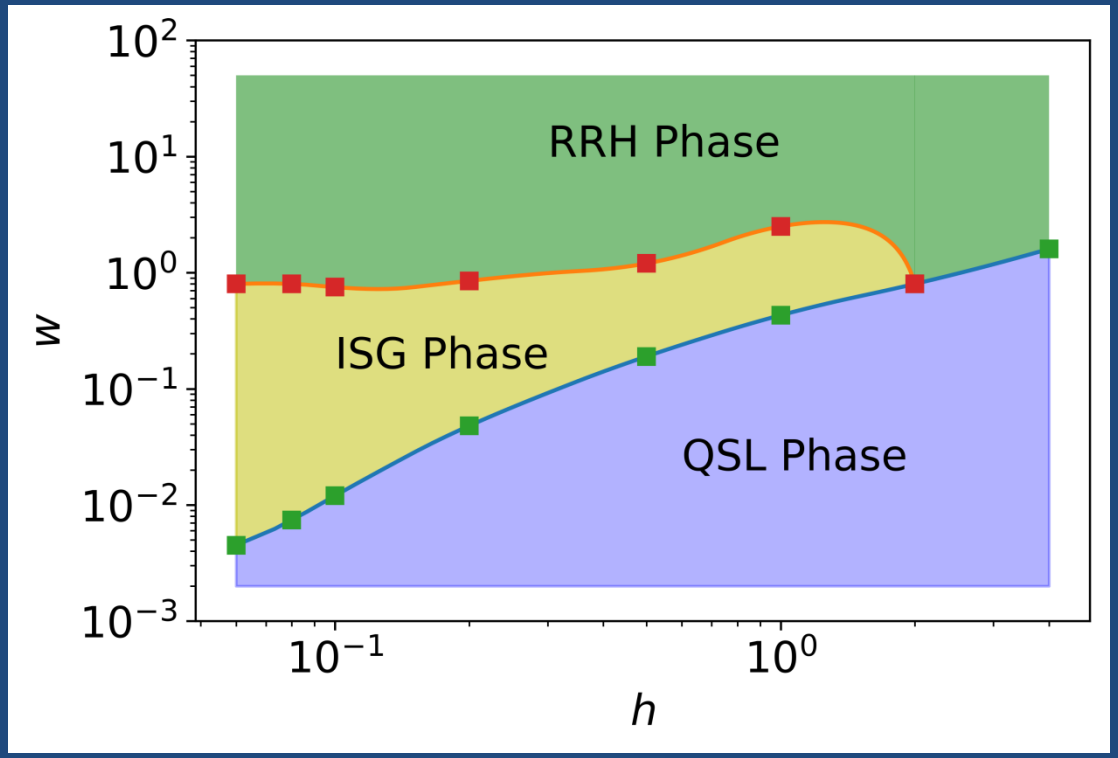
$$\mathcal{H} = \frac{1}{48}\sum_{<i,j>} h_i^2 h_j^2 \sigma_i^z \sigma_j^z - \frac{63}{256}\sum_u K_u(\sigma_1^+\sigma_2^-\sigma_3^+\sigma_4^-\sigma_5^+\sigma_6^- + h.c.)$$



No spinons allowed in the model: restricted to ice subspace

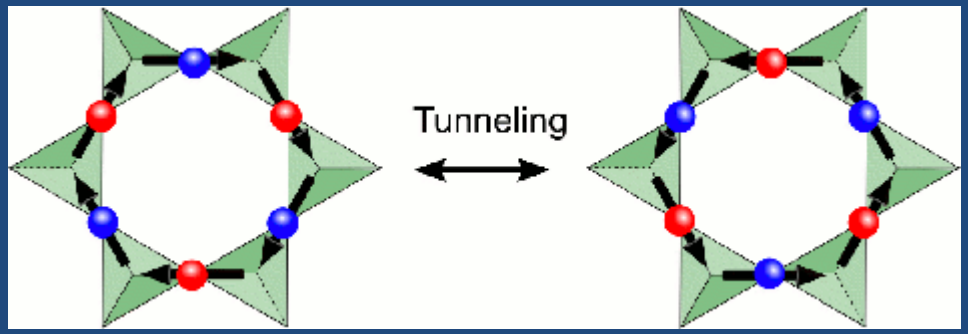
Derived from perturbation theory (Benton)
Couplings depend on h and w : Treat as independent parameters (like t-J model)

Phase Diagram



RRH may be GCQSL of Savary and Balents

Uniform system w=0: Ising couplings do not matter
Same as model studied by Shannon et all: QSL phase

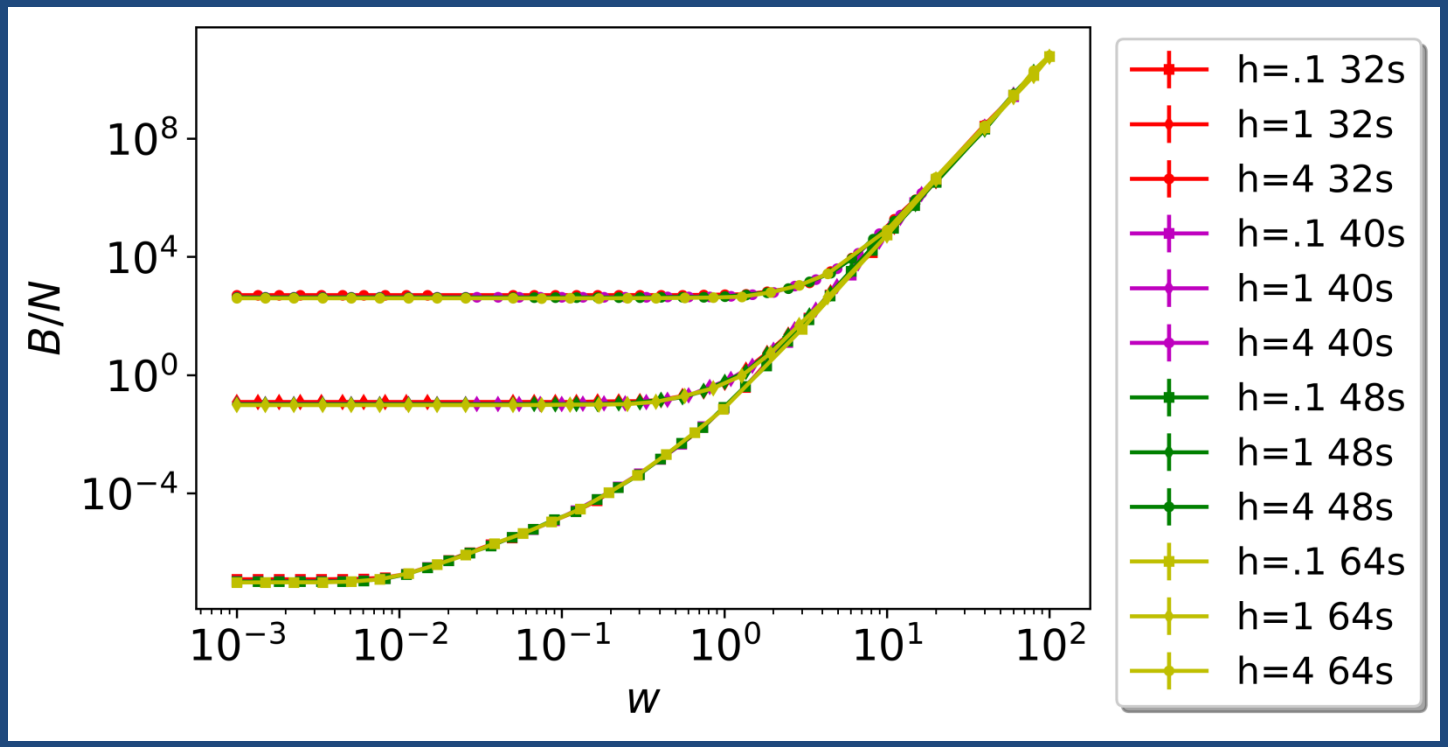


In the effective model, we study sizes:

N = 16, 32, 40, 48, 64 systems with PBC : 2^N vs $(\frac{3}{2})^{\frac{N}{2}}$

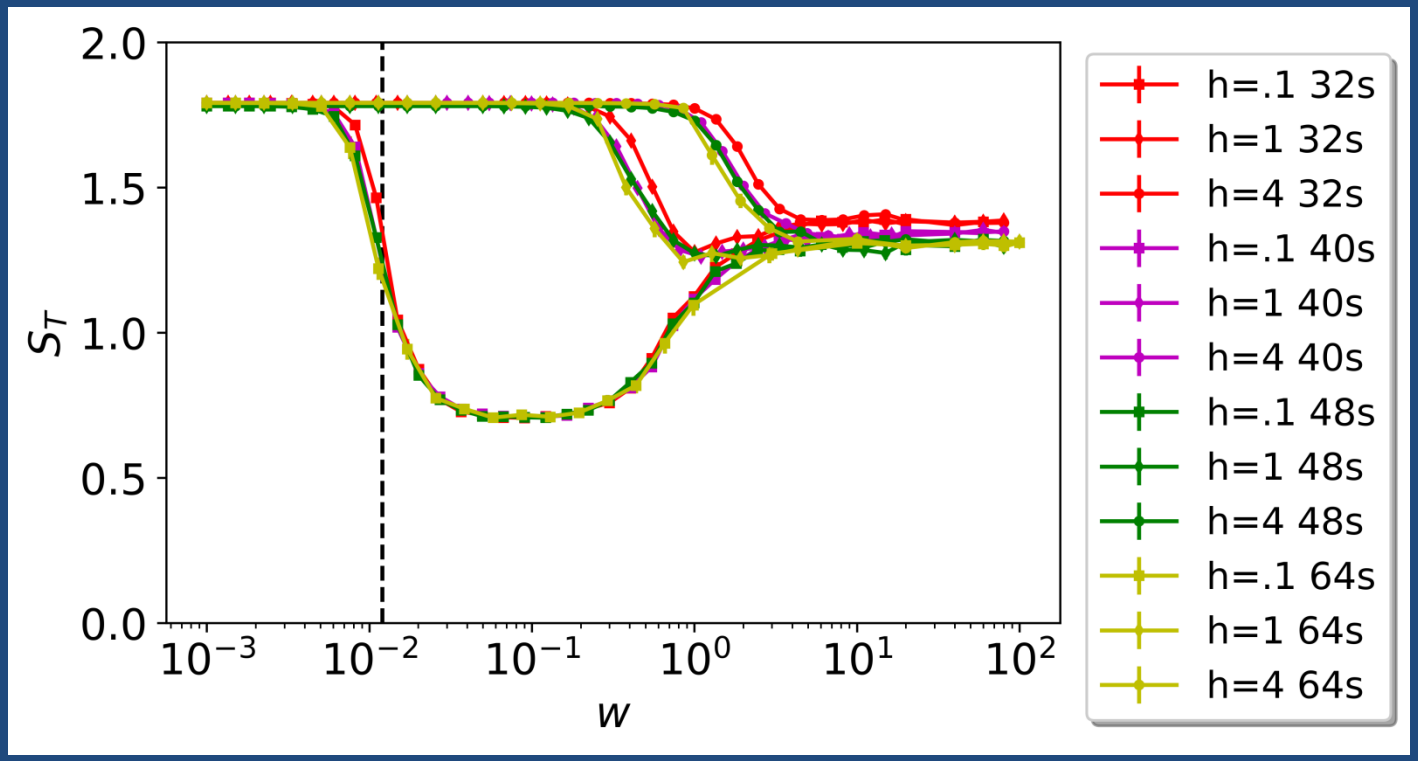
Hilbert space segments into many sectors
Find all the sectors, find ground state in each sector, find global ground state and compute properties

Many-body band-width



h^6 w^2h^2 w^6

Entanglement entropy

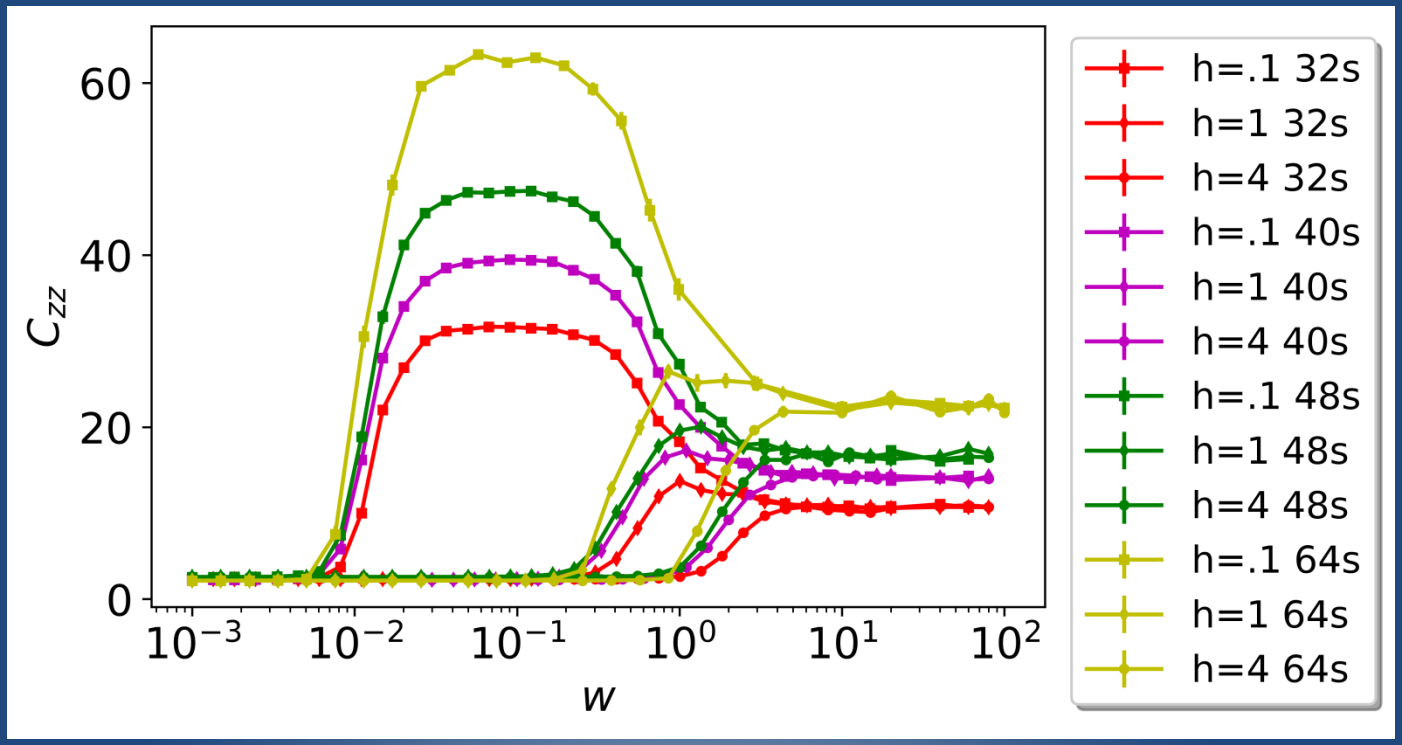


$\ln 6, \quad \ln 2$

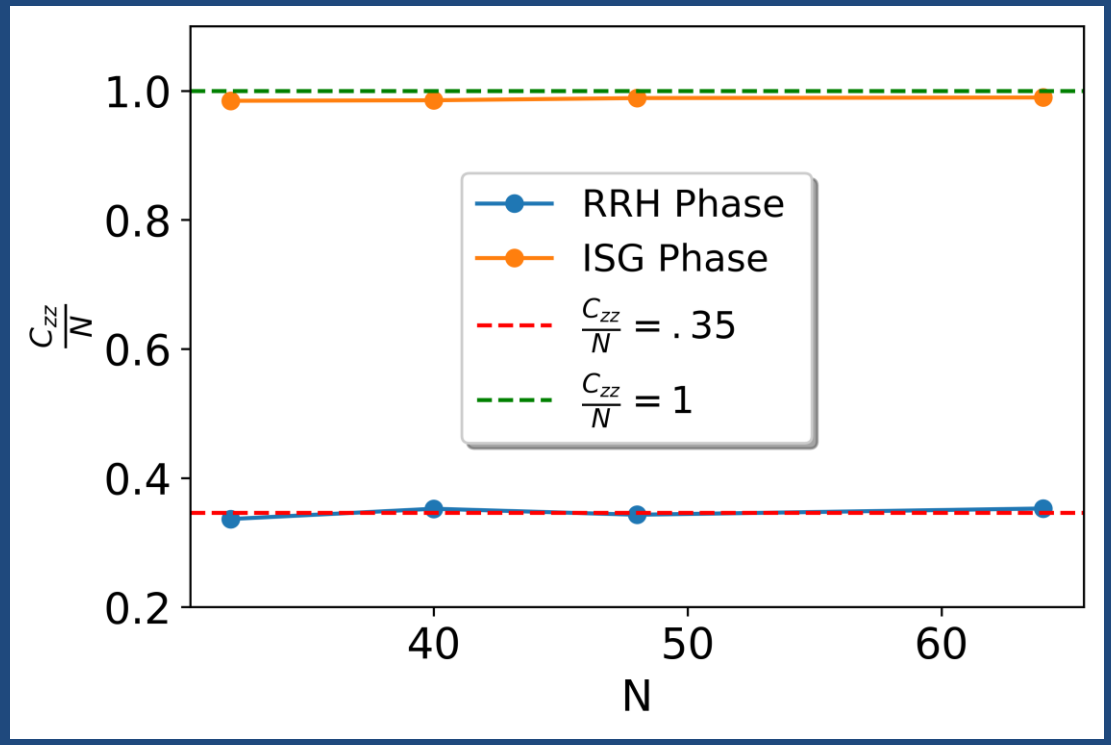
Ising Spinglass Correlation Sum

$$C_{zz} = [\frac{1}{N^2}\sum_{i,j} | < \sigma_i^z \sigma_j^z > |],$$

x N



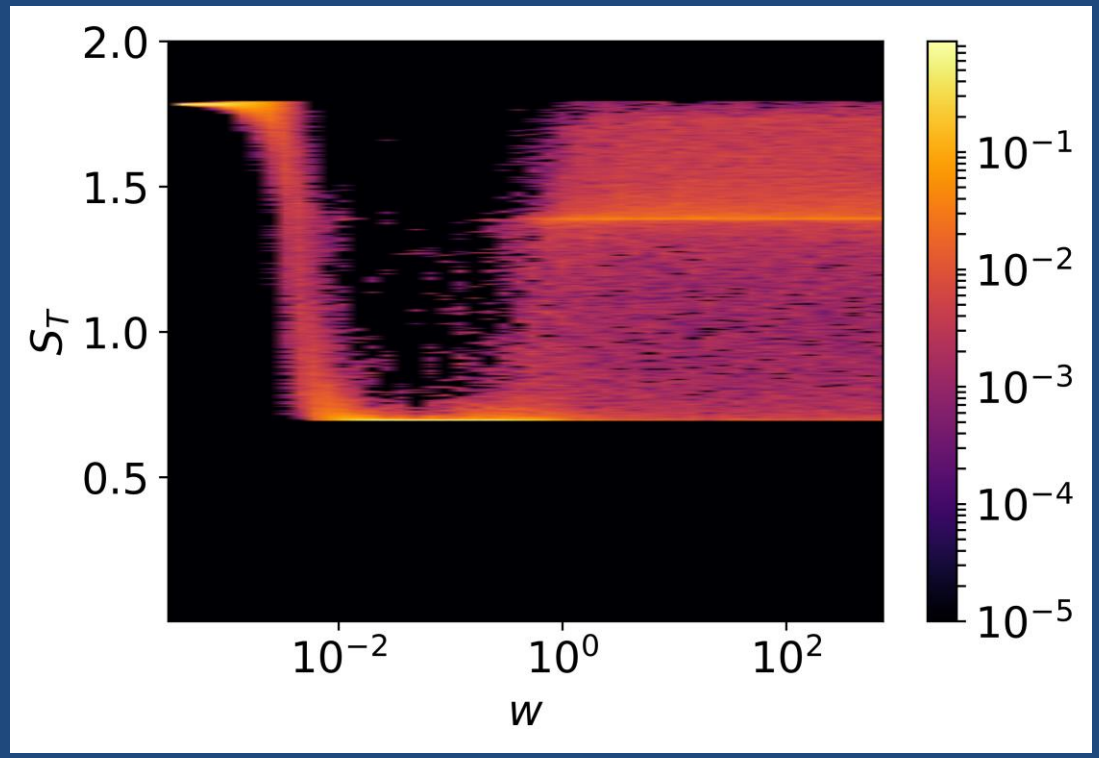
Both phases have long-range Ising spin-glass order



Spinglass order nearly saturates in the Ising spin-glass phase

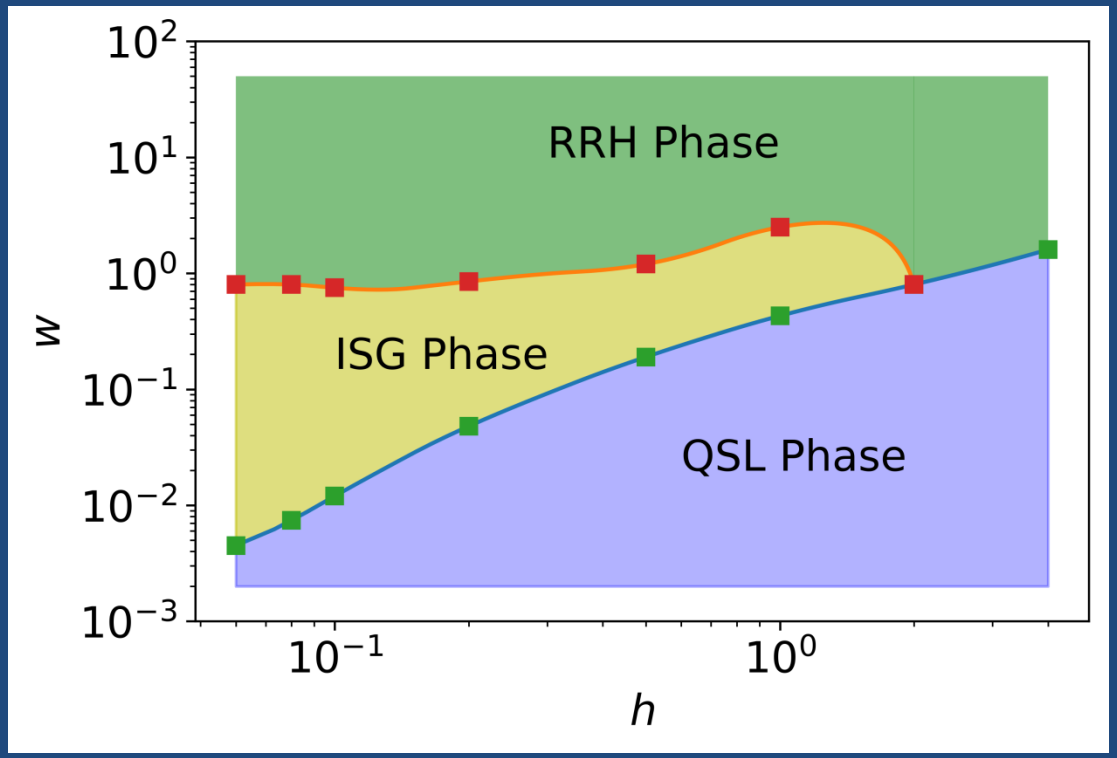
In the RRH phase, we should consider Ising model in transverse-field on the backbone. No Ising order if fields are large.

Distribution of entanglement entropy



Transition regions and RRH phase have a broad distribution

Phase Diagram

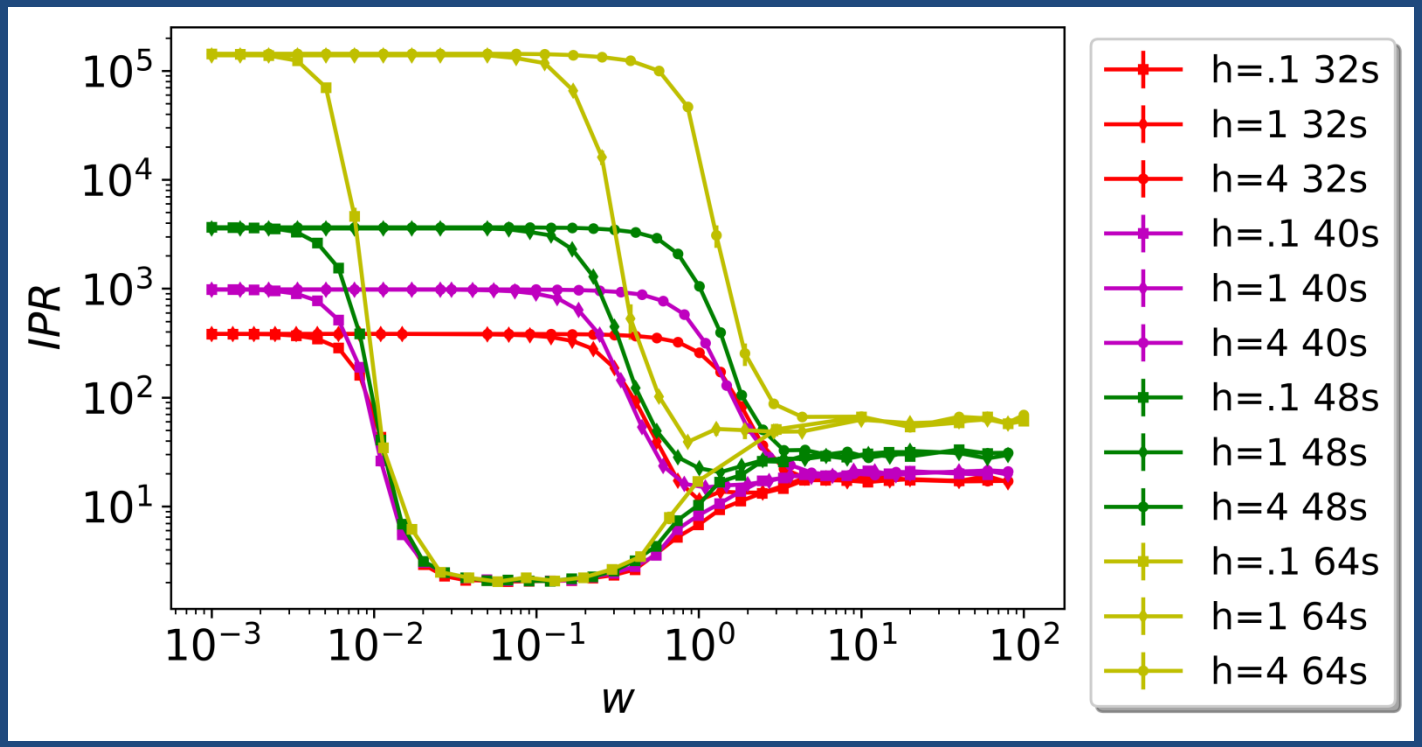


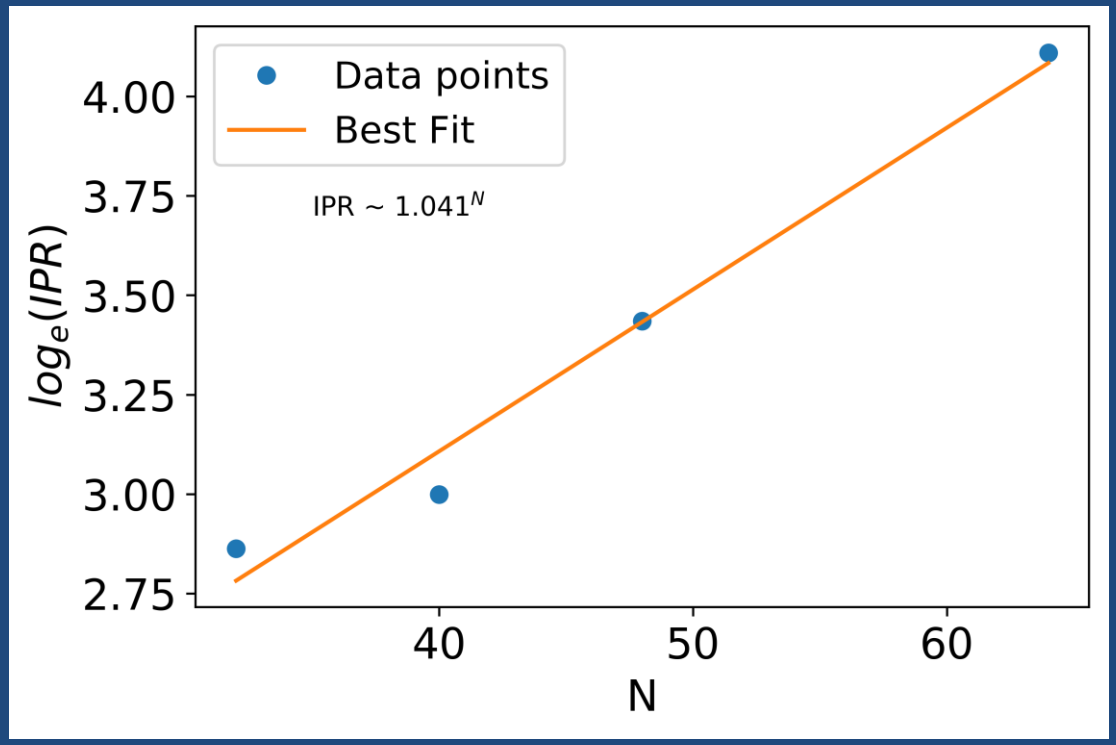
Spin-glass order is further promoted by having a constrained subspace --- reduces thermal fluctuations (Chalker, Sherrington and collaborators)

Random resonating hexagon phase is a variant of random singlet phase

Many-body Inverse Participation Ratio

How many Ising states is the ground state made of?





Participation also grows exponentially with size, though very slowly.
A fluctuating cluster (2 states) every 12-16 spins.

A resonating hexagon constraints another 6 or more spins. Two states per hexagon

Experiments on non-Kramers systems

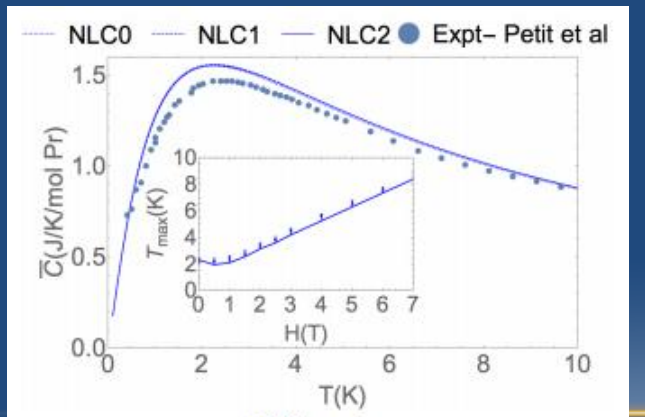
Disordered Route to the Coulomb Quantum Spin Liquid: Random Transverse Fields on Spin Ice in $Pr_2Zr_2O_7$

J.-J. Wen,[1,2,3] S. M. Koohpayeh,[1] K. A. Ross,[1,4] B. A. Trump,[5] T. M. McQueen,[1,5,6] K. Kimura,[7,8] S. Nakatsuji,[7,9] Y. Qiu,[4] D. M. Pajerowski,[4] J. R. D. Copley,[4] and C. L. Broholm[1,4,6]

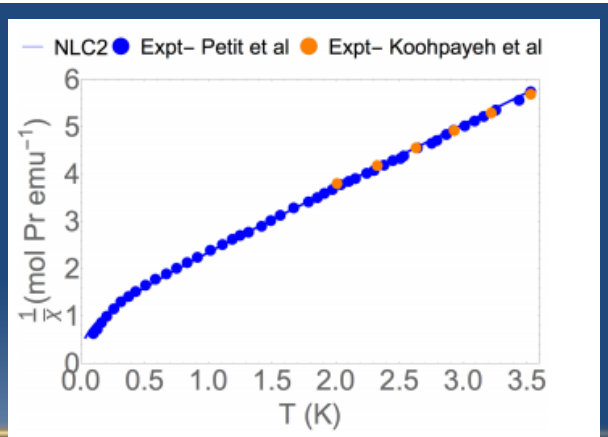
Disorder is an order of magnitude too large.
Good for NLC convergence

Instabilities of a U(1) quantum spin liquid in disordered non-Kramers pyrochlores

Owen Benton[1]



(a) Heat capacity



(b) Inverse susceptibility

No more than pockets of entanglement

Evidence for resonating hexagons?
Can disorder be reduced by material preparation?

How can one have a U(1) QSL in the rare-earth pyrochlores?

Very low disorder large mean h : Or it could turn into a spin-glass

Very dilute site disorder (bond disorder will be disruptive)

Correlated disorder (due to strain)

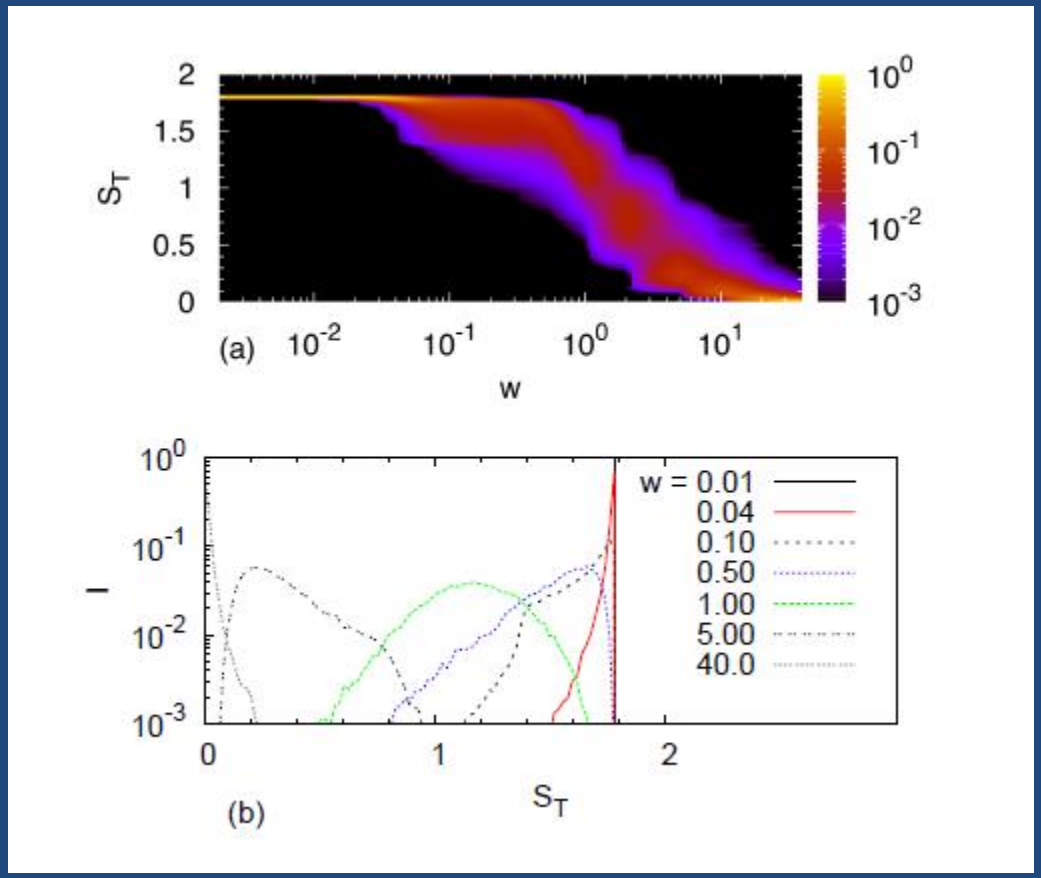
Random direction, uniform magnitude disorder

NON-EQUILIBRIUM DYNAMICS?

SUMMARY AND FUTURE DIRECTIONS

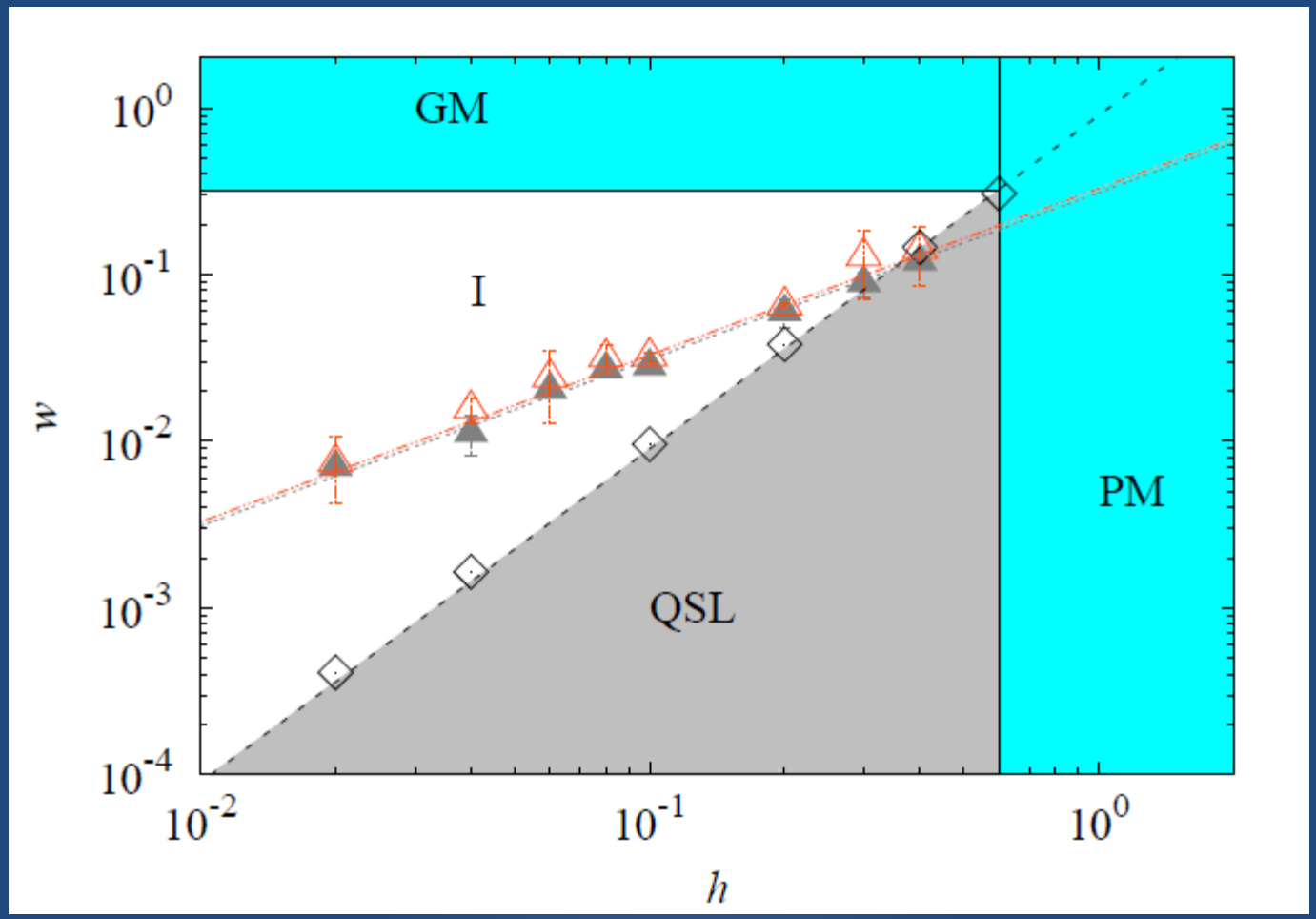
- QSL phases: emergent degrees of freedom
- Random Transverse-Fields added to spin-ice leads to a confined phase with spin-glass order
- Disorder comparable or larger than J can lead to RRH phase
- PrZrO material has too large randomness to be in a QSL phase (RRH? Evidence for resonating clusters?)
- How can a U(1) QSL phase be realized in rare earth pyrochlores?
- Equilibrium and non-equilibrium dynamics would be interesting to study in future

THE END



A distribution of entanglement, persists to very high randomness

Phase Diagram



Is there an MBL phase deep inside GM? (Savary and Balents: Yes)

What is the nature of the Ising phase?