Resonating three colouring wavefunctions for the Kagome antiferromagnet

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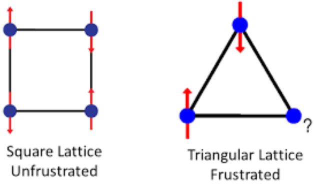
Outline of the Talk

- quick intro to Kagome AFM
- The three colouring (3c) solvable point (H_{XXZ0})
- The problem statement in higher magnetization sectors / 3c solutions for $J_z > -1/2$
- Localized (flat-band) magnon modes ($J_z > 0$)
- Mapping of magnons to three colourings
- Resolves the problem AND adiabaticity in these high mag sectors
- DMRG evidence for adiabaticity in zero mag sector
- Colouring perspective on bipartite *XXZ*

Introduction

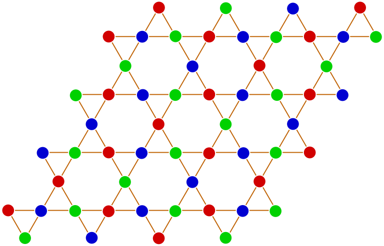
- Classic Issue of frustrated Heisenberg magnets



- Triangle motifs: Triangular, Kagome, etc. (2d)
- Kagome lattice - Herbertsmithite ($ZnCu_3(OH)_6Cl_2$)
- No magnetic order till 50 mK ($\theta_{CW} \sim O(100K)$)
- Candidate for a Quantum Spin Liquid (QSL)
- Z_2 QSL, $U(1)$ QSL proposals have gotten attention..
- Ordered states also, e.g. Ralko et al PRB (2018)
- Which QSL? : NOT Focus of this talk
- Broader perspective: the XXZ phase diagram (See Essafi et al, Nature Comm (2016) and precursors)

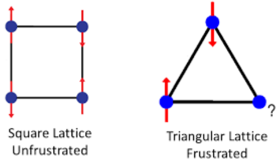
The three colouring solvable point

- Recently, a new colouring perspective on Kagome AFM: Changlani et al, PRL (2018)
- $H_{XXZ0} = \sum_{\langle i,j\rangle \in \text{Kagome}} \left(S_i^x S_j^x + S_i^y S_j^y - \frac{1}{2} S_i^z S_j^z \right)$
- Exact solutions representable as three colourings
- For Triangular lattice by Momoi & Suzuki in 1994

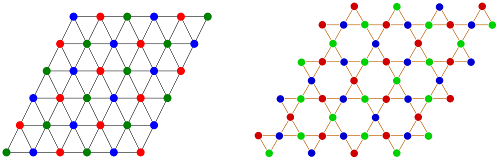


- RGB $\rightarrow$ 120° states in XY plane of Bloch sphere
- e.g. $|\bullet\rangle = |\uparrow\rangle + |\downarrow\rangle$, $|\bullet\rangle = |\uparrow\rangle + \omega|\downarrow\rangle$, $|\bullet\rangle = |\uparrow\rangle + \omega^2|\downarrow\rangle$,

Three Colouring POV on frustration



now goes to



- only finite 3c's on triangle ... essentially, 120° order
- Exponentially many 3c's on Kagome...
- IMP *XXZ*0 holds together the Kagome phase diagram

Details of the three colouring solution

- On a single $\triangle$, H_{XXZ0} ground state manifold is fully polarized — $|\uparrow\uparrow\uparrow\rangle$
  chiral state 1 — $|\downarrow\uparrow\uparrow\rangle + \omega|\uparrow\downarrow\uparrow\rangle + \omega^2|\uparrow\uparrow\downarrow\rangle$
  chiral state 2 — $|\downarrow\uparrow\uparrow\rangle + \omega^2|\uparrow\downarrow\uparrow\rangle + \omega|\uparrow\uparrow\downarrow\rangle$
  & $\uparrow\rightarrow\downarrow$ above (6 states in total)
- $\implies$ Full Kagome $H_{XXZ0} \propto \sum_\triangle P_\triangle$ where $P_\triangle = |+\rangle\langle+| + |-\rangle\langle-|$
- $|+\rangle = |\downarrow\uparrow\uparrow\rangle + |\uparrow\downarrow\uparrow\rangle + |\uparrow\uparrow\downarrow\rangle$,
  $|-\rangle = |\uparrow\downarrow\downarrow\rangle + |\downarrow\uparrow\downarrow\rangle + |\downarrow\downarrow\uparrow\rangle$ achiral states
- $P_\triangle$ are non-commuting
- Any $|3c\rangle$ is manifestly a ground state (e.g. $|\bullet\bullet\bullet\rangle$ on a $\triangle$)
- XXZ has total Sz conserved, $\therefore |GS\rangle = P_{Sz}|3c\rangle$
- Exponentially degenerate GS manifold in each Sz sector at $XXZ0$ point .. NOT CLEAR which state gets selected towards $J_z = 1$

Our Problem Statement

- 3c solns away from $XXZ0$, on whole $J_z > -\frac{1}{2}$ segment in high magnetization sectors..

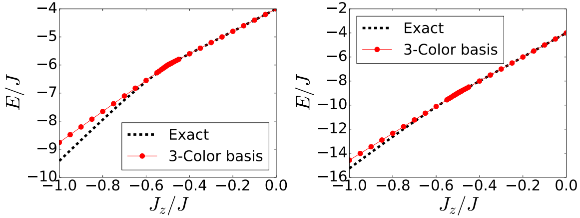
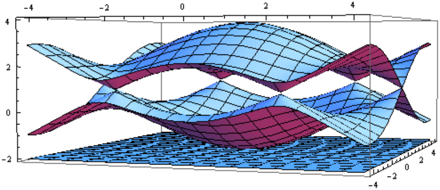


Figure: LEFT: $L = 4 \times 2 \times 3$ narrow cylinder (total $Sz = 8$ or $1/6$ boson filling)
RIGHT: 36-site cluster (total $Sz = 14$ or $1/9$ boson filling)

- In 3c diagonalization, 3c mat elems need to be evaluated efficiently .. Changlani et al, PRL supp
- What are these 3c states?? .. Ans: Resonating 3c's

Localized magnons ($J_z > 0$) 1

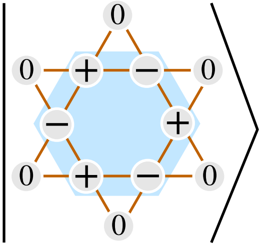
- For $J_z > 0$, Schulenberg et al PRL (2002), Zhitormitsky-Tsunetsugu PRB (2004), Bergmann et al PRB (2008)
- $J_z > 0$ is repulsive interactions for bosons ($H_{XXZ} = \frac{1}{2}\sum_{\langle i,j\rangle} b_i^\dagger b_j + h.c. + J_z n_i n_j$)
- At single particle level..



- Lowest states are flat band states
- One extra state from the second band

Localized magnons ($J_z > 0$) 2

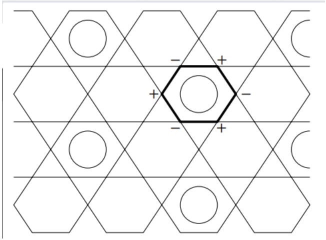
- Can be understood as localized magnons



- $\pm$ amplitudes give destructive interference
- leads to localizing the boson/$\downarrow$
- Only $N - 1$ hexagons linearly independent
- Actual counting N flatband states $+$ 1 from second band
- Extra two states ... "topological" magnons

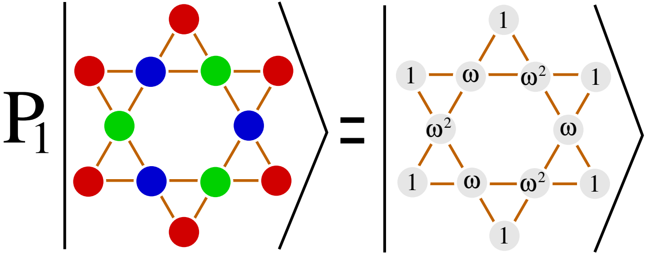
Close-packing of Localized magnons

- To get the many-body ground state, closely-pack these localized magnons!
- The 0 amplitude sites avoid any $J_z > 0$ repulsion costs
- Thus, simultaneously minimizes XY and J_z pieces
- This gives the required filling ...
  e.g. 1/9 on Kagome lattice (and finite clusters that accomodate the associated root 3 pattern)



Mapping from magnons to three colourings

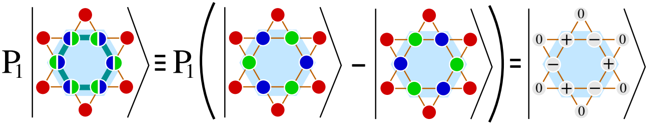
- Previous $J_z > 0$ or repulsive bosons
- How to go to $J_z > -1/2$ or attractive bosons
- Quite clearly magnons are playing a role
- Thus, find a mapping btn. 3c's and magnons
- NOW projection (P_{S_z}) becomes crucial...
- Step 1



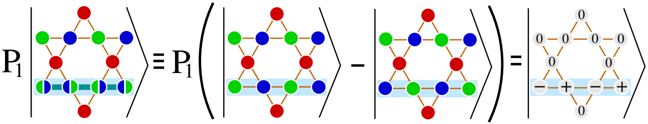
Recall $|\bullet\rangle = |\uparrow\rangle + |\downarrow\rangle$, $|\bullet\rangle = |\uparrow\rangle + \omega|\downarrow\rangle$,
$|\bullet\rangle = |\uparrow\rangle + \omega^2|\downarrow\rangle$

Mapping from magnons to three colourings

- Step 2 ... Resonate on a 2c loop (RCL)

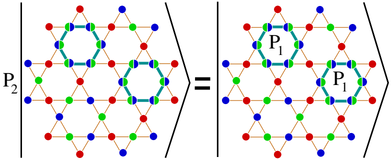


- Also above P_0 gives ZERO, ie. $P_0(|3c_1\rangle - |3c_2\rangle) = 0$
- Mapping to **1** particle magnons DONE, including topo magnons

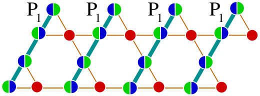


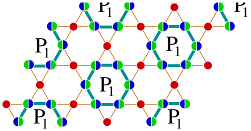
Mapping from magnons to three colourings

- Step 3 ... Localize bosons



- Projection forces to put 1 boson on each RCL
- Closely pack the RCLs to get the desired filling





- Finally why $J_z > -1/2$??
- Decompose H as $H_{XXZ0} + \left(J_z + \frac{1}{2}\right) n_i n_j$
- NOW the 0 amplitude sites avoid $\left(J_z + \frac{1}{2}\right) n_i n_j$ repulsive costs ... simulatenous minimization DONE

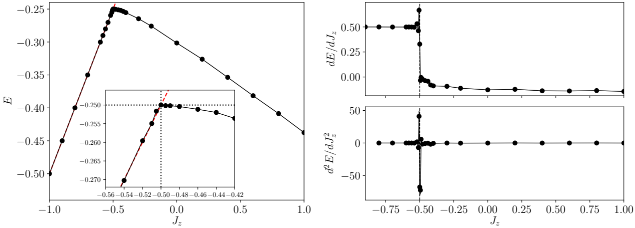
Adiabaticity to $XXZ0$

- For these high magnetization sectors, Ising $\leftrightarrow$ Heisenberg $\leftrightarrow$ XY $\leftrightarrow$ $XXZ0$
- Zero mag sector, NOT clear how to apply 3c's yet
- Above adiabaticity evidence exists!
- He & Chen, PRL (2015) .. using DMRG for XY $\leftrightarrow$ *Heisenberg* $\leftrightarrow$ *Ising*
- Changlani et al, PRL (2018) ... ED data on 36 sites $XXZ0$ $\leftrightarrow$ XY $\leftrightarrow$ *Heisenberg* (realistically, upto $J_z = -0.4$)
- Highly suggestive of state stabilizing near $XXZ0$ IMP to Kagome physics
- Doing this pert theory HARD ... (Exp. colorings) ...suspect further insights to be learned
- Similar adiabaticity from $XXZ0$ to 120° on triangle

Adiabaticity to $XXZ0$

DMRG data in absence of analytics ($O(150)$ sites)

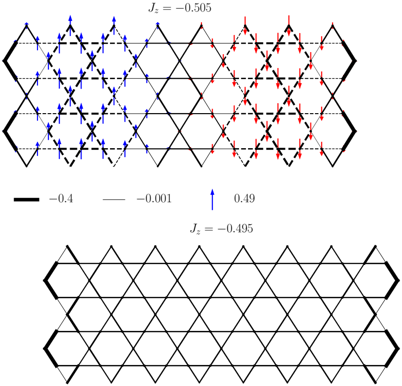
- Track energy vs. J_z



- NO HINT of any other discontinuity
- strengthens indications from Changlani et al, PRL.

Adiabaticity to $XXZ0$

- Below $J_z < -1/2$, polarized FM state (provable)



- Converging DMRG challenging near $J_z = -0.5$
- FM, start with two domains
- AFM, multiple initial states to get to lowest energies...

Are colourings vis-à-vis triangles special?

- Main Message till now: $XXZ0 + \delta J_z$ IMP to Kagome
- How to exploit this insight?

Recent work with H. Changlani

- More generally, are triangles and 3c's any special?
- 4c's and (non-XXZ) parent Hamiltonian written down..
- Recall $XXZ0$ sits at QCP between FM and non-FM
- Same true for classical Heisenberg model via Luttinger-Tisza analysis
- For bipartite XXZ, Luttinger-Tisza rather gives $J_z = -1$ between FM and AFM
- And indeed, it is an exactly solvable QCP as well!
- Second message: Exact solvability at FM/AFM for XXZ magnets more general

Details of bipartite XXZ solution

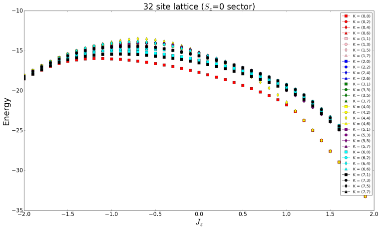
- $H_{XXZ1} = \sum_{\langle i,j\rangle \in \text{bipartite}} \left(S_i^x S_j^x + S_i^y S_j^y - 1 S_i^z S_j^z \right)$
- Solution is a "two-colouring" now
- $|2c\rangle = P_{S_z} \left(\prod_{i \in \mathbf{A}} \otimes |\bullet\rangle \prod_{j \in \mathbf{B}} \otimes |\bullet\rangle \right)$ (Néel state in XY plane)
- Unique solution due to bipartiteness in each S_z sector
- Choose $|\bullet\rangle = |\uparrow\rangle + |\downarrow\rangle$, $|\bullet\rangle = |\uparrow\rangle - |\downarrow\rangle$
- Solution proof again similar starting with a bond instead of $\triangle$
- Exact correlators using 2c version of 3c mat elem formulas computable thanks to finite solutions

(L_x, L_y) PBC/OBC	$\frac{E_{\lvert C\rangle}}{\text{\#-bonds}}$	$\frac{E_{ED}}{\text{\#-bonds}}$	$\#_{\lvert C\rangle}$ $(L_x L_y + 1)$	$\#_{ED}$	$\langle \hat{\mathbf{S}}_i^z \hat{\mathbf{S}}_j^z \rangle_{\lvert C\rangle}$ $(-\frac{1}{4}\frac{1}{L_x L_y - 1})$	$\langle \hat{\mathbf{S}}_i^z \hat{\mathbf{S}}_j^z \rangle_{ED}$	$\epsilon_{ij} \langle \hat{\mathbf{S}}_i^x \hat{\mathbf{S}}_j^x \rangle_{\lvert C\rangle}$ $(\frac{1}{8}\frac{L_x L_y}{L_x L_y - 1})$	$\epsilon_{ij} \langle \hat{\mathbf{S}}_i^x \hat{\mathbf{S}}_j^x \rangle_{ED}$
(2,2)/(4,1)	-0.25	-0.2500000...	5	5	-1/12	-0.0833333...	1/6	0.166666...
(4,2)	-0.25	-0.2500000...	9	9	-1/28	-0.0357143...	1/7	0.142857...
(6,2)	-0.25	-0.2500000...	13	13	-1/44	-0.0227273...	3/22	0.136364...
(4,4)	-0.25	-0.2500000...	17	—				
(6,6)	-0.25	-0.2500000...	37	—				

- sums of powers of cosines, Ramanujan J, J. Integer sequences

Adiabaticity to $XXZ1$

- Adiabaticity studies on...



- Contrast with Kagome adiabaticity
- Another contrast: hidden "SU(2) symmetry"
  H_{XXZ1} has GS: $\{|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle, -|\downarrow\downarrow\rangle\}$ w/h $E = 0$ and ES: $|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle$ w/h $E = 1$
  H_{XXX} has GS: $|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$ w/h $E = 0$ and ES: $\{|\uparrow\uparrow\rangle, |\downarrow\downarrow\rangle, |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\}$ w/h $E = 1$
- Thus, UV/IR duality at operator level
- For wavefunctions, get a -1 phase for $|\downarrow\rangle_B$

Conclusion

- Details in arXiv:1808.08633
- RCLs as exact solutions in high mag sectors for $J_z > -1/2$
- Applicability in zero mag sector?
- 3c's may provide useful variational ansatz (eg Capponi et al PRB (2013)) similar to RVBs
- Adiabaticity to $XXZ0$ in high AND zero mag sectors
- Exactly solvable critical point between AFM and FM XXZ bipartite magnets (with Changlani, manuscript in prep)
- Adiabaticity to $XXZ1$ in bipartite? SEEMS SO. Similar to triangular lattice
- General statement: Physics of Heisenberg XXX emerge from $XXZ0/1$ points
- However, Resonances/RCL special to Kagome

Open Issues

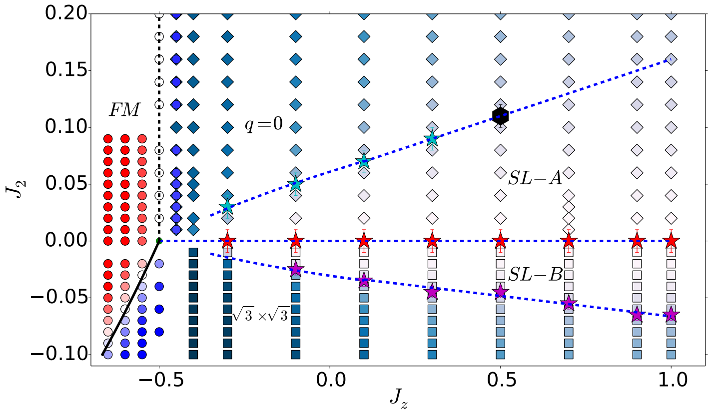
Some Open issues:

- Pert theory near $XXZ0$
- Few particles on top of closely-packed RCLs ?
- Can increasing density melt close-packing of RCLs?
- 3c map of non-flat band states? (technical)
- How to write highly entangled states as 3c wavefunctions?
  (Note: we can write down ordered states as 3/2c's)

Acknowledgements

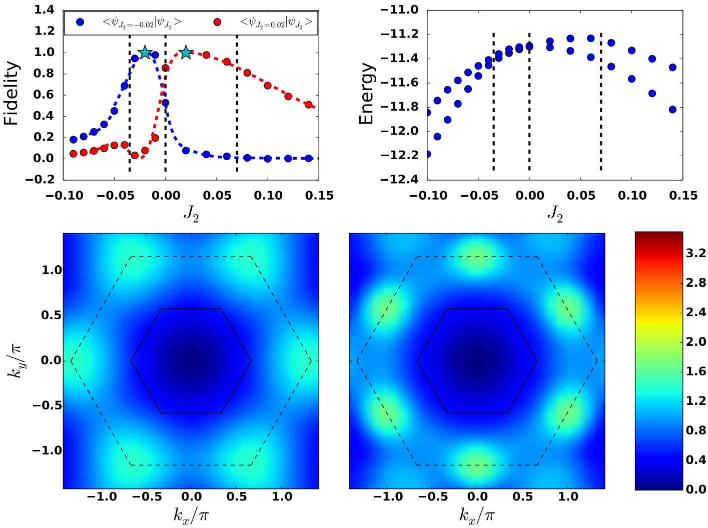
- Thank you!
- IRCC, IIT Bombay for support

Extra slides 1



from Changlani PRL (2018)

Extra slides 2



from Changlani PRL (2018)