A sign-problem-free effective model of triangular lattice antiferromagnetism

Henry Shackleton November 4, 2022

Harvard University



Outline of talk

- Geeral discussion of quantum antiferromagnets and sign problems
- \bullet Derivation of effective model bosonic spinons coupled to $\textit{odd}\ \mathbb{Z}_2$ gauge field
- Sign-problem-free mapping generalized particle/vortex dualities

 $H = \sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$, trivial phase for half-integer spin precluded by LSM theorem

 $H = \sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$, trivial phase for half-integer spin precluded by LSM theorem



 $H = \sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$, trivial phase for half-integer spin precluded by LSM theorem





 $H = \sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$, trivial phase for half-integer spin precluded by LSM theorem





Numerics generally restricted to small system sizes, resolution of ordered phases difficult

"Wavefunction-based" numerics (MPS, PEPS, ED...)

"Wavefunction-based" numerics (MPS, PEPS, ED...)

- Minimize energy of trial $|\psi_0
 angle$
- Generic ansatzes, can be tried on any Hamiltonian
- Generally restricted to small system sizes
- Certain ground states may fall outside the range of applicability of an ansatz

"Wavefunction-based" numerics (MPS, PEPS, ED...)

- Minimize energy of trial $|\psi_0\rangle$
- Generic ansatzes, can be tried on any Hamiltonian
- Generally restricted to small system sizes
- Certain ground states may fall outside the range of applicability of an ansatz

"Partition function-based" numerics (PIMC, DQMC, SSE...)

"Wavefunction-based" numerics (MPS, PEPS, ED...)

- Minimize energy of trial $|\psi_0
 angle$
- Generic ansatzes, can be tried on any Hamiltonian
- Generally restricted to small system sizes
- Certain ground states may fall outside the range of applicability of an ansatz

"Partition function-based" numerics (PIMC, DQMC, SSE...)

- Direct evaluation of tr $\left[e^{-\beta H}\right]$
- Stochastic methods allow for much larger system sizes
- "Sign problem" prevents generic applicability
- Can cure sign problem through clever mappings, designer Hamiltonians, etc

Bosonic spinon description captures orderd phases



Sachdev 1992.

Mean-field spinon solution supports gapped vison excitations



Spinon condensation \rightarrow magnetic order

Sachdev 1992; Huh, Punk, and Sachdev 2011.

Mean-field spinon solution supports gapped vison excitations



Vison condensation \rightarrow VBS order

Sachdev 1992; Huh, Punk, and Sachdev 2011.

Effective model of triangular lattice antiferromagnetism

$$egin{aligned} \mathcal{Z} &= \sum_{s_{j,j+\widehat{\mu}}=\pm 1} \prod_{j,lpha} \int \mathrm{d} z_{jlpha} \, \delta \left(\sum_{lpha=1,2} \left| z_{jlpha}^2
ight| - 1
ight) \ & imes \left[\prod_j s_{j,j+ au}
ight] \exp \left(- \mathcal{H}[z_lpha,s]
ight) \ &\mathcal{H}[z_lpha,s] &= -rac{J}{2} \sum_{\langle j,\mu
angle} s_{j,j+\widehat{\mu}} \left(z_{j,lpha}^* z_{j+\widehat{\mu},lpha} + \ \mathrm{c.c}
ight) \ &- \mathcal{K} \sum_{egin{aligned} \sum_{egin{aligned} \sum_{\Delta \Box}} s_{j,j+\widehat{\mu}} \ &. \end{array} \end{aligned}$$



Jian et al. 2018.

Effective model of triangular lattice antiferromagnetism

$$\begin{aligned} \mathcal{Z} &= \sum_{s_{j,j+\widehat{\mu}} = \pm 1} \prod_{j,\alpha} \int \mathrm{d}z_{j\alpha} \,\delta \left(\sum_{\alpha=1,2} |z_{j\alpha}^2| - 1 \right) \\ &\times \left[\prod_j s_{j,j+\tau} \right] \exp\left(-H[z_{\alpha},s]\right) \\ H[z_{\alpha},s] &= -\frac{J}{2} \sum_{\langle j,\mu \rangle} s_{j,j+\widehat{\mu}} \left(z_{j,\alpha}^* z_{j+\widehat{\mu},\alpha} + \text{ c.c} \right) \\ &- \mathcal{K} \sum_{\Delta \Box} \prod_{\Delta \Box} s_{j,j+\widehat{\mu}} . \end{aligned}$$

Jian et al. 2018.

Effective model of triangular lattice antiferromagnetism

$$\begin{split} \mathcal{Z} &= \sum_{s_{j,j+\widehat{\mu}} = \pm 1} \prod_{j,\alpha} \int \mathrm{d} z_{j\alpha} \, \delta \left(\sum_{\alpha = 1,2} \left| z_{j\alpha}^2 \right| - 1 \right) \\ &\times \left[\prod_j s_{j,j+\tau} \right] \exp\left(-H[z_\alpha,s] \right) \\ H[z_\alpha,s] &= -\frac{J}{2} \sum_{\langle j,\mu \rangle} s_{j,j+\widehat{\mu}} \left(z_{j,\alpha}^* z_{j+\widehat{\mu},\alpha} + \ \mathrm{c.c} \right) \\ &- \mathcal{K} \sum_{\Delta \Box} \prod_{\Delta \Box} s_{j,j+\widehat{\mu}} \, . \end{split}$$

Jian et al. 2018.



$$\mathcal{Z} = \prod_{i} \int_{0}^{2\pi} rac{\mathrm{d} heta_{i}}{2\pi} \exp\left[-H
ight] \quad , \quad H = -rac{J}{\pi} \sum_{\langle ij
angle} \cos(heta_{i} - heta_{j}) = -rac{J}{\pi} \sum_{i\mu} \cos\left(\Delta_{\mu} heta_{i}
ight)$$

$$\mathcal{Z} = \prod_i \int_0^{2\pi} rac{\mathrm{d} heta_i}{2\pi} \exp\left[-H
ight] \quad, \quad H = -rac{J}{\pi} \sum_{\langle ij
angle} \cos(heta_i - heta_j) = -rac{J}{\pi} \sum_{i\mu} \cos\left(\Delta_\mu heta_i
ight)$$

Using the Villain representation,

$$e^{-J(1-\cos(heta))/\pi} pprox \sum_{n=-\infty}^{\infty} e^{-J(heta-2\pi n)^2/(2\pi)},$$

$$\mathcal{Z} = \prod_{i} \int_{0}^{2\pi} rac{\mathrm{d} heta_{i}}{2\pi} \exp\left[-H
ight] \quad, \quad H = -rac{J}{\pi} \sum_{\langle ij
angle} \cos(heta_{i} - heta_{j}) = -rac{J}{\pi} \sum_{i\mu} \cos\left(\Delta_{\mu} heta_{i}
ight)$$

Using the Villain representation,

$$e^{-J(1-\cos(heta))/\pi} pprox \sum_{n=-\infty}^{\infty} e^{-J(heta-2\pi n)^2/(2\pi)},$$

and

$$\sum_{m=-\infty}^{\infty} e^{-J(\theta-2\pi n)^2/(2\pi)} = \frac{1}{\sqrt{2J}} \sum_{p=-\infty}^{\infty} e^{i\pi p^2/(2J)-ip\theta} \,,$$

we get

$$\mathcal{Z} = \sum_{p_{i\mu}} \prod_{i} \int_{0}^{2\pi} \frac{\mathrm{d}\theta_{i}}{2\pi} e^{-H} \quad , \quad H = \frac{\pi}{2J} \sum_{i,\mu} p_{i\mu}^{2} + i p_{i\mu} \Delta_{\mu} \theta_{i}$$

Integrating out θ_i enforces $\Delta_{\mu} p_{i\mu} = 0$. $p_{i\mu}$ must form *closed current loops*. Can be enforced by taking $p_{i\mu} = \epsilon_{\mu\nu\lambda} \Delta_{\nu} h_{\bar{i}\lambda}$



$$\mathcal{Z} = \sum_{s_{ij}=\pm 1} \prod_{i} \int_{0}^{2\pi} \frac{\mathrm{d} heta_{i}}{2\pi} \exp\left[-H
ight] \quad , \quad H = -\frac{J}{\pi} \sum_{i\mu} s_{i,i+\mu} \cos\left(\Delta_{\mu} heta_{i}
ight) + K \sum_{\Box} \prod_{\Box} s_{ij}$$

Carefully following s_{ij} through Villain representation gives mutual Chern-Simons coupling between $h_{\bar{i},\mu}$ and s_{ij} ,

$$i\pi\epsilon_{\mu\nu\lambda}\Delta_{\nu}h_{\overline{i},\lambda}rac{1-s_{i,i+\mu}}{2}=i\pi h_{\overline{i},\mu}rac{1-\prod_{\Box}s_{i,i+\mu}}{2}$$

Claim: integration over s_{ij} can be accomplished by independently summing over possible plaquette values $\prod_{\Box} s_{ij} \equiv \Phi_{\bar{i}\mu} = \pm 1$.

Claim: integration over s_{ij} can be accomplished by independently summing over possible plaquette values $\prod_{\Box} s_{ij} \equiv \Phi_{\bar{i}\mu} = \pm 1$. This is not true generally! Fluxes are not independent - product of $\Phi_{\bar{i}\mu}$ over any closed surface must be 1. Alternatively, $\Delta_{\mu} \Phi_{\bar{i}\mu} = 0 \mod 4$.



Claim: integration over s_{ij} can be accomplished by independently summing over possible plaquette values $\prod_{\Box} s_{ij} \equiv \Phi_{\bar{i}\mu} = \pm 1$. This is not true generally! Fluxes are not independent - product of $\Phi_{\bar{i}\mu}$ over any closed surface must be 1. Alternatively, $\Delta_{\mu}\Phi_{\bar{i}\mu} = 0 \mod 4$.

This constraint

is enforced *dynamically* by the redundant degrees of freedom present in the height field representation

$$h_{\bar{i}\mu} \to h_{\bar{i}\mu} + \Delta_{\mu} f_{\bar{i}}$$
$$\exp\left[i\pi\Delta_{\mu} f_{\bar{i}} \frac{1 - \Phi_{\bar{i}\mu}}{2}\right] = \exp\left[-i\frac{\pi}{2} f_{\bar{i}}\Delta_{\mu} \Phi_{\bar{i}\mu}\right]$$



Claim: integration over s_{ij} can be accomplished by independently summing over possible plaquette values $\prod_{\Box} s_{ij} \equiv \Phi_{\bar{i}\mu} = \pm 1$. This is not true generally! Fluxes are not independent - product of $\Phi_{\bar{i}\mu}$ over any closed surface must be 1. Alternatively, $\Delta_{\mu}\Phi_{\bar{i}\mu} = 0 \mod 4$.

This constraint

is enforced *dynamically* by the redundant degrees of freedom present in the height field representation

$$\begin{split} h_{\bar{i}\mu} &\to h_{\bar{i}\mu} + \Delta_{\mu} f_{\bar{i}} \\ \exp\left[i\pi\Delta_{\mu} f_{\bar{i}} \frac{1 - \Phi_{\bar{i}\mu}}{2}\right] = \exp\left[-i\frac{\pi}{2} f_{\bar{i}}\Delta_{\mu} \Phi_{\bar{i}\mu}\right] \end{split}$$



Because of this, we are allowed to independently integrate over $\Phi_{\overline{i}\mu} = \pm 1$.

$$\begin{split} \mathcal{Z} &= \sum_{h=-\infty}^{\infty} \exp\left[-H\right] \\ H &= \frac{\pi}{2J} \sum_{i,\mu} \left(\epsilon_{\mu\nu\lambda} \Delta_{\nu} h_{\bar{i},\lambda}\right)^2 + \mathcal{K}_d \sum_{i,\mu} \sigma_{i,i+\mu} \\ \sigma_{\bar{i},\bar{i}+\mu} &\equiv \left(2h_{\bar{i},\mu} - 1\right) \mod 2 \\ \tanh \mathcal{K}_d &\equiv e^{-2\mathcal{K}} \end{split}$$

 $J \rightarrow 0$ limit recovers 3D Ising model - dual to even \mathbb{Z}_2 gauge theory.

Accomodation of Berry phase

Berry phase introduces an extra phase factor, $H \to H - i\pi \sum_j \frac{1-s_{j,j+\tau}}{2}$.

Park and Sachdev 2002.

Accomodation of Berry phase

Berry phase introduces an extra phase factor, $H \rightarrow H - i\pi \sum_{j} \frac{1-s_{j,j+\tau}}{2}$. Can be absorbed by a shift of *h* because of CS coupling

$$\begin{split} H &= \frac{\pi}{2J} \sum_{i,\mu} \left(\epsilon_{\mu\nu\lambda} \Delta_{\nu} h_{\bar{i},\lambda} \right)^2 + i\pi \epsilon_{\mu\nu\lambda} \Delta_{\nu} \tilde{h}_{\bar{i},\lambda} \frac{1 - s_{i,i+\mu}}{2} + K \sum_{\Box} \prod_{\Box} s_{ij} \\ \tilde{h} &\equiv h + h^0 \quad , \quad \epsilon_{\mu\nu\lambda} \Delta_{\nu} h_{\bar{i}\lambda}^0 = \delta_{\mu\tau} \end{split}$$

Accomodation of Berry phase

Berry phase introduces an extra phase factor, $H \to H - i\pi \sum_j \frac{1-s_{j,j+\tau}}{2}$. Can be absorbed by a shift of *h* because of CS coupling

$$H = \frac{\pi}{2J} \sum_{i,\mu} \left(\epsilon_{\mu\nu\lambda} \Delta_{\nu} h_{\bar{i},\lambda} \right)^2 + i\pi \epsilon_{\mu\nu\lambda} \Delta_{\nu} \tilde{h}_{\bar{i},\lambda} \frac{1 - s_{i,i+\mu}}{2} + K \sum_{\Box} \prod_{\Box} s_{ij}$$

$$\tilde{h} \equiv h + h^0 \quad , \quad \epsilon_{\mu\nu\lambda} \Delta_{\nu} h_{\bar{i}\lambda}^0 = \delta_{\mu\tau} \quad 1.5$$
Ising term is now $K_d \sum_{i,\mu} \varepsilon_{i,i+\mu} \sigma_{i,i+\mu}$,
where $\prod_{\Box} \varepsilon_{i,i+\mu} = -1$ for spatial plaquettes 1.0
 K_d
0.5
Fark and Sachdev 2002.
Park and Sachdev 2002.

13

Elevation to O(4) model

Two complex DOFs, $z_{ilpha}\equiv r_{ilpha}e^{i heta_{lpha}}$, constraint $\sum_{lpha}r_{ilpha}^2=1$

Hopping $z_{i,\alpha}^* z_{i+\mu,\alpha} + c.c \rightarrow r_{i,\alpha} r_{j,\alpha} \cos(\Delta_\mu \theta_{i,\alpha})$

Elevation to O(4) **model**

Two complex DOFs, $z_{ilpha}\equiv r_{ilpha}e^{i heta_{lpha}}$, constraint $\sum_{lpha}r_{ilpha}^2=1$

Hopping $z_{i,\alpha}^* z_{i+\mu,\alpha} + c.c \rightarrow r_{i,\alpha} r_{j,\alpha} \cos(\Delta_{\mu} \theta_{i,\alpha})$ Performing Villain approximation on each θ_{α} breaks O(4) symmetry to O(2) \otimes O(2), must use exact identity

$$e^{J\cos heta}\propto\sum_{p=-\infty}^{\infty}e^{ip heta}l_p(J)\quad \ln l_p(J\gg1)pproxrac{2}{J}p^2$$

Elevation to O(4) **model**

H

Two complex DOFs, $z_{ilpha}\equiv r_{ilpha}e^{i heta_{lpha}}$, constraint $\sum_{lpha}r_{ilpha}^2=1$

Hopping $z_{i,\alpha}^* z_{i+\mu,\alpha} + c.c \rightarrow r_{i,\alpha} r_{j,\alpha} \cos(\Delta_{\mu} \theta_{i,\alpha})$ Performing Villain approximation on each θ_{α} breaks O(4) symmetry to O(2) \otimes O(2), must use exact identity

$$e^{J\cos\theta} \propto \sum_{p=-\infty}^{\infty} e^{ip\theta} I_p(J) \quad \ln I_p(J \gg 1) \approx \frac{2}{J} p^2$$
$$\mathcal{Z} = \sum_{h_{\overline{j},\alpha,\mu}=-\infty}^{\infty} \prod_{j\alpha} \int_0^1 r_{j,\alpha} \, \mathrm{d}r_{j,\alpha} \, \delta\left(\sum_{\alpha} r_{j,\alpha}^2 - 1\right) \exp\left(-H[r_{\alpha}, h_{\alpha}]\right)$$
$$[r_{\alpha}, h_{\alpha}] = \sum_{\langle j,\mu \rangle} \left[-\ln I_{\rho_{j,\alpha,\mu}}(Jr_{j,\alpha}r_{j+\widehat{\mu},\alpha}) + K_d \varepsilon_{\overline{j},\mu} \sigma_{\overline{j},\mu} \right]$$

Generalizations of mapping to other models

Bose-Hubbard model in 2 + 1D coupled to \mathbb{Z}_2 gauge field - what happens at non-integer filling?

$$H = J \sum_{i\lambda} s_{i,i+\lambda} \cos \left(\Delta_{\lambda} \theta_{i} + i\mu \delta_{\lambda\tau} \right) + K \sum_{\Box} \prod_{\Box} s_{ij}$$
$$\Rightarrow \frac{1}{2J} \sum_{i\lambda} \left(p_{i\lambda} - n_{0} \delta_{\lambda\tau} \right)^{2} + K_{d} \sum_{i,\mu} \sigma_{i,i+\mu}$$

Fluctuations of non-contractible loops crucial - cluster/worm updates may be necessary for large system sizes



Homeier et al. 2022.

Future directions

• Large-N expansion for O(2N) DQCP - matchup between numerics and theory?

Future directions

- Large-N expansion for O(2N) DQCP matchup between numerics and theory?
- More sophisticated simulations continuous time, cluster updates for DQCP, etc

Future directions

- Large-N expansion for O(2N) DQCP matchup between numerics and theory?
- More sophisticated simulations continuous time, cluster updates for DQCP, etc
- Generalization of mapping to non-Abelian gauge groups?