# <span id="page-0-0"></span>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
- Derivation of effective model bosonic spinons coupled to odd  $\mathbb{Z}_2$  gauge field
- Sign-problem-free mapping generalized particle/vortex dualities

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

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



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





 $H=\sum_{ij}J_{ij}{\bf S}_i\cdot{\bf S}_j$ , 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  $|\psi_0\rangle$
- 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

"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  $|\psi_0\rangle$
- 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. . . )

- Direct evaluation of tr  $[e^{-\beta H}]$
- 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.](#page-0-0)

### Mean-field spinon solution supports gapped vison excitations



Spinon condensation  $\rightarrow$  magnetic order

Sachdev [1992;](#page-0-0) Huh, Punk, and Sachdev [2011.](#page-0-0)

### Mean-field spinon solution supports gapped vison excitations



Vison condensation  $\rightarrow$  VBS order

Sachdev [1992;](#page-0-0) Huh, Punk, and Sachdev [2011.](#page-0-0)

### Effective model of triangular lattice antiferromagnetism

$$
\mathcal{Z} = \sum_{\mathbf{s}_{j,j+\widehat{\mu}}=\pm 1} \prod_{j,\alpha} \int dz_{j\alpha} \delta\left(\sum_{\alpha=1,2} |z_{j\alpha}^2| - 1\right)
$$

$$
\times \left[\prod_j s_{j,j+\tau}\right] \exp\left(-H[z_\alpha, s]\right)
$$

$$
H[z_\alpha, s] = -\frac{J}{2} \sum_{\langle j,\mu \rangle} s_{j,j+\widehat{\mu}} (z_{j,\alpha}^* z_{j+\widehat{\mu},\alpha} + \text{c.c})
$$

$$
-K \sum_{\triangle \Box} \prod_{\Delta \square} s_{j,j+\widehat{\mu}}.
$$



Jian et al. [2018.](#page-0-0)

### Effective model of triangular lattice antiferromagnetism

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

Jian et al. [2018.](#page-0-0)

#### Effective model of triangular lattice antiferromagnetism

$$
\mathcal{Z} = \sum_{\substack{\mathbf{s}_{j,j+\widehat{\mu}}=\pm 1 \ j,\alpha}} \prod_{j,\alpha} \int dz_{j\alpha} \delta\left(\sum_{\alpha=1,2} |z_{j\alpha}^2| - 1\right)
$$

$$
\times \left[\prod_j \mathbf{s}_{j,j+\tau}\right] \exp\left(-H[z_{\alpha}, \mathbf{s}]\right)
$$

$$
H[z_{\alpha}, \mathbf{s}] = -\frac{J}{2} \sum_{\langle j,\mu \rangle} \mathbf{s}_{j,j+\widehat{\mu}} (z_{j,\alpha}^* z_{j+\widehat{\mu},\alpha} + \text{c.c})
$$

$$
-K \sum_{\triangle \Box} \prod_{\Delta \square} \mathbf{s}_{j,j+\widehat{\mu}}.
$$

Jian et al. [2018.](#page-0-0)



$$
\mathcal{Z} = \prod_i \int_0^{2\pi} \frac{\mathrm{d}\theta_i}{2\pi} \exp\left[-H\right] \quad , \quad H = -\frac{J}{\pi} \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j) = -\frac{J}{\pi} \sum_{i\mu} \cos(\Delta_\mu \theta_i)
$$

$$
\mathcal{Z} = \prod_i \int_0^{2\pi} \frac{\mathrm{d}\theta_i}{2\pi} \exp\left[-H\right] \quad , \quad H = -\frac{J}{\pi} \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j) = -\frac{J}{\pi} \sum_{i\mu} \cos(\Delta_\mu \theta_i)
$$

Using the Villain representation,

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

$$
\mathcal{Z} = \prod_i \int_0^{2\pi} \frac{\mathrm{d}\theta_i}{2\pi} \exp\left[-H\right] \quad , \quad H = -\frac{J}{\pi} \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j) = -\frac{J}{\pi} \sum_{i\mu} \cos\left(\Delta_\mu \theta_i\right)
$$

Using the Villain representation,

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

and

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

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



$$
\mathcal{Z} = \sum_{s_{ij}=\pm 1} \prod_i \int_0^{2\pi} \frac{\mathrm{d}\theta_i}{2\pi} \exp\left[-H\right] \quad , \quad H = -\frac{J}{\pi} \sum_{i\mu} s_{i,i+\mu} \cos\left(\Delta_\mu \theta_i\right) + K \sum_{\square} \prod_{\square} s_{ij}
$$

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

$$
i\pi\epsilon_{\mu\nu\lambda}\Delta_{\nu}h_{\bar{i},\lambda}\frac{1-s_{i,i+\mu}}{2}=i\pi h_{\bar{i},\mu}\frac{1-\prod_{\square} s_{i,i+\mu}}{2}
$$

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

Claim: integration over  $s_{ii}$  can be accomplished by independently summing over possible plaquette values  $\prod_{\square} s_{ij} \equiv \Phi_{\overline{i}\mu} = \pm 1.$ This is not true generally! Fluxes are not independent - product of  $\Phi_{\bar{i}\mu}$  over any closed

surface must be 1. Alternatively,  $\Delta_{\mu} \Phi_{\bar{j} \mu} = 0$  mod 4.



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

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



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

#### This constraint

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

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



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

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

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

### Accomodation of Berry phase

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

Park and Sachdev [2002.](#page-0-0)

#### Accomodation of Berry phase

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

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

$$
\tilde{h} \equiv h + h^0 \quad , \quad \epsilon_{\mu\nu\lambda} \Delta_{\nu} h_{\bar{i}\lambda}^0 = \delta_{\mu\tau}
$$

#### Accomodation of Berry phase

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

$$
H = \frac{\pi}{2J} \sum_{i,\mu} \left( \epsilon_{\mu\nu\lambda} \Delta_{\nu} h_{\overline{i},\lambda} \right)^2 + i \pi \epsilon_{\mu\nu\lambda} \Delta_{\nu} \widetilde{h}_{\overline{i},\lambda} \frac{1 - s_{i,i+\mu}}{2} + K \sum_{\square} \prod_{\square} s_{ij}
$$
  
\n
$$
\widetilde{h} \equiv h + h^0 , \quad \epsilon_{\mu\nu\lambda} \Delta_{\nu} h_{\overline{i}\lambda}^0 = \delta_{\mu\tau} 1.5
$$
  
\nIsing term is now  $K_d \sum_{i,\mu} \epsilon_{i,i+\mu} \sigma_{i,i+\mu}$ ,  
\nwhere  $\prod_{\square} \epsilon_{i,i+\mu} = -1$  for spatial plaquettes  
\n $K_d$   
\n $0.5$   
\n $\epsilon_{\mu\nu\lambda} \Delta_{\nu} h_{\overline{i}\lambda}^0 = \delta_{\mu\tau} 1.5$   
\n $K_d$   
\n $\epsilon_{\mu\nu\lambda} \Delta_{\nu} h_{\overline{i}\lambda}^0 = \delta_{\mu\tau} 1.5$   
\n $K_d$   
\n $\epsilon_{\mu\nu\lambda} \Delta_{\nu} h_{\overline{i}\lambda}^0 = \delta_{\mu\tau} 1.5$   
\n $K_d$   
\n $\epsilon_{\mu\nu\lambda} \Delta_{\nu} h_{\overline{i}\lambda}^0 = \delta_{\mu\tau} 1.5$   
\n $K_d$   
\n $\epsilon_{\mu\nu\lambda} \Delta_{\nu} h_{\overline{i}\lambda}^0 = \delta_{\mu\tau} 1.5$   
\n $\epsilon_{$ 

13

### Elevation to O(4) model

Two complex DOFs,  $z_{i\alpha}\equiv r_{i\alpha}e^{i\theta_{\alpha}}$ , constraint  $\sum_{\alpha}r_{i\alpha}^2=1$ 

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

### Elevation to O(4) model

Two complex DOFs,  $z_{i\alpha}\equiv r_{i\alpha}e^{i\theta_{\alpha}}$ , constraint  $\sum_{\alpha}r_{i\alpha}^2=1$ 

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

$$
e^{J\cos\theta} \propto \sum_{p=-\infty}^{\infty} e^{ip\theta} I_p(J) \quad \ln I_p(J \gg 1) \approx \frac{2}{J}p^2
$$

#### Elevation to O(4) model

Two complex DOFs,  $z_{i\alpha}\equiv r_{i\alpha}e^{i\theta_{\alpha}}$ , constraint  $\sum_{\alpha}r_{i\alpha}^2=1$ 

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

must use exact identity

$$
e^{J\cos\theta} \propto \sum_{p=-\infty}^{\infty} e^{ip\theta} I_p(J) \quad \ln I_p(J \gg 1) \approx \frac{2}{J} p^2
$$

$$
\mathcal{Z} = \sum_{h_{\tilde{J},\alpha,\mu}=-\infty}^{\infty} \prod_{j\alpha} \int_0^1 r_{j,\alpha} \, dr_{j,\alpha} \, \delta\left(\sum_{\alpha} r_{j,\alpha}^2 - 1\right) \exp\left(-H[r_{\alpha}, h_{\alpha}]\right)
$$

$$
H[r_{\alpha}, h_{\alpha}] = \sum_{\langle j,\mu\rangle} \left[-\ln I_{p_{j,\alpha,\mu}}(Jr_{j,\alpha}r_{j+\widehat{\mu},\alpha}) + K_d \varepsilon_{\tilde{j},\mu} \sigma_{\tilde{j},\mu}\right]
$$

### 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?

$$
H = J \sum_{i\lambda} s_{i,i+\lambda} \cos(\Delta_{\lambda} \theta_i + i\mu \delta_{\lambda \tau}) + K \sum_{\square} \prod_{\square} s_{ij}
$$

$$
\Rightarrow \frac{1}{2J} \sum_{i\lambda} (p_{i\lambda} - n_0 \delta_{\lambda \tau})^2 + K_d \sum_{i,\mu} \sigma_{i,i+\mu}
$$

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



Homeier et al. [2022.](#page-0-0)

### 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?