New Frontiers of Strongly Correlated Materials

Exact Solution to a Class of Generalized Kitaev Spin-1/2 Models in Arbitrary Dimensions

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References:

[1] J. J. Miao, H. K. Jin, F. Wang, F. C. Zhang, YZ, arXiv:1806.06495 (2018).

[2] J. J. Miao, H. K. Jin, F. C. Zhang, YZ, arXiv: 1806.10960 (2018).

Outline

- □ A brief introduction to Kitaev honeycomb model
- □ The construction of exactly solvable models
- □ Generating new models: 1D, 2D and 3D
- □ A particular example in 2D: a Mott insulator model
- 3D examples and possible realization in real materials

Kitaev Honeycomb model

Spin-1/2 model (compass model)

$$H = -J_x \sum_{x \text{ link}} K_{ij} - J_y \sum_{y \text{ link}} K_{ij} - J_z \sum_{z \text{ link}} K_{ij}$$

where K_{ij} is defined as

 $K_{ij} = \begin{cases} \sigma_i^x \sigma_j^x, & \text{if } (i, j) \text{ is a } x \text{ link,} \\ \sigma_i^y \sigma_j^y, & \text{if } (i, j) \text{ is a } y \text{ link,} \\ \sigma_i^z \sigma_j^z, & \text{if } (i, j) \text{ is a } z \text{ link.} \end{cases}$

Brick-wall representation





Feng, Zhang, Xiang (2007); Chen, Nussinov (2008)

Kitaev (2006)



- Exact solvability
- > Quantum paramagnet
 - > SU(2) invariant ground state
 - > Emergent SU(2) symmetry
- Fractional spin excitations
- Topologically distinct phases
- > Two spins per unit cell

Existing generalizations

✓ Spin-1/2 models in 2D

Yao, Kivelson (2007); Yang, Zhou, Sun (2007); Baskaran, Santhosh, Shankar (2009); Tikhonov, Feigelman (2010); Kells, Kailasvuori, Slingerland, Vala (2011); ...

✓ Spin-1/2 models in 3D

✓ Si, Yu (2007); Ryu (2009); Mandal, Surendran (2009); Kimchi, Analytis, Vishwanath (2014); Nasu, Udagawa, Motome (2014); Hermanns, O'Brien, Trebst (2015); Hermanns, Trebst (2016); …

✓ Multiple-spin interactions

✓ Kitaev (2006); Lee, Zhang, Xiang (2007); Yu, Wang (2008); …

✓ SU(2)-invariant models

✓ F. Wang(2010); Yao, Lee (2011); Lai and O. I. Motrunich (2011); …

✓ Higher spin models

Yao, Zhang, Kivelson (2009); Wu, Arovas, Hung (2009); Chern (2010); Chua, Yao, Fiete (2011); Nakai, Ryu, Furusaki (2012); Nussinov, van den Brink, (2013); ...

Our goals

- Provide some generic rules for searching generalized Kitaev spin-1/2 models in arbitrary dimensions.
- □ Constrict ourselves on spin-1/2 models.
- Demonstrate some models of particular interest.

Construction of spin-1/2 models

Basic idea: (1) Construct exactly solvable 1D spin chains and (2) then couple them to form a connected lattice in arbitrary dimensions.

Steps:

- Construct spin-1/2 chains that can be exactly solved by the Jordan-Wigner transformation.
- 2 Couple these chains to form a connected lattice on which the spin-1/2 model can be still exactly solved by the Jordan-Wigner transformation.

Parquet rules:

Elementary rules
 Supplementary rules

Sites and links on a lattice

- **Consider a** *d*-dimensional cube, $d = 2, 3, 4, \cdots$
- **Site labelling:** $n = (n_1, n_2, \cdots, n_d), \ 1 \le n_j \le L_j, \ j = 1, \cdots, d$

Ordering of sites

D Define a number, $N = n_1 + \sum_{j=2}^d (n_j - 1) \prod_{l=1}^{j-1} L_j$, for each site n;

 $\Box \quad \text{If } N < M \text{, then } n < m.$

Link: a pair of sites (n, m)

D Local link:
$$\sum_{j=1}^{d} |n_j - m_j| = 1$$

D Nonlocal link:
$$\sum_{j=1}^d \left| n_j - m_j \right| > 1$$



ordering of sites



local and nonlocal links

Model Hamiltonian

$$H = H_{local}^{(2)} + H_{nonlocal}^{(2)} + H_{nonlocal}^{(M)}$$

Interactions

- $\square H_{local}^{(2)}: \text{ local two-spin terms, } J_{n\,n+\hat{1}}^{\alpha\beta}\sigma_n^{\alpha}\sigma_{n+\hat{1}}^{\beta} \text{ and } J_{n,n+\hat{k}}^{zz}\sigma_n^{z}\sigma_{n+\hat{k}}^{z};$
- $\square H_{nonlocal}^{(2)}: \text{ nonlocal two-spin terms, } J_{nm}^{ZZ} \sigma_n^Z \sigma_m^Z;$ $\square H_{nonlocal}^{(M)}: \text{ nonlocal multiple-spin terms, } J_{nm}^{\alpha\beta} \sigma_n^{\alpha} [\prod_{n < l < m} \sigma_l^Z] \sigma_m^{\beta}, \text{ etc.,}$ where $\alpha, \beta = x, y$, and $\hat{k} = \hat{1}, \cdots, \hat{d}$.

Firstly, divide the lattice into white (w) and black (b) sublattices arbitrary.

Elementary rules:

- For a (local or nonlocal) link (n, m): an x-bond is allocated for n ∈ w and m ∈ b; a y-bond is allocated for n ∈ b and m ∈ w; an xy-bond is allocated for n ∈ w and m ∈ w; a yx-bond is allocated for n ∈ b and m ∈ b;
- 2 Different *z*-bonds are not allowed to share the same site.



beyond compass models

Exactly solvability: quadratic fermion terms

Jordan-Wigner transformation

$$\begin{array}{rcl}
\sigma_m^+ &=& c_m^\dagger e^{i\pi\left(\sum_{l < m} \hat{n}_l\right)}, \\
\sigma_m^z &=& 2\hat{n}_m - 1,
\end{array}$$

Majorana fermion representation

$$n \in w, \ \eta_n = c_n^{\dagger} + c_n \text{ and } \gamma_n = i \left(c_n^{\dagger} - c_n \right)$$

 $n \in b, \ \eta_n = i \left(c_n^{\dagger} - c_n \right) \text{ and } \gamma_n = c_n^{\dagger} + c_n$

$$J_{n,n+\hat{1}}^{\alpha\beta}\sigma_{n}^{\alpha}\sigma_{n+\hat{1}}^{\beta}$$

$$\sigma_{n\in w}^{x}\sigma_{n+\hat{1}\in b}^{x} = -i\gamma_{n}\gamma_{n+\hat{1}},$$

$$\sigma_{n\in b}^{y}\sigma_{n+\hat{1}\in w}^{y} = i\gamma_{n}\gamma_{n+\hat{1}},$$

$$\sigma_{n\in w}^{x}\sigma_{n+\hat{1}\in w}^{y} = -i\gamma_{n}\gamma_{n+\hat{1}},$$

$$\sigma_{n\in b}^{y}\sigma_{n+\hat{1}\in b}^{x} = i\gamma_{n}\gamma_{n+\hat{1}},$$

All the possible quadratic γ -fermion terms by J-W transformation.

$$\begin{split} & J_{nm}^{\alpha\beta}\sigma_{n}^{\alpha}\left[\prod_{n < l < m}\sigma_{l}^{z}\right]\sigma_{m}^{\beta}\\ & \sigma_{n \in w}^{x}\left[\prod_{n < l < m}(-\sigma_{l}^{z})\right]\sigma_{m \in b}^{x} = -i\gamma_{n}\gamma_{m},\\ & \sigma_{n \in b}^{y}\left[\prod_{n < l < m}(-\sigma_{l}^{z})\right]\sigma_{m \in w}^{y} = i\gamma_{n}\gamma_{m},\\ & \sigma_{n \in w}^{x}\left[\prod_{n < l < m}(-\sigma_{l}^{z})\right]\sigma_{m \in w}^{y} = -i\gamma_{n}\gamma_{m},\\ & \sigma_{n \in b}^{y}\left[\prod_{n < l < m}(-\sigma_{l}^{z})\right]\sigma_{m \in b}^{y} = i\gamma_{n}\gamma_{m}, \end{split}$$

Exactly solvability: biquadratic fermion terms

 $J_{nm}^{zz}\sigma_n^z\sigma_m^z$ $\sigma_n^z\sigma_m^z = i\hat{D}_{nm}\gamma_n\gamma_m$

Static Z_2 gauge field

 $\hat{D}_{nm} = \pm i\eta_n\eta_m$

" - ": $n \& m \in$ the same sublattice " + ": $n \& m \in$ opposite sublattice

The eigenstates can be divided into different sectors according to {*D_{nm}*}.
 In each sector, allowed spin terms are trasformed to quadratic γ-fermion terms.

Majorana fermion representation

$$n \in w, \ \eta_n = c_n^{\dagger} + c_n \text{ and } \gamma_n = i \left(c_n^{\dagger} - c_n \right)$$

 $n \in b, \ \eta_n = i \left(c_n^{\dagger} - c_n \right) \text{ and } \gamma_n = c_n^{\dagger} + c_n$



Separation of degrees of freedom $H = H_{\gamma} \otimes H_{\eta}$

Majorana fermion representation

$$n \in w, \ \eta_n = c_n^{\dagger} + c_n \text{ and } \gamma_n = i \left(c_n^{\dagger} - c_n \right)$$

 $n \in b, \ \eta_n = i \left(c_n^{\dagger} - c_n \right) \text{ and } \gamma_n = c_n^{\dagger} + c_n$

It is possible that some isolated η_n do not show up in $H_\eta \Rightarrow$ **local degeneracy**

To lift the local degeneracy: couple isolated η_n using nonlocal terms

$$\begin{array}{l} \begin{array}{l} \displaystyle \operatorname{quadratic} \eta - \operatorname{fermion \ terms} & \operatorname{quadratic} \gamma - \operatorname{fermion \ terms} \\ \\ \sigma_{n \in b}^{x} \left[\prod_{n < l < m} (-\sigma_{l}^{z}) \right] \sigma_{m \in w}^{x} = -i\eta_{n}\eta_{m}, \\ \\ \sigma_{n \in w}^{y} \left[\prod_{n < l < m} (-\sigma_{l}^{z}) \right] \sigma_{m \in b}^{y} = i\eta_{n}\eta_{m}, \\ \\ \sigma_{n \in b}^{x} \left[\prod_{n < l < m} (-\sigma_{l}^{z}) \right] \sigma_{m \in b}^{y} = -i\eta_{n}\eta_{m}, \\ \\ \sigma_{n \in w}^{y} \left[\prod_{n < l < m} (-\sigma_{l}^{z}) \right] \sigma_{m \in w}^{y} = -i\eta_{n}\eta_{m}, \\ \\ \sigma_{n \in w}^{y} \left[\prod_{n < l < m} (-\sigma_{l}^{z}) \right] \sigma_{m \in w}^{y} = -i\eta_{n}\eta_{m}, \\ \\ \sigma_{n \in w}^{y} \left[\prod_{n < l < m} (-\sigma_{l}^{z}) \right] \sigma_{m \in w}^{y} = -i\eta_{n}\eta_{m}, \\ \end{array} \right]$$

Duality



 A similar duality relates topological trivial and non-trivial phases in interacting Kitaev chains.
 J.J. Miao, H.K. Jin, F.C. Zhang, YZ (2017)

A way to construct new models



Shortcut multiple-spin interactions



New multiple-spin interaction

Supplementary rules:

- 1 To add η -fermion quadratic terms using a nonlocal link (n, m): n and m are not allowed to coincide with site connected by existing z-bonds in the original Hamiltonian constructed subjected to the two elementary rules.
- 2 To add shortcut multiple-spin interactions: for a step along the 1-direction, the two-spin term should be $\sigma_l^{\alpha} \sigma_{l+1}^{\beta}$ with $\alpha, \beta = x, y$; for a step along the other directions, the two-spin terms should be $\sigma_l^z \sigma_{l+\delta}^z$ with $\delta \neq 1$, and there must exist a local *z*-bond on this step in the original Hamiltonian.
- ③ In the above, the indices α and β should be chosen as follows: for $l \in w$ and $l + \hat{1} \in b$, $(\alpha, \beta) = (x, x)$; for $l \in b$ and $l + \hat{1} \in w$, $(\alpha, \beta) = (y, y)$; for $l \in w$ and $l + \hat{1} \in w$, $(\alpha, \beta) = (x, y)$; for $l \in b$ and $l + \hat{1} \in b$, $(\alpha, \beta) = (y, x)$.

Generating new models: 1D examples

Three parent models in 1D



Generating new models: 1D examples

Three parent models in 1D



Generating new models: 1D examples



Generating new models: from 1D to 2D

Two parent models in 2D



Generating new models: 2D examples

Duality transformation can be performed along each chain independently.



Generating new models: 2D examples

Split sites and insert nonlocal bonds



Generating new models: 3D examples



Three types of unit cells





$$\begin{split} H &= H_0 + H_1, \quad (1a) \\ H_0 &= \sum_{\vec{r}} J_x \sigma^x_{\vec{r},1} \sigma^x_{\vec{r},2} + J_{yx} \sigma^y_{\vec{r},2} \sigma^x_{\vec{r},3} + J_y \sigma^y_{\vec{r},3} \sigma^y_{\vec{r}+\hat{x},1} \\ &+ J_z \sigma^z_{\vec{r},1} \sigma^z_{\vec{r}-\hat{x}+\hat{y},2}, \quad (1b) \\ H_1 &= \sum_{\vec{r}} t_x \sigma^x_{\vec{r},3} \sigma^z_{\vec{r}+\hat{x},1} \sigma^z_{\vec{r}+\hat{x},2} \sigma^y_{\vec{r}+\hat{x},3} \\ &+ t_y \sigma^x_{\vec{r},3} \sigma^x_{\vec{r}+\hat{x},1} \sigma^x_{\vec{r}+\hat{y},2} \sigma^y_{\vec{r}+\hat{y},3}, \quad (1c) \end{split}$$



 H_0 : two-spin interactions

 $\begin{array}{l} H_1: \ \text{four-spin interactions} \\ \rightarrow \ \text{lift local degeneracy} \end{array}$



Elementary plaquette & Flux operator

$$\hat{\phi}_p = -\sigma_{\vec{r},1}^y \sigma_{\vec{r},2}^z \sigma_{\vec{r},3}^z \sigma_{\vec{r}+\hat{x},1}^x \sigma_{\vec{r}+\hat{y},2}^y \sigma_{\vec{r}+\hat{y},1}^z \sigma_{\vec{r}-\hat{x}+\hat{y},3}^z \sigma_{\vec{r}-\hat{x}+\hat{y},2}^x$$

Majorana representation

•
$$\eta_n = c_n^{\dagger} + c_n \text{ and } \beta_n = i \left(c_n^{\dagger} - c_n \right)$$

$$\Box \circ \eta_n = i (c_n^{\dagger} - c_n) \text{ and } \beta_n = c_n^{\dagger} + c_n$$





Static Z_2 gauge field: $\hat{D}_{\vec{r}} = i\eta_{\vec{r},1}\eta_{\vec{r}-\hat{x}+\hat{y},2}$

$$\begin{split} \sigma^{x}_{\vec{r},1}\sigma^{x}_{\vec{r},2} &= -i\beta_{\vec{r},1}\beta_{\vec{r},2},\\ \sigma^{y}_{\vec{r},2}\sigma^{x}_{\vec{r},3} &= -i\beta_{\vec{r},2}\beta_{\vec{r},3},\\ \sigma^{y}_{\vec{r},3}\sigma^{y}_{\vec{r}+\hat{x},1} &= i\beta_{\vec{r},3}\beta_{\vec{r}+\hat{x},1},\\ \sigma^{z}_{\vec{r},1}\sigma^{z}_{\vec{r}-\hat{x}+\hat{y},2} &= i\hat{D}_{\vec{r}}\beta_{\vec{r},1}\beta_{\vec{r}-\hat{x}+\hat{y},2}, \end{split}$$





$$\begin{split} \sigma^x_{\vec{r},3} \sigma^z_{\vec{r}+\hat{x},1} \sigma^z_{\vec{r}+\hat{x},2} \sigma^y_{\vec{r}+\hat{x},3} &= i\eta_{\vec{r},3} \eta_{\vec{r}+\hat{x},3}, \\ \sigma^x_{\vec{r},3} \sigma^x_{\vec{r}+\hat{x},1} \sigma^x_{\vec{r}+\hat{y},2} \sigma^y_{\vec{r}+\hat{y},3} &= -i\hat{D}_{\vec{r}+\hat{x}} \eta_{\vec{r},3} \eta_{\vec{r}+\hat{y},3}, \end{split}$$

$$\hat{\phi}_p = \hat{D}_{\vec{r}} \hat{D}_{\vec{r}+\hat{x}}$$



Exact solvability: Given $\{D_{\vec{r}} = \pm 1\} \rightarrow \text{Both } H_0$ and H_1 are quadratic form.

 H_0 : Absence of $\eta_3 \rightarrow 2^{L_{\chi}L_y/2}$ —fold degeneracy H_1 : Lift the local degeneracy

Lift the local degeneracy

 H_1 : Free Majorana fermions η_3 on a square lattice, coupled to a static Z_2 gaugefield $D_{\vec{r}}$



Ground state: π – flux state, $\phi_p = -1$, on every plaquette

Energy dispersion: π – flux state

$$\epsilon_{\eta_3}(\vec{k}) = \pm \sqrt{(t_x \sin k_x)^2 + (t_y \sin k_y)^2}$$



Boundary conditions: open BC vs. periodic BC



Boundary terms — JW transformation $\sigma_{L_x,n_y,3}^y \sigma_{1,n_y,1}^y = i\beta_{L_x,n_y,3}\beta_{1,n_y,1}\hat{F}_{n_y}$ $\hat{F}_{n_y} = e^{i\pi\hat{N}_{n_y}} \quad \hat{N}_{n_y} = \sum_{n_x,\mu} \hat{n}_{n_x,n_y,\mu}$ Fluxes on edge plaquettes

$$\hat{\phi}_{p} = \hat{D}_{L_{x},n_{y}}\hat{D}_{1,n_{y}}\hat{F}_{n_{y}}$$
$$\hat{\phi}_{p} = \hat{D}_{1,n_{y}}\hat{D}_{2,n_{y}}\hat{F}_{n_{y}+1}$$

Open boundary condition

- **Good** quantum #s: $D_{\vec{r}}$
- \square 2^{*L*_y}-fold degeneracy: Majorana zero modes at edges

Periodic boundary condition

- **Good quantum #s:** $\{\phi_p, \Phi_x, \Phi_y\}$
- \square Z₂ global fluxes: Φ_x, Φ_y

$$\hat{\Phi}_x = \hat{F}_{n_y=1} \quad \hat{\Phi}_y = \prod_{n_y} \hat{D}_{\vec{r}=(1,n_y)}$$

Degrees of freedom: a $3 \times L_x \times L_y$ lattice



Projection: to remove the unphysical states

$$\hat{P} = (1 + F\hat{F})/2$$

total fermion # parity:
$$\hat{F} = \prod_{n_y} \hat{F}_{n_y}$$

Deductions:

- (1) For a given set of $\{\phi_p, \phi_x, \phi_y\}$, the projection \hat{P} survives half fermionic states with compatible *F*.
- 2 A physical spin excitation should be composed of even number of fermions.

Ground states: topological degeneracy

- □ Ground states: π flux states □ Unprojected degenerate ground states: $\Phi_x = \pm 1, \Phi_y = \pm 1$ □ Topological degeneracy: $\Delta E \propto 1/L$ □ Projection: survives 3 ground states $\hat{P}|G\rangle_{\Phi_x=\Phi_y=1} = 0$ for L_x , $L_y = even$
 - **D** Pairing terms vanish at $q_x = q_y = 0$

Robust against disorders

3-fold topological degeneracy on a torus



Bulk spinon excitations

π – flux states: magnetic unit cell
 6 sites in each magnetic unit cell
 Six bands for β-Majorana fermions
 Two point nodes: (0,0) and (0, π)
 Dirac-like dispersion around nodes





Breaking time-reversal symmetry (TRS)

□ Chern numbers

$$C\# = (-1, -1, 1, -1, 1, 1)$$

D 5th order perturbation: open a gap for η_3 MFs



Breaking time-reversal symmetry (TRS)

$\Box Z_2$ vortices

PBC: even # of vortices

□ A pair of vortices

- One Majorana zero mode (MZM) in each vortex core center
- Extra double degeneracy due to MZMs?
- □ MZM changes Fermion # parity
 → Projection removes half states.
- 4-fold GS degeneracy regarding global fluxes Φ_x and Φ_y
- \square 2*n* well-separated vortices
 - \square 2^{*n*+1}-fold degeneracy





Summary

- □ Mott insulator model: odd number of spin-1/2 per unit cell.
- □ Algebraic quantum spin liquid ground state.
- Ground states are of three-fold topological degeneracy.
- Bulk spinon excitations: two Dirac nodes.
- Breaking TRS
 - □ Topologically nontrivial spinon bands: odd Chern numbers.
 - \square Z_2 vortices obey non-Abelian statistics.

More models in 3D

Generate new models from an existing model.



hyperhoneycomb

hyperoctagon

Si, Yu (2007); Ryu (2009); Mandal, Surendran (2009); Kimchi, Analytis, Vishwanath (2014); Nasu, Udagawa, Motome (2014); Hermanns, O'Brien, Trebst (2015); Hermanns, Trebst (2016)

Possible material realization

Metal organic framework (MOF)



Hyerhoneycomb: Cu-network

Zhang, Baker, ..., Pratt, et. al. (2018)

Summary

□ Construct a class of generalized Kitaev spin-1/2 models in arbitrary dimensions

□ Beyond the category of quantum compass models

- Provide some methods to generate new models from existing models.
- □ A particular 2D example: Pristine Mott insulator.



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Thank you for attention

and make

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