Majorana stripe order on the surface of a three-dimensional topological insulator

arXiv: 1711.03632

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Talk plan

- **Brief introduction**
- **Model of *interacting* Majorana fermions**
  - Symmetry considerations at the noninteracting level
  - Map to a quantum spin model in the special “neutrality” condition
  - Application of the world-line QMC methods
  - Further duality mapping to a quantum compass model
  - Away from the neutrality condition : mean-field theory
- **Summary**

Majorana zero modes (MZMs)

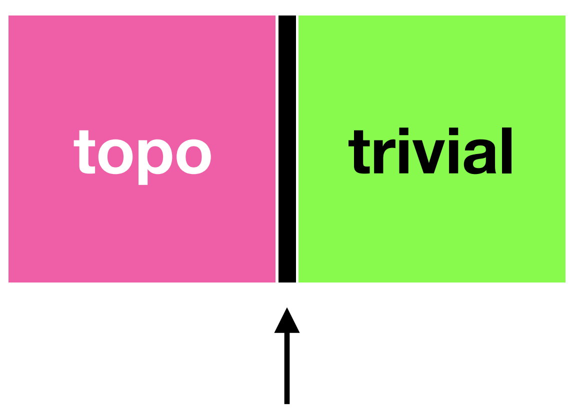
- (Generalized) bulk-boundary correspondence

topological class of the bulk

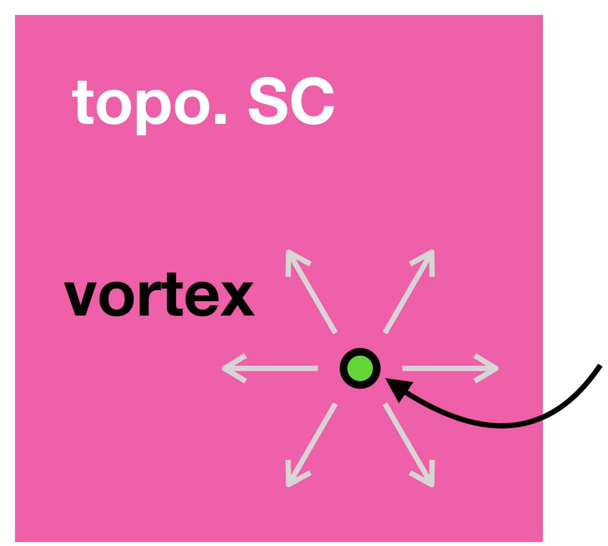
$\Updownarrow$

number of gapless edge states

number of zero modes bound to topological defects (e.g., vortices)



gapless edge state



Majorana zero mode bound to a vortex

Teo and Kane, PRB 2010

- *Effect of interactions* on the edge/vortex states ?

Setup for a Majorana lattice

- **Surface of a 3D TI subject to a SC proximity effect**

Fu and Kane, PRL 2008

— *Topological surface state resembling 2D p+ip SC*

— *Majorana zero modes (MZMs) bound to vortices*

— *Introduce Abrikosov vortex lattice* (Chiu et al, PRB 2015)

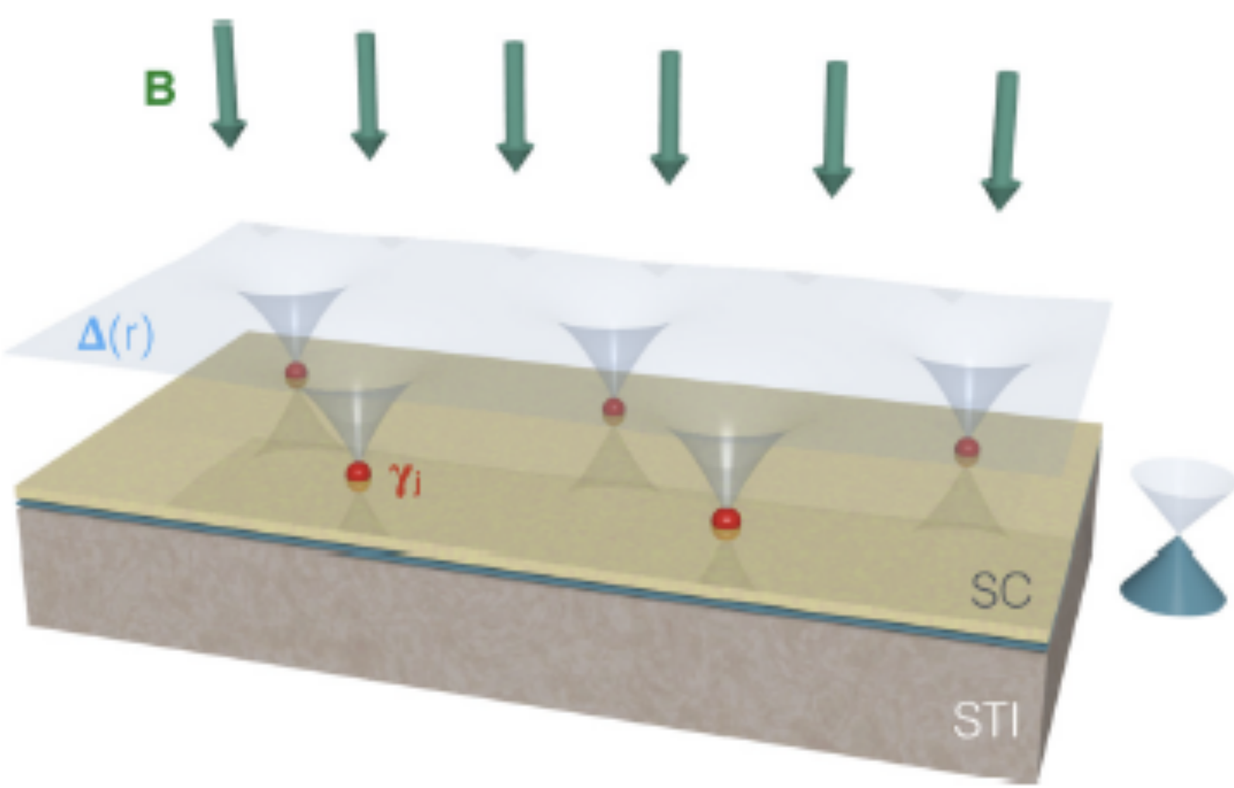
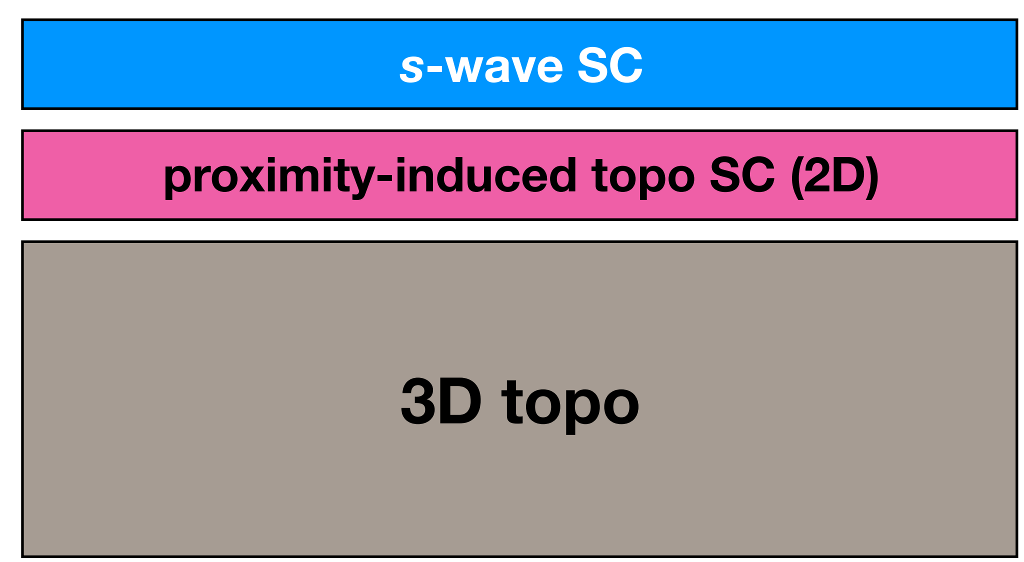


Figure credit: C.-K. Chiu *et al.*



Vortex state in the Fu-Kane model

Fu and Kane, PRL 2008

cf. Symposium talk by Hiroki Isobe (Nov. 9)

$$\hat{H}_{\mathrm{FK}} = \frac{1}{2}\int d^2\mathbf{r}\,\hat{\Psi}^\dagger_{\mathbf{r}}\mathcal{H}_{\mathrm{FK}}(\mathbf{r})\,\hat{\Psi}_{\mathbf{r}}\,; \quad \hat{\Psi}_{\mathbf{r}} = (\hat{\psi}_{\uparrow\mathbf{r}}, \hat{\psi}_{\downarrow\mathbf{r}}, \hat{\psi}^\dagger_{\downarrow\mathbf{r}}, -\hat{\psi}^\dagger_{\uparrow\mathbf{r}})^{\mathrm{T}}$$

$$\boxed{\mathcal{H}_{\mathrm{FK}} = \tau^z\left(-iv_{\mathrm{F}}\boldsymbol{\sigma}\cdot\nabla - \mu_{\mathrm{F}}\right) + \mathrm{Re}\,\Delta(\mathbf{r})\tau^x + \mathrm{Im}\,\Delta(\mathbf{r})\tau^y,}$$

$\tau^{x,y,z}$ $(\sigma^{x,y,z})\cdots$ Pauli matrices in the Nambu (spin) basis

$\Delta(\mathbf{r})\cdots$ proximity-induced pair potential

$v_{\mathrm{F}}\cdots$ velocity of the surface Dirac mode for $\Delta = 0$

- **Solution in the presence of a vortex** $\Delta(\mathbf{r}) = \Delta_0(r)e^{-i(n\varphi+\vartheta)}$

$$\hat{\gamma} = \int d^2\mathbf{r}\left(u(\mathbf{r})\psi_{\downarrow\mathbf{r}} + u^*(\mathbf{r})\psi^\dagger_{\downarrow\mathbf{r}}\right) = \hat{\gamma}^\dagger$$

MZM

$$u(\mathbf{r}) = u(r) = \mathcal{N}^{-1}e^{i\left(\frac{\vartheta}{2}-\frac{\pi}{4}\right)}\exp\left(-\int_0^r \Delta_0(r')dr'\right)$$

Symmetry considerations

- **Different sym. classes for $\mu_F = 0$ and $\mu_F \neq 0$** Chiu *et al*., PRB 2015

$$\boxed{\begin{aligned}\mathcal{H}_{\mathrm{FK}} &= \tau^z\left(-iv_{\mathrm{F}}\boldsymbol{\sigma}\cdot\nabla - \mu_{\mathrm{F}}\right) + \mathrm{Re}\,\Delta(\mathbf{r})\tau^x + \mathrm{Im}\,\Delta(\mathbf{r})\tau^y,\\ \hat{\Psi}_{\mathbf{r}} &= (\hat{\psi}_{\uparrow\mathbf{r}}, \hat{\psi}_{\downarrow\mathbf{r}}, \hat{\psi}^\dagger_{\downarrow\mathbf{r}}, -\hat{\psi}^\dagger_{\uparrow\mathbf{r}})^{\mathrm{T}}\end{aligned}}$$

— **General case ($\mu_F \neq 0$) : symmetry class D**

1. *Time-reversal symmetry is absent due to the applied magnetic field*
2. *Only particle-hole symmetry* $\Xi = \sigma^y\tau^y K$

— ***"neutrality condition"*** **($\mu_F = 0$) : symmetry class BDI**

3. *Additional* ***artificial time-reversal symmetry*** Θ_{eff}

$$\Theta_{\mathrm{eff}} = \sigma^x\tau^x K, \quad \Theta_{\mathrm{eff}}^2 = 1$$

Important consequences of Θ_{eff}

Chiu *et al.*, PRB 2015

- MZM for a vortex is a spin-down state

$$\hat{\gamma} = \int d^2\mathbf{r} \left(u(\mathbf{r})\psi_{\downarrow\mathbf{r}} + u^*(\mathbf{r})\psi^\dagger_{\downarrow\mathbf{r}} \right)$$

- The usual quadratic hybridization term is prohibited

$$\hat{\Theta}_{\text{eff}}\hat{\gamma}\,\hat{\Theta}^{-1}_{\text{eff}} = \hat{\gamma}$$

$$\hat{\Theta}_{\text{eff}}\,i\,\hat{\Theta}^{-1}_{\text{eff}} = -i$$

$\Rightarrow$ $i\gamma_1\gamma_2$ is *not allowed*

- Consequently, the corresponding interacting model *must be in the strong coupling limit* under the neutrality condition.

$$\hat{H}_{\text{int}} = \sum_{i>j} it_{ij}\hat{\gamma}_i\hat{\gamma}_j + \sum_{i>j>k>\ell} g_{ijk\ell}\hat{\gamma}_i\hat{\gamma}_j\hat{\gamma}_k\hat{\gamma}_\ell + \ldots$$

kinetic energy completely suppressed

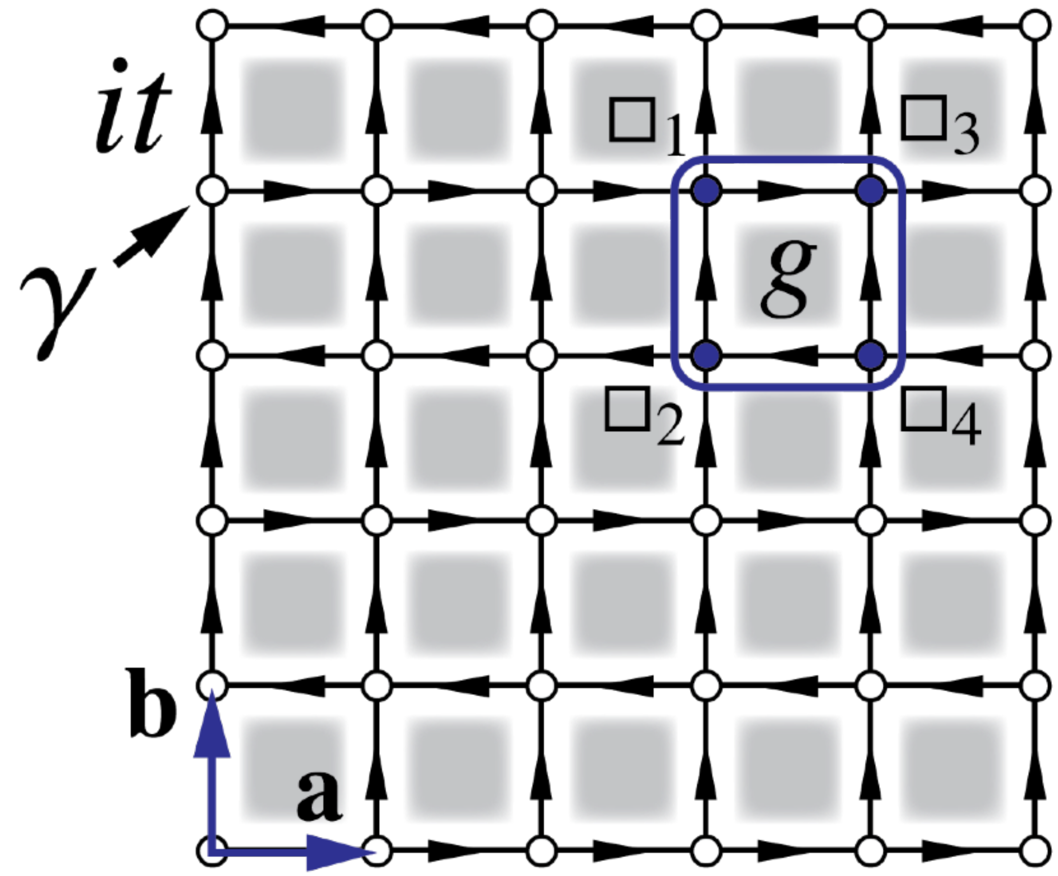
Square-lattice Majorana model

Simplest local interactions in the neutrality condition ($\mu_F = 0$)

$$\hat{H}_g = g \sum_{\square} \hat{\gamma}_{\square_1} \hat{\gamma}_{\square_2} \hat{\gamma}_{\square_3} \hat{\gamma}_{\square_4}$$

$$\hat{\gamma}^{\dagger}_{\mathbf{r}} = \hat{\gamma}_{\mathbf{r}}, \quad \{\hat{\gamma}_{\mathbf{r}}, \hat{\gamma}_{\mathbf{r}'}\} = 2\delta_{\mathbf{r},\mathbf{r}'}$$

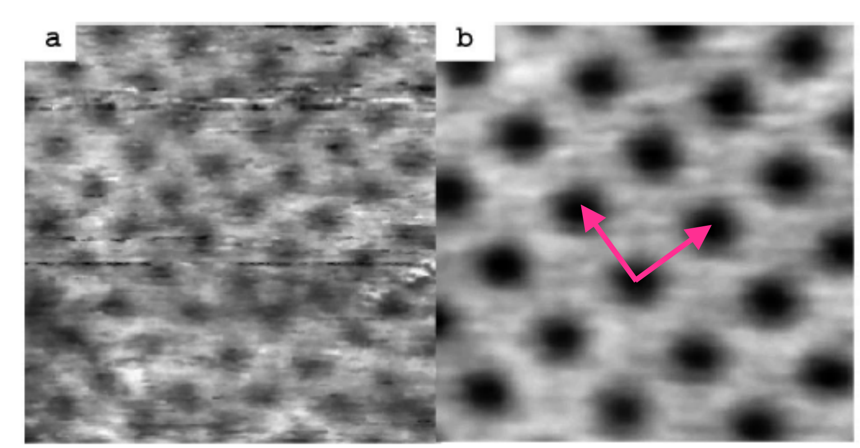
—*Assume a square-lattice Abrikosov vortices (e.g., due to an array of pinning impurities and/or lattice anisotropies)*



Additional term for $\mu_F \neq 0$

$$\hat{H}_t = it \sum_{\mathbf{r}} \left[\hat{\gamma}_{\mathbf{r}} \hat{\gamma}_{\mathbf{r}+\mathbf{b}} + (-1)^{r_y} \hat{\gamma}_{\mathbf{r}} \hat{\gamma}_{\mathbf{r}+\mathbf{a}} \right]$$

—*π-flux due to underlying vortices*



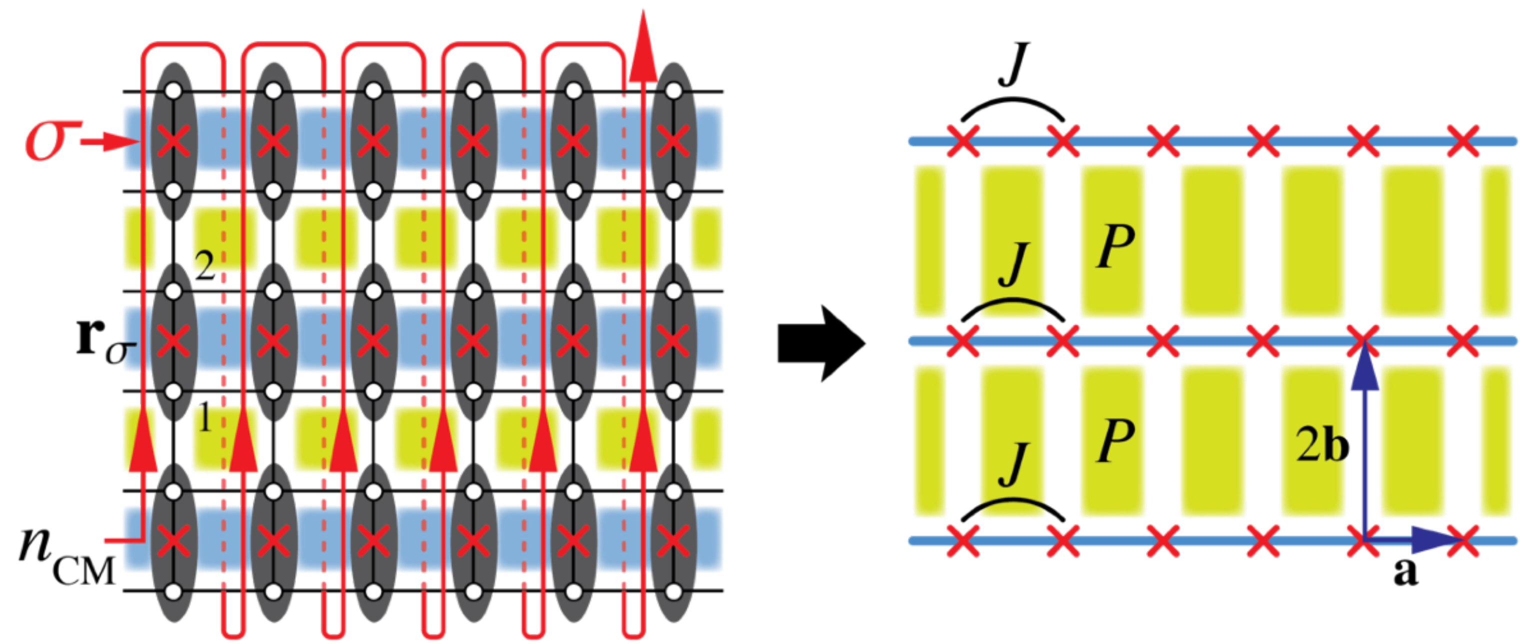
cf. $LuNi_2B_2C$ (De Wilde *et al.*, PRL 1997)

Mapping to a spin model at $\mu_F = 0$

1. Introduce pairings

$$\hat{c}_{\mathbf{r}_\sigma} = \frac{1}{2}(\hat{\gamma}_{\mathbf{r}_\sigma,1} + i\hat{\gamma}_{\mathbf{r}_\sigma,2})$$

complex fermion　　“bottom”　　“top”

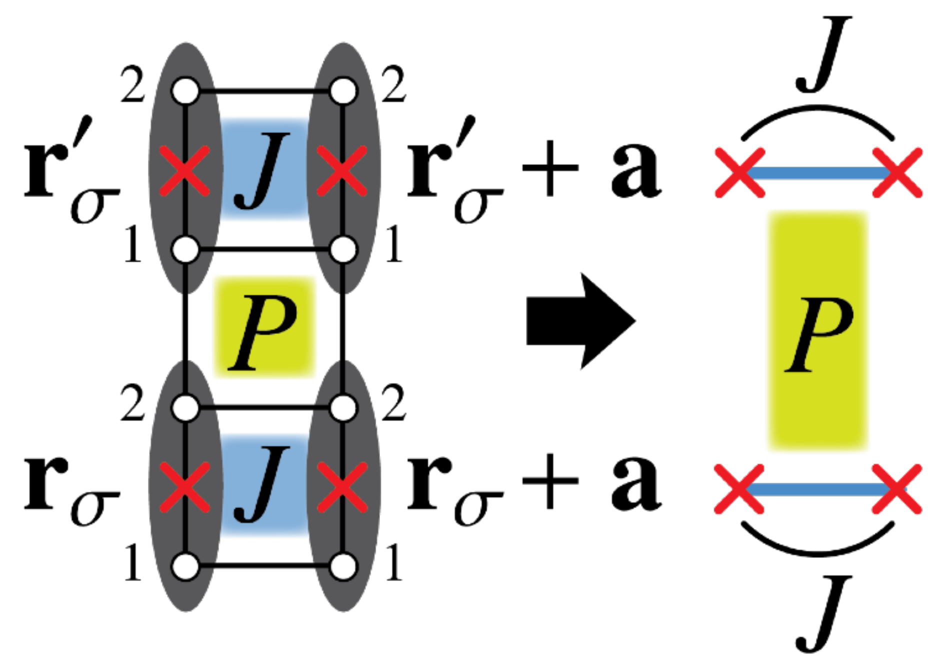


2. Jordan-Wigner transformation

(assuming OBC in the *b* direction)

$$\hat{c}^\dagger_{\mathbf{r}_\sigma}\hat{c}_{\mathbf{r}_\sigma} = \frac{1}{2}(1 + \hat{\sigma}^z_{\mathbf{r}_\sigma})$$

$$\hat{c}^\dagger_{\mathbf{r}_\sigma} = \frac{1}{2}\left(\prod_{n_{\mathrm{CM}}(\mathbf{r}'_\sigma)<n_{\mathrm{CM}}(\mathbf{r}_\sigma)} \hat{\sigma}^z_{\mathbf{r}'_\sigma}\right)(\hat{\sigma}^x_{\mathbf{r}_\sigma} + i\hat{\sigma}^y_{\mathbf{r}_\sigma})$$



$$\boxed{\hat{H}_{g,\sigma} = -J\sum_{\mathbf{r}_\sigma}\hat{\sigma}^z_{\mathbf{r}_\sigma}\hat{\sigma}^z_{\mathbf{r}_\sigma+\mathbf{a}} - P\sum_{\square_\sigma}\left(\prod_{\mathbf{r}_\sigma\in\square_\sigma}\hat{\sigma}^x_{\mathbf{r}_\sigma}\right), \quad J = P = g}$$

Faithful spin representation with only local interactions

Application of (bosonic) QMC

- The spin representation for $\mu_F = 0$ does not have the sign problem in the world-line QMC simulation
- Thermodynamic properties can be investigated in an unbiased way!

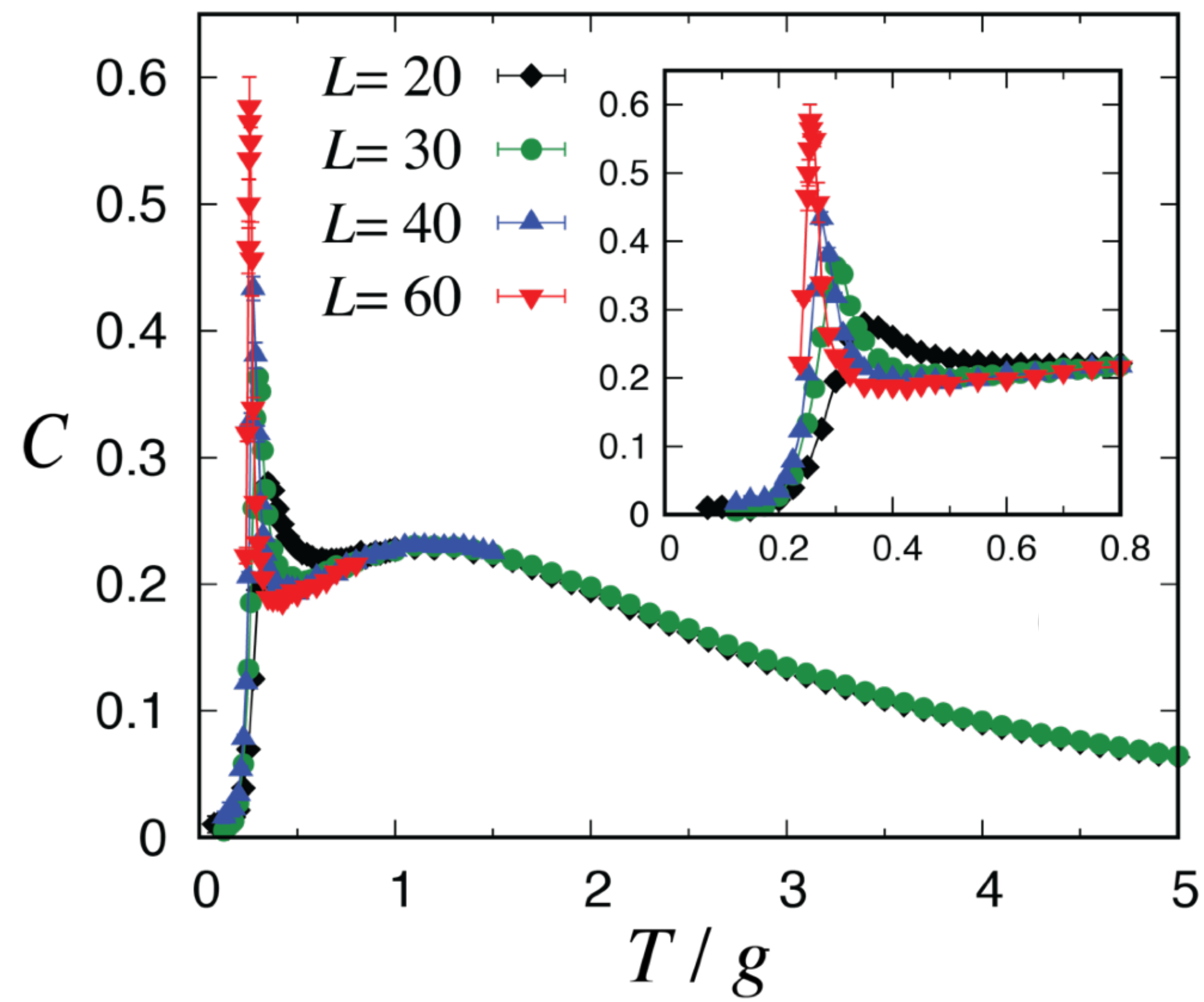
Specific heat

— *Broad peak in the specific heat at around T ~ g*

— *Additional divergent peak at T ~ 0.25 g, indicating a finite-temperature transition*

— *Inconsistent with the previous conjecture of QCP by Chiu et al. (PRB, 2015)*

— *What's the nature of the low-T phase?*



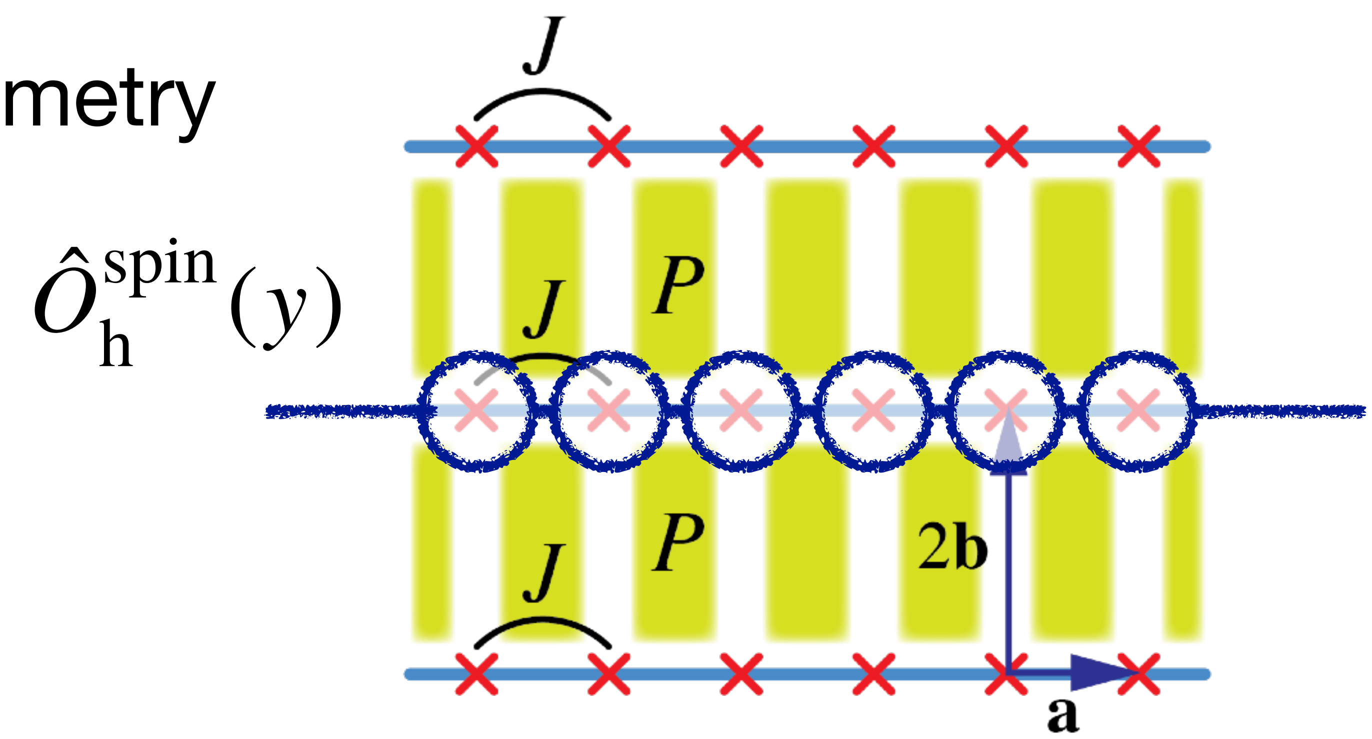
Possibility of usual order of "spins"?

- There is a 1D "gauge-like" symmetry in the model for $\mu_F = 0$

$$\left[\hat{H}_{g,\sigma}, \hat{O}^{\rm spin}_{\rm h}(y)\right] = 0, \ \forall y$$

$$\hat{O}^{\rm spin}_{\rm h}(y) = \prod_{r^x_\sigma} \hat{\sigma}^x_{\mathbf{r}_\sigma = (r^x_\sigma, y)}$$

Flipping the whole spins in a row



$$\hat{H}_{g,\sigma} = -J \sum_{\mathbf{r}_\sigma} \hat{\sigma}^z_{\mathbf{r}_\sigma} \hat{\sigma}^z_{\mathbf{r}_\sigma + \mathbf{a}} - P \sum_{\Box_\sigma} \left(\prod_{\mathbf{r}_\sigma \in \Box_\sigma} \hat{\sigma}^x_{\mathbf{r}_\sigma} \right)$$

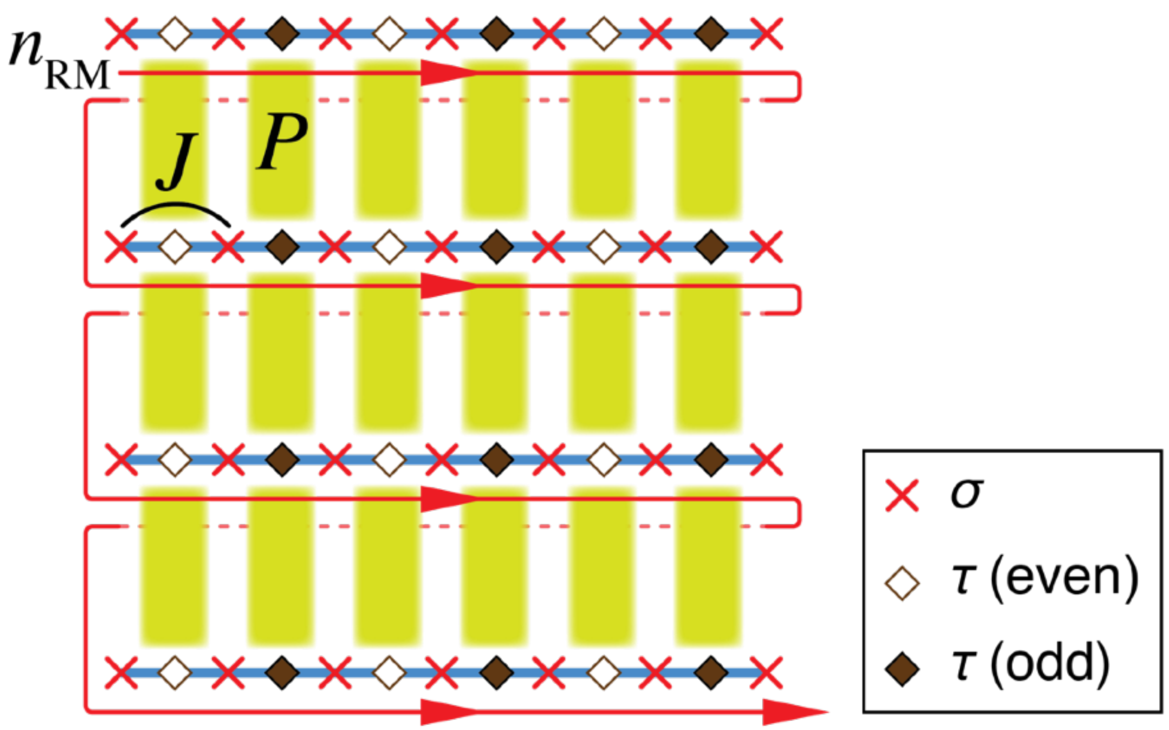
- These 1D symmetries cause a dimensional reduction from 2D to 1D for the order parameter field σ^z

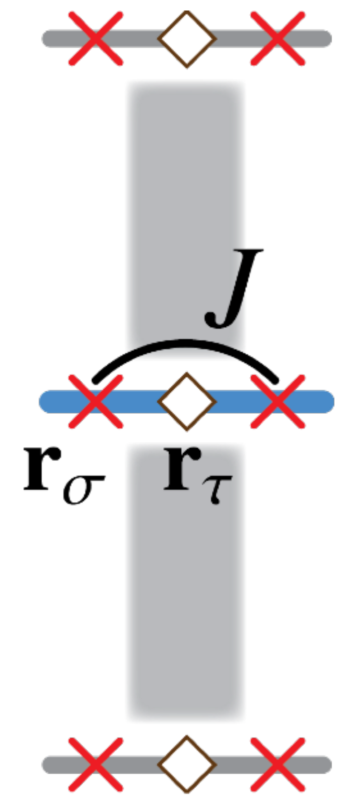
- ***No long-range order of σ^z is possible at $T > 0$*** at any momentum, as known as "generalized Elitzur's theorem"

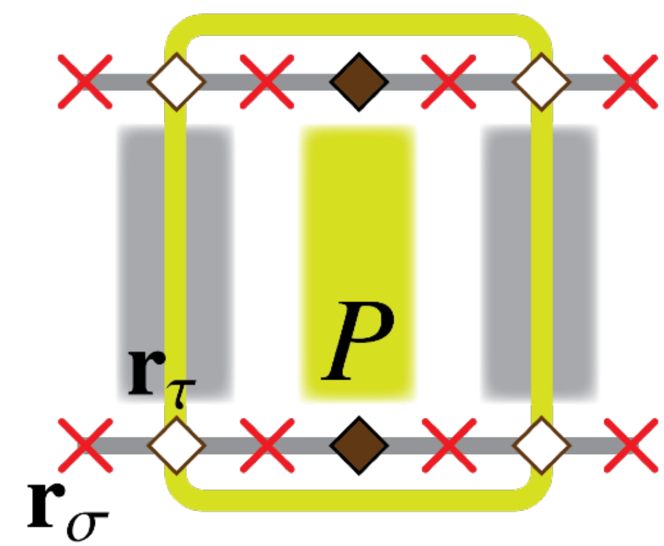
Batista and Nussinov, PRB 2005

Kramers-Wannier transformation

- To elucidate the nature of the low-T phase, we invoke a *two-step* duality mapping







P term : XXXX ➛ XXXX

K.-W. trans. #1 (σ ➛ τ)

J term : ZZ ➛ Z

$$\hat{\tau}^z_{\mathbf{r}_\tau} = \hat{\sigma}^z_{\mathbf{r}_\sigma}\hat{\sigma}^z_{\mathbf{r}_\sigma+\mathbf{a}},$$

$$\hat{\tau}^x_{\mathbf{r}_\tau} = \prod_{n_{\mathrm{RM}}(\mathbf{r}'_\sigma)\le n_{\mathrm{RM}}(\mathbf{r}_\sigma)} \hat{\sigma}^x_{\mathbf{r}'_\sigma}$$

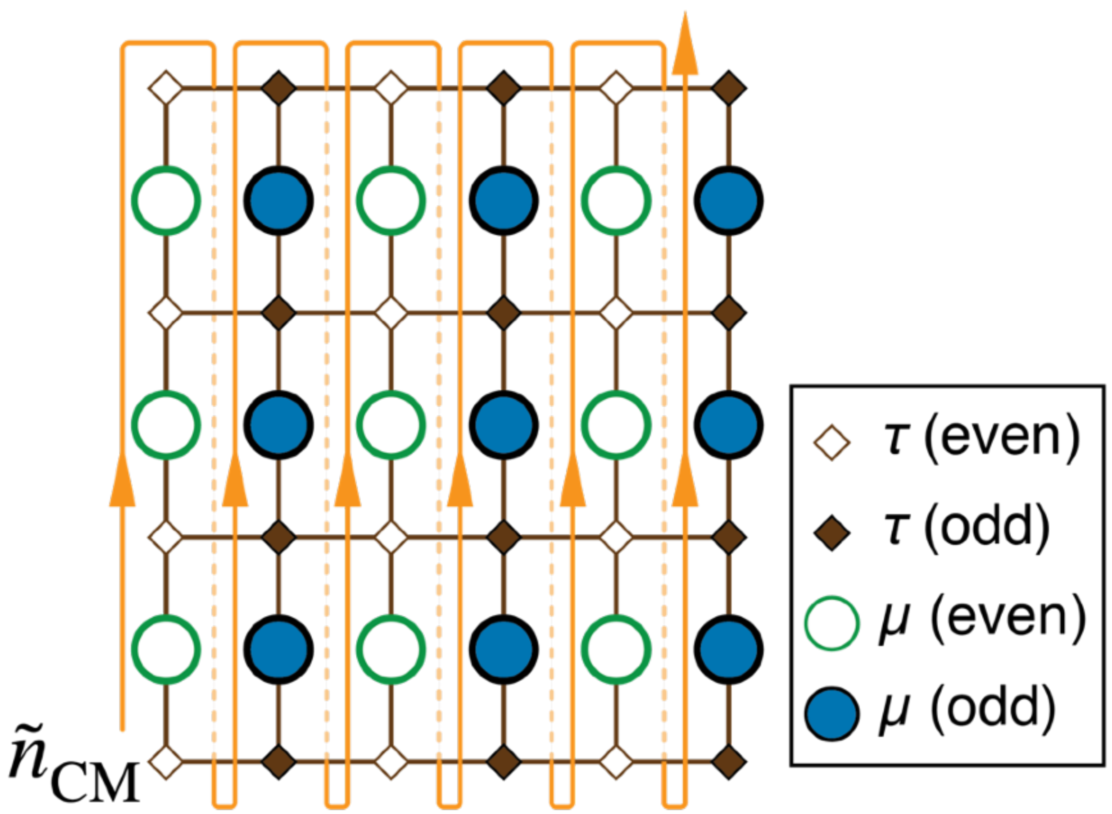
$$\hat{H}_{g,\tau} = \hat{H}^{\mathrm{e}}_{g,\tau} + \hat{H}^{\mathrm{o}}_{g,\tau}$$

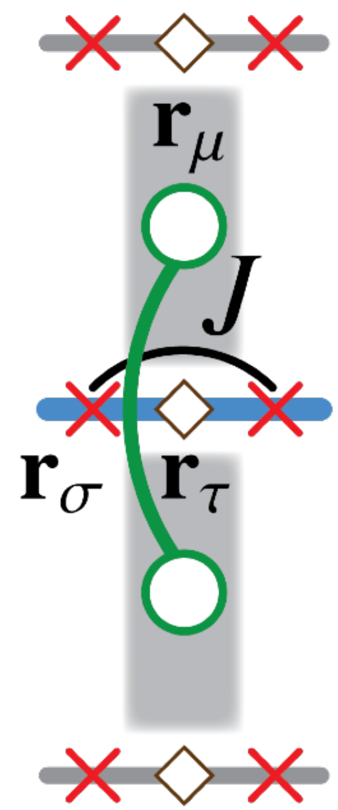
$$\hat{H}^{\mathrm{e(o)}}_{g,\tau} = \sum_{\mathbf{r}_\tau \in \text{even (odd) columns}} \left(-J\hat{\tau}^z_{\mathbf{r}_\tau} - P\hat{\tau}^x_{\mathbf{r}_\tau}\hat{\tau}^x_{\mathbf{r}_\tau+2\mathbf{a}}\hat{\tau}^x_{\mathbf{r}_\tau+2\mathbf{b}}\hat{\tau}^x_{\mathbf{r}_\tau+2\mathbf{a}+2\mathbf{b}}\right)$$

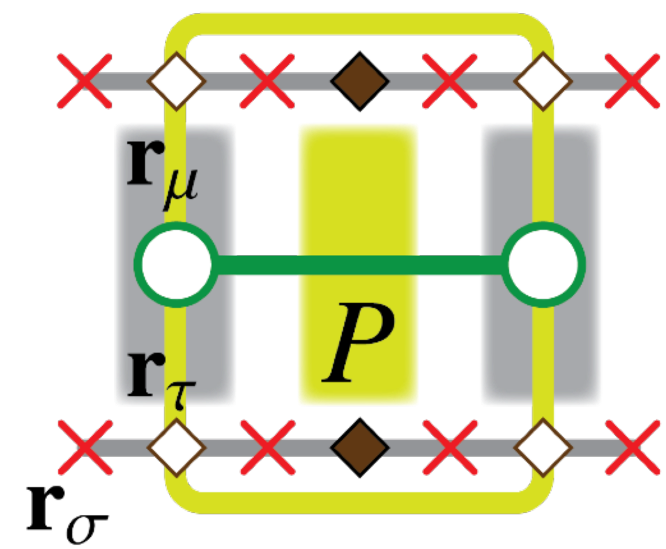
K.-W. transformation (cont'd)

- Finally, we obtain two decoupled copies of the *quantum compass model*

Nussinov and van der Brink, RMP, 2015







***P* term :**
XXXX* ➛ *XXXX* ➛ *XX

***J* term :**
ZZ* ➛ *Z* ➛ *ZZ

K.-W. trans. #2 (τ ➛ μ)

$$\hat{\mu}^x_{\mathbf{r}_\mu} = \hat{\tau}^x_{\mathbf{r}_\tau}\hat{\tau}^x_{\mathbf{r}_\tau+2\mathbf{b}}$$

$$\hat{\mu}^z_{\mathbf{r}_\mu} = \prod_{\tilde{n}_{\mathrm{CM}}(\mathbf{r}'_\tau)\leq\tilde{n}_{\mathrm{CM}}(\mathbf{r}_\tau)} \hat{\tau}^z_{\mathbf{r}'_\tau}$$

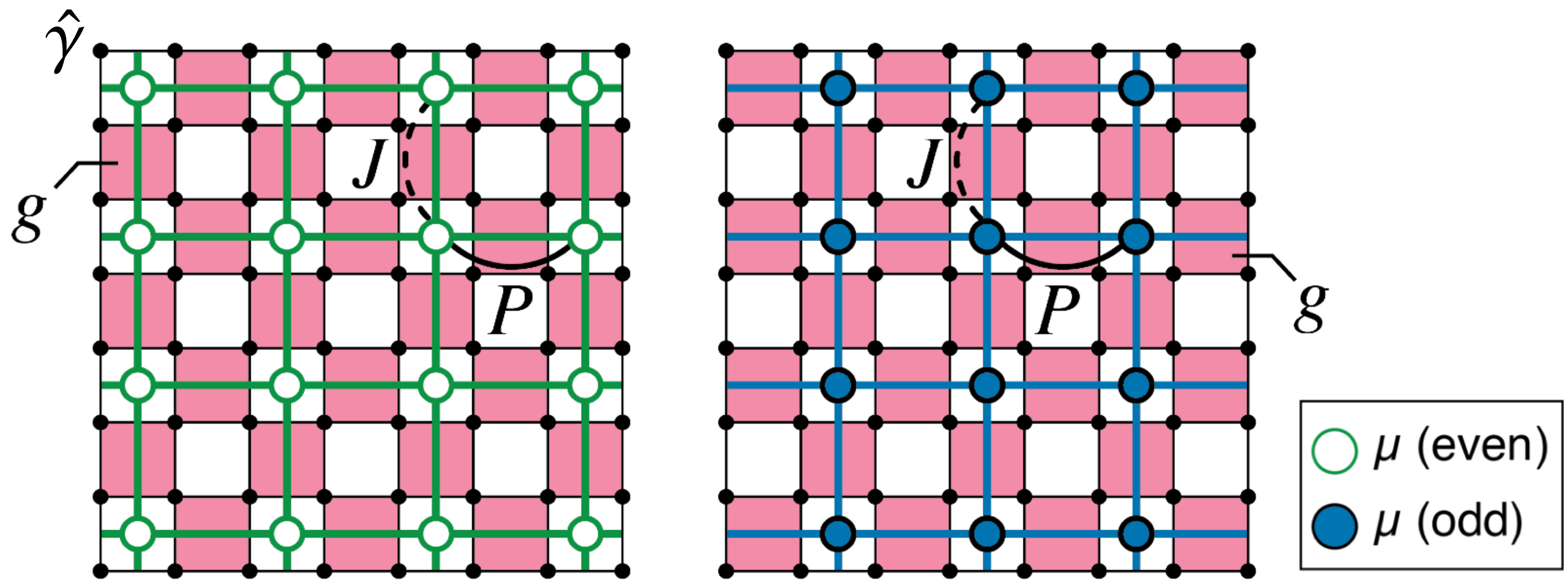
$$\boxed{\begin{aligned}\hat{H}_{g,\mu} &= \hat{H}^{\mathrm{e}}_{g,\mu} + \hat{H}^{\mathrm{o}}_{g,\mu}\\ \hat{H}^{\mathrm{e(o)}}_{g,\mu} &= \sum_{\mathbf{r}_\mu\,\in\,\text{even (odd) column}} \left(-P\hat{\mu}^x_{\mathbf{r}_\mu}\hat{\mu}^x_{\mathbf{r}_\mu+2\mathbf{a}} - J\hat{\mu}^z_{\mathbf{r}_\mu}\hat{\mu}^z_{\mathbf{r}_\mu+2\mathbf{b}}\right)\end{aligned}}$$

Correspondence of the interactions

$$\hat{H}_g = g \sum_{\square} \hat{\gamma}_{\square_1} \hat{\gamma}_{\square_2} \hat{\gamma}_{\square_3} \hat{\gamma}_{\square_4}$$

1. Jordan-Wigner transformation
2. Duality transformation

$$\hat{H}_{g,\mu} = \hat{H}^{\mathrm{e}}_{g,\mu} + \hat{H}^{\mathrm{o}}_{g,\mu}, \quad \hat{H}^{\mathrm{e(o)}}_{g,\mu} = \sum_{\mathbf{r}_\mu \in \text{even (odd) column}} \left(-P \hat{\mu}^x_{\mathbf{r}_\mu} \hat{\mu}^x_{\mathbf{r}_\mu + 2\mathbf{a}} - J \hat{\mu}^z_{\mathbf{r}_\mu} \hat{\mu}^z_{\mathbf{r}_\mu + 2\mathbf{b}} \right)$$

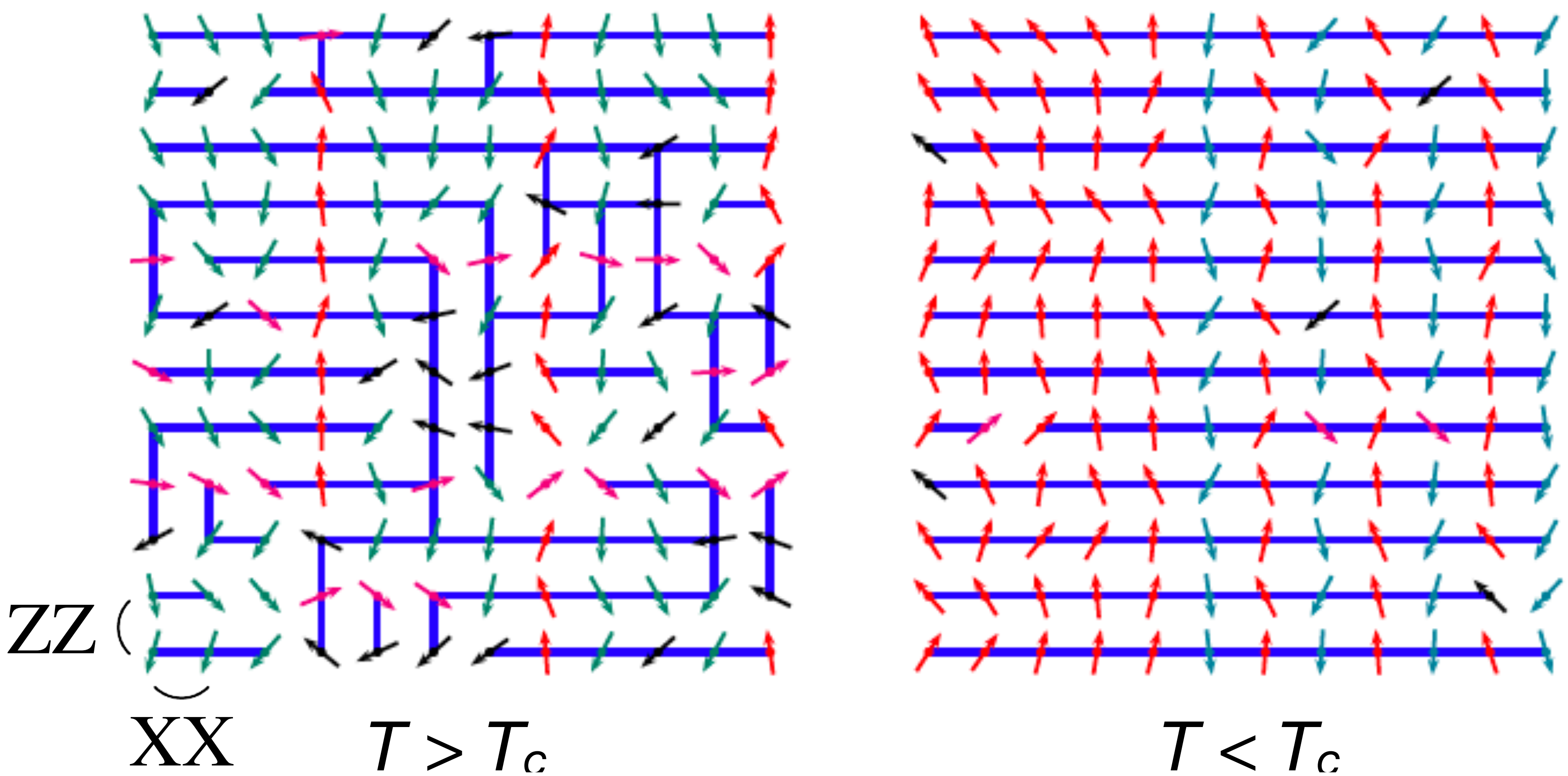


- The even-odd decoupling of the compass model corresponds to the *checkerboard decomposition* of the Majorana model

“Nematic” order of the compass model

Nussinov and van der Brink, RMP, 2015

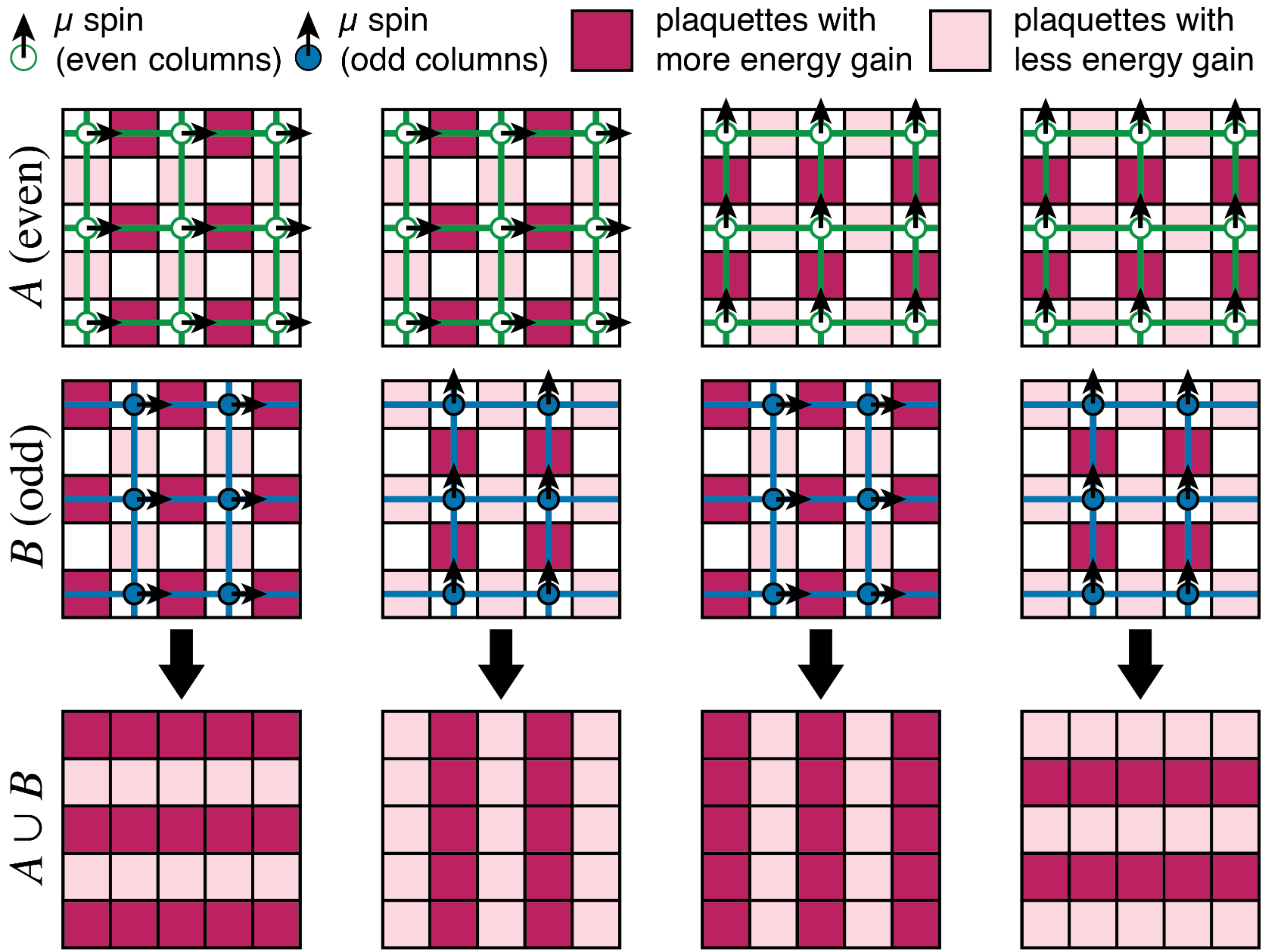
- Any spin-spin correlation function is short-ranged at $T > 0$
- Breaking of the spin-lattice Z_2 reflection symmetry $\begin{cases} \mathbf{a} \leftrightarrow \mathbf{b} \\ x \leftrightarrow z \end{cases}$



Order parameter $\quad \hat{D}_\mu(\mathbf{r}_\mu) = \hat{\mu}^x_{\mathbf{r}_\mu} \hat{\mu}^x_{\mathbf{r}_\mu + 2\mathbf{a}} - \hat{\mu}^z_{\mathbf{r}_\mu} \hat{\mu}^z_{\mathbf{r}_\mu + 2\mathbf{b}}$

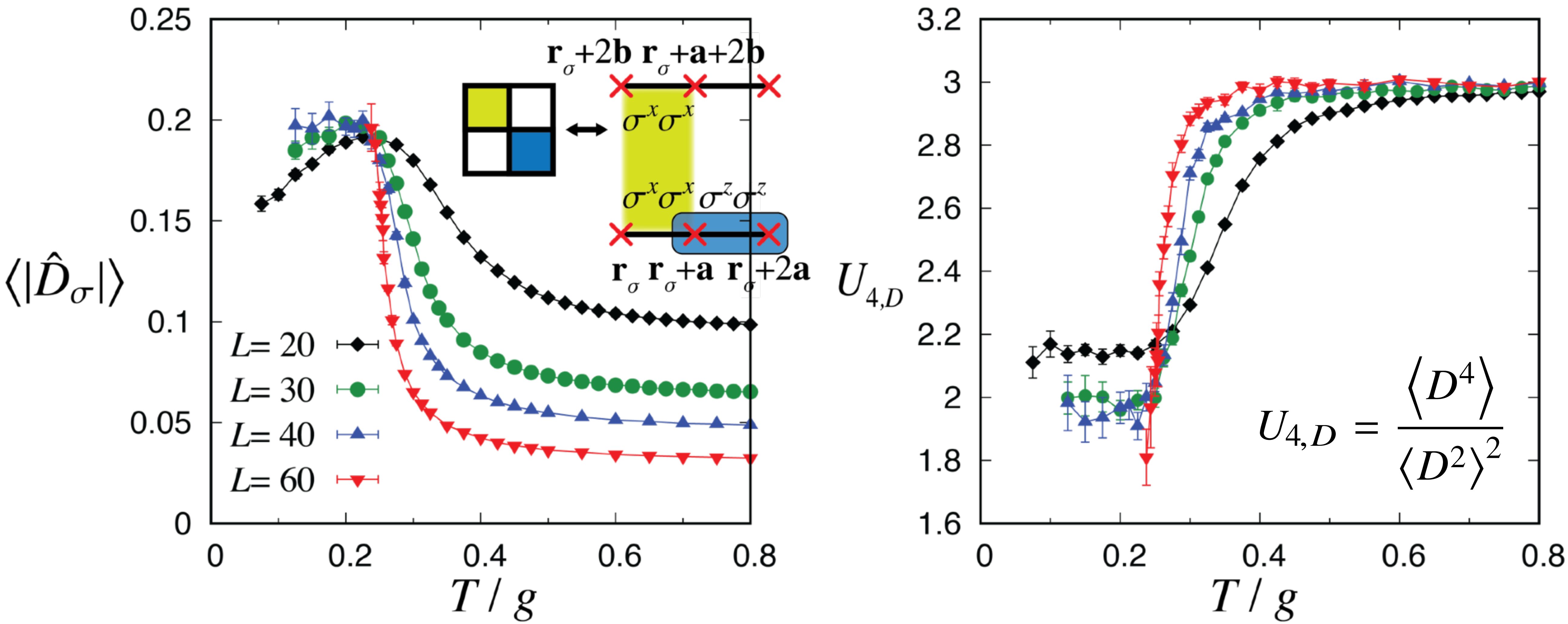
Figure credit: Wenzel and Janke, PRB (2008)

“Majorana stripe” order



Confirmation by QMC

- The Majorana stripe order appears at $T \sim 0.25g$, consistent with the location of the divergent peak in the specific heat.



Order parameter $\hat{D}_\sigma(\mathbf{r}_\sigma) = \hat{\sigma}^z_{\mathbf{r}_\sigma+\mathbf{a}}\hat{\sigma}^z_{\mathbf{r}_\sigma+2\mathbf{a}} - \hat{\sigma}^x_{\mathbf{r}_\sigma+2\mathbf{b}}\hat{\sigma}^x_{\mathbf{r}_\sigma}\hat{\sigma}^x_{\mathbf{r}_\sigma+\mathbf{a}+2\mathbf{b}}\hat{\sigma}^x_{\mathbf{r}_\sigma+\mathbf{a}}$

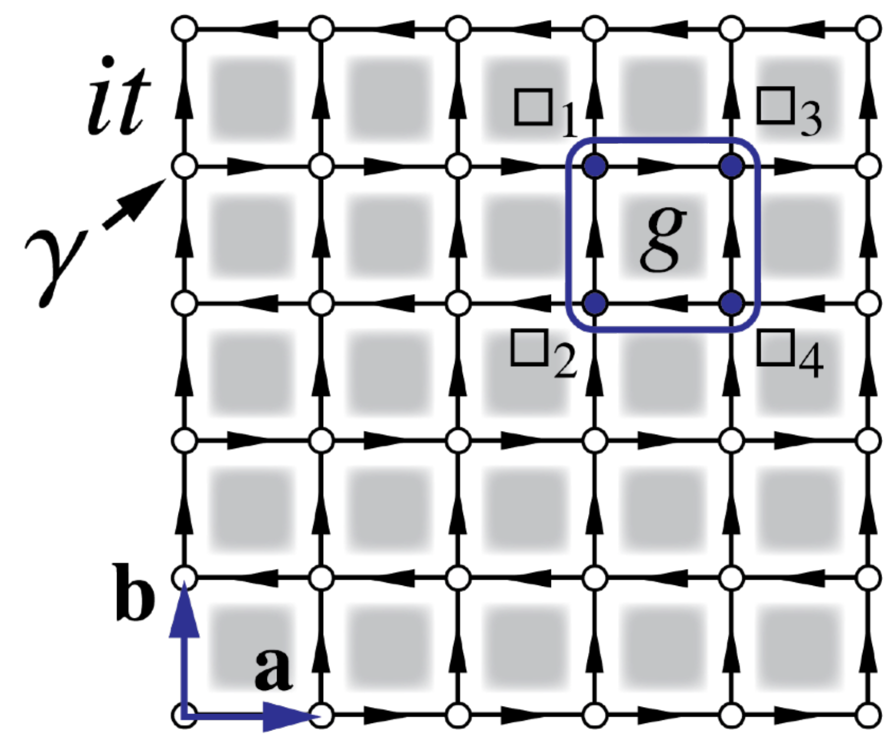
$$\left(\hat{D}_\mu(\mathbf{r}_\mu) = \hat{\mu}^x_{\mathbf{r}_\mu}\hat{\mu}^x_{\mathbf{r}_\mu+2\mathbf{a}} - \hat{\mu}^z_{\mathbf{r}_\mu}\hat{\mu}^z_{\mathbf{r}_\mu+2\mathbf{b}}\right)$$

Away from the neutrality condition

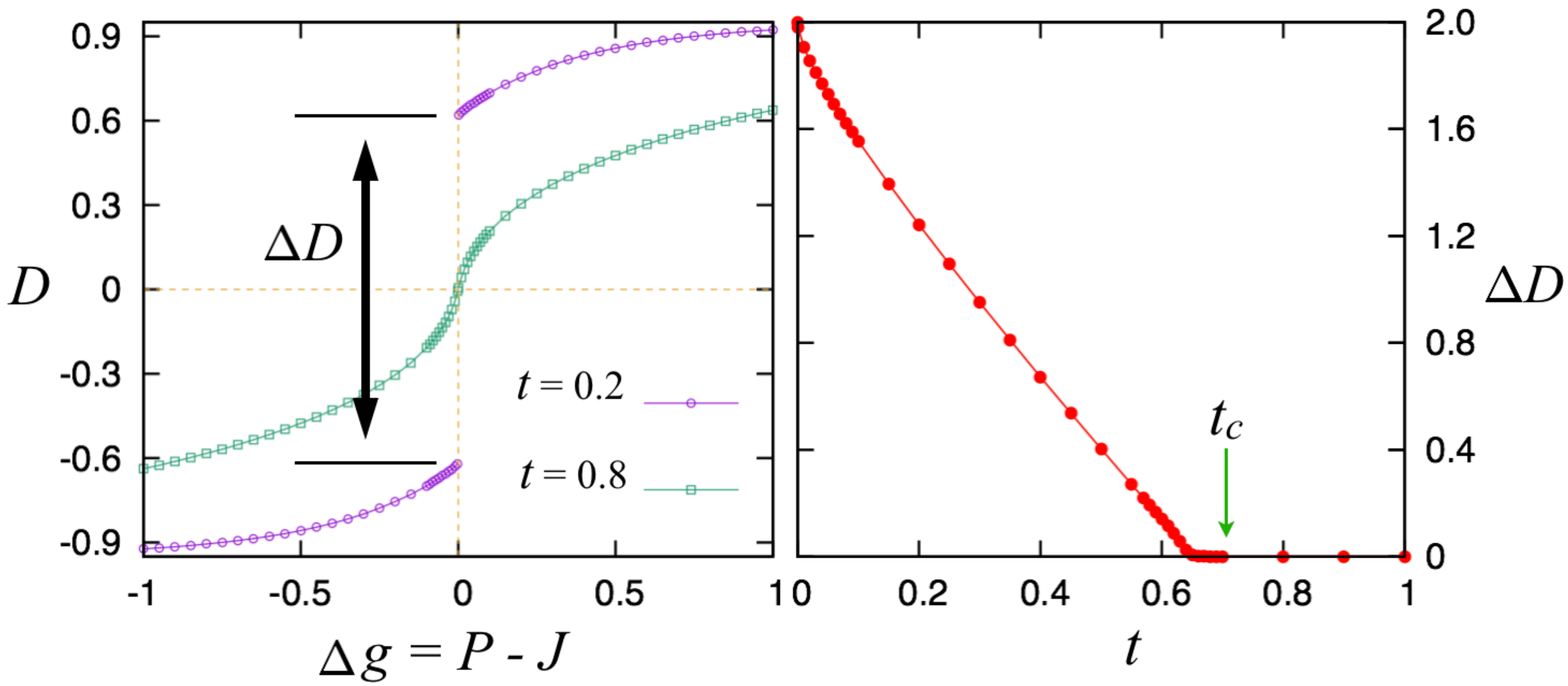
$$\boxed{\hat{H} = \hat{H}_g + \hat{H}_t}$$

$$\hat{H}_g = g \sum_{\Box} \hat{\gamma}_{\Box_1} \hat{\gamma}_{\Box_2} \hat{\gamma}_{\Box_3} \hat{\gamma}_{\Box_4}$$

$$\hat{H}_t = it \sum_{\mathbf{r}} \left[\hat{\gamma}_{\mathbf{r}} \hat{\gamma}_{\mathbf{r}+\mathbf{b}} + (-1)^{r_y} \hat{\gamma}_{\mathbf{r}} \hat{\gamma}_{\mathbf{r}+\mathbf{a}} \right]$$



- MF approximation $\hat{H} \to \hat{H}_{\mathrm{MF}}$

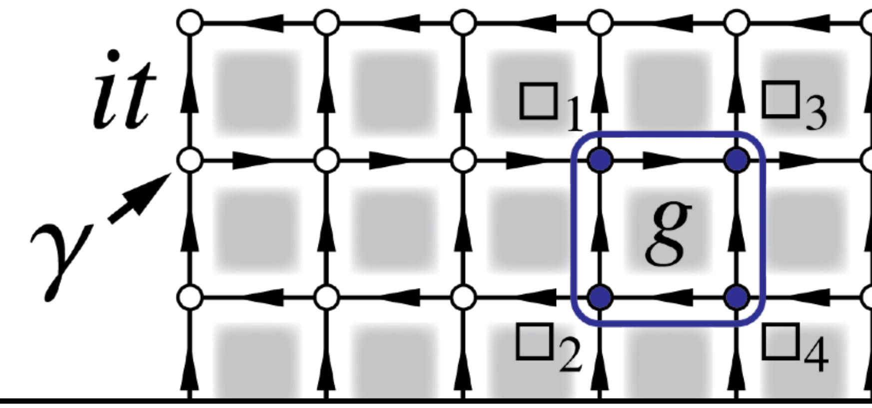


Away from the neutrality condition

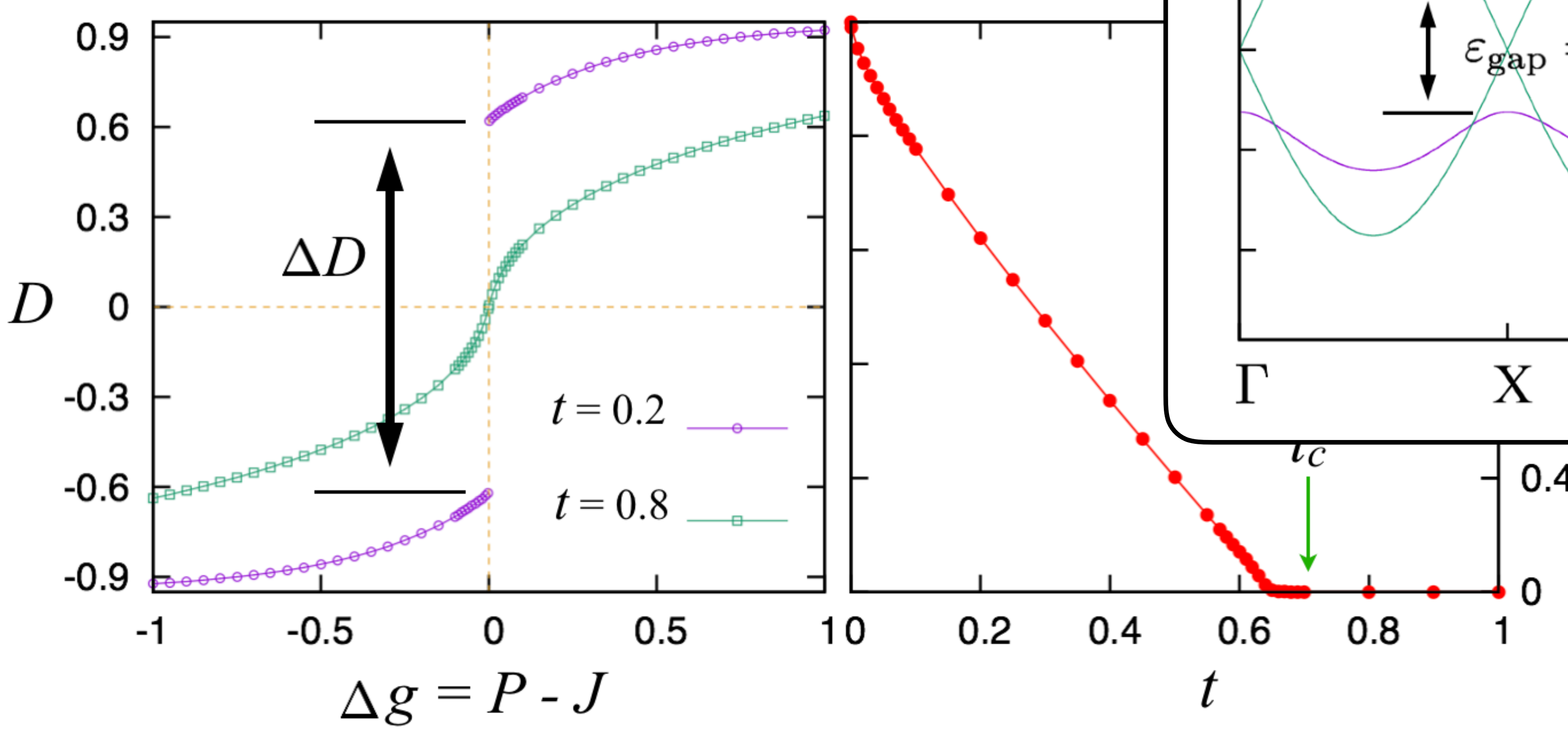
$$\boxed{\hat{H} = \hat{H}_g + \hat{H}_t}$$

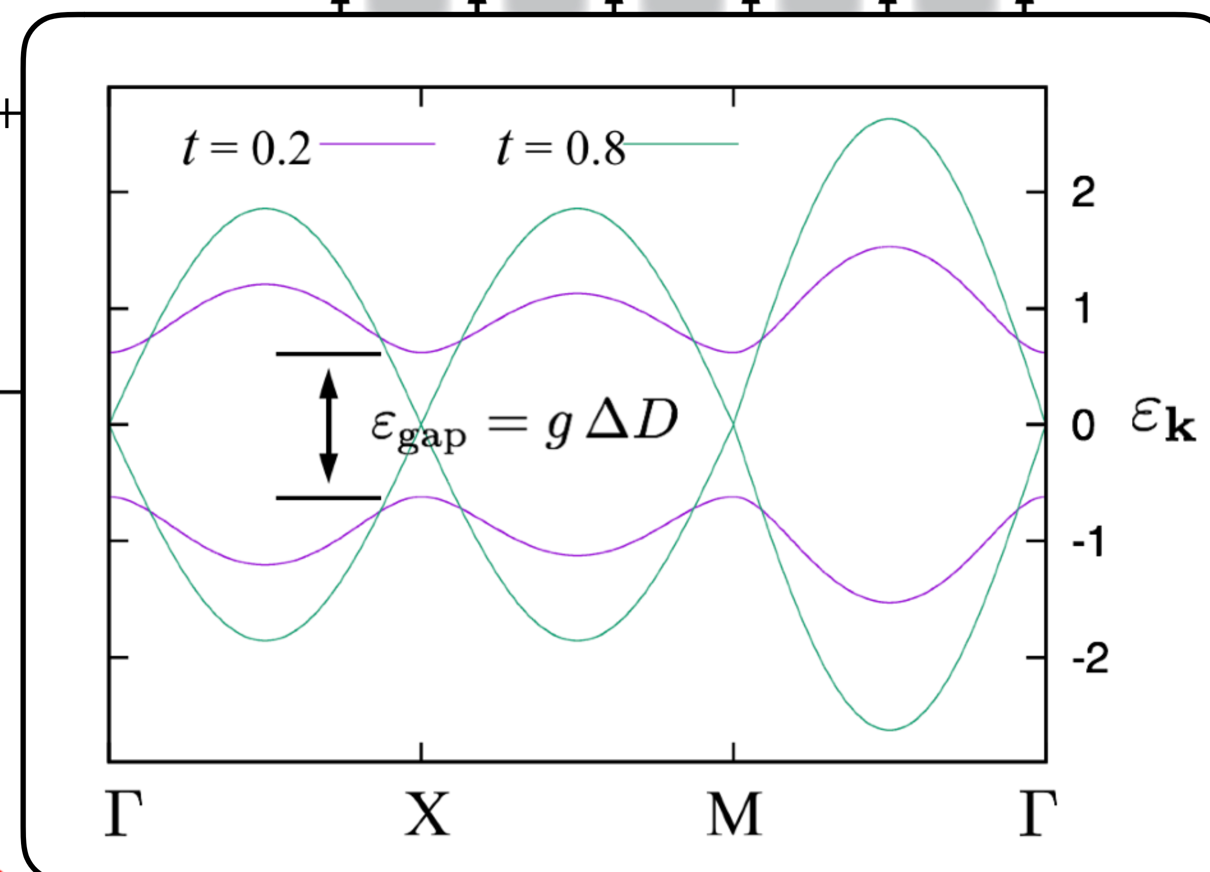
$$\hat{H}_g = g \sum_{\square} \hat{\gamma}_{\square_1} \hat{\gamma}_{\square_2} \hat{\gamma}_{\square_3} \hat{\gamma}_{\square_4}$$

$$\hat{H}_t = it \sum_{\mathbf{r}} \left[\hat{\gamma}_{\mathbf{r}} \hat{\gamma}_{\mathbf{r}+\mathbf{b}} + (-1)^{r_y} \hat{\gamma}_{\mathbf{r}} \hat{\gamma}_{\mathbf{r}+} \right.$$



- MF approximation $\hat{H} \rightarrow \hat{H}_{\mathrm{MF}}$

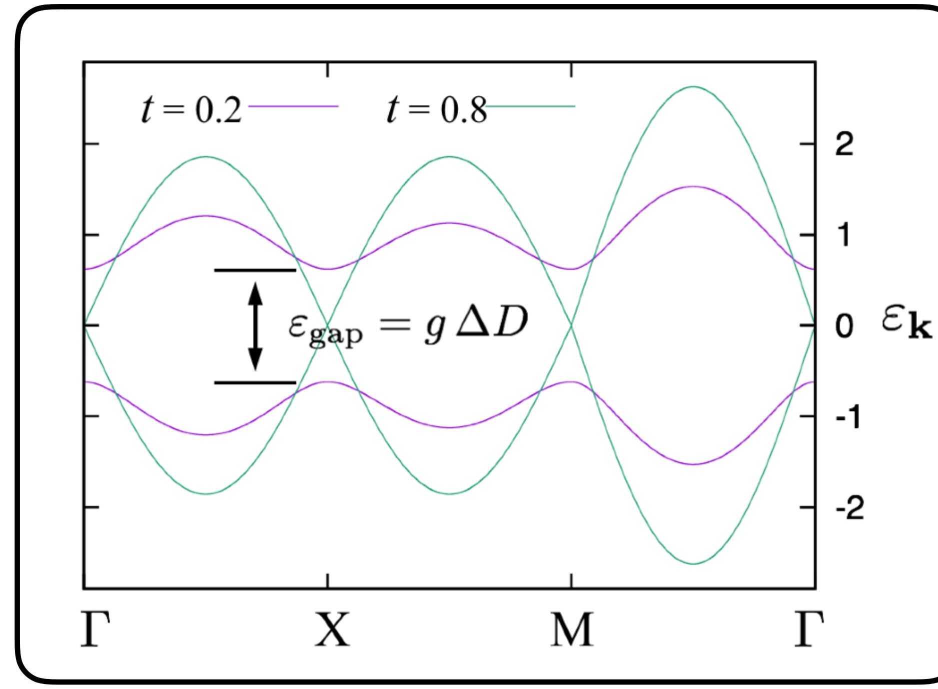


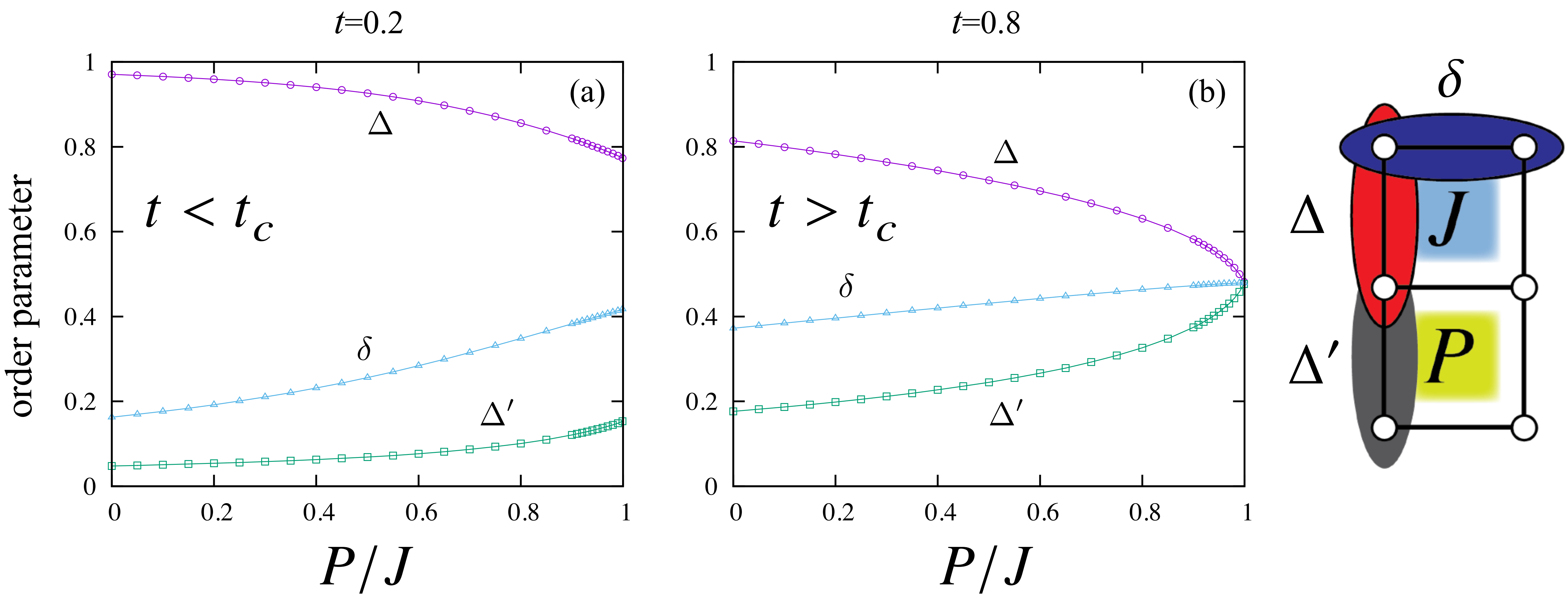


Gap closing induced by the Majorana hybridization

Phenomenology at $t = t_c$

- Gap closing
- Restoration of the broken translational & rotational symmetries

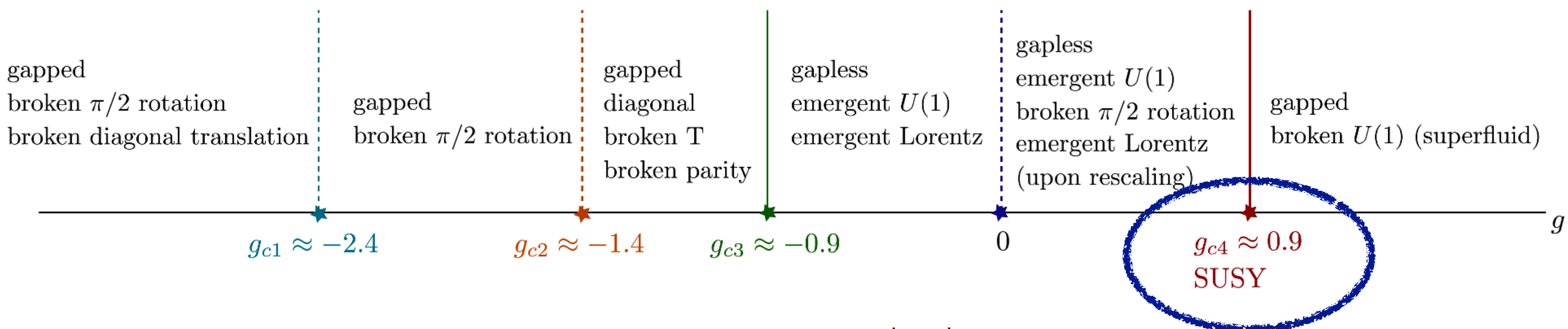




Recent work by Affleck *et al.*

PRB **96**, 125121 (2017)

- Mean-field approx. (similar to ours)
- Low-energy effective model, RG analysis, *etc*.: weak-coupling instabilities



$$\mathcal{L} = \bar{\psi} i \gamma^{\mu} \partial_{\mu} \psi + |\partial_{\mu}\phi|^2 - m^2|\phi|^2 + g_1(\psi_1^{\dagger}\psi_2^{\dagger}\phi + \text{H.c.}) - g_2|\phi|^4 \quad (g > 0),$$

ψ ... fermion field

ϕ ... bosonic field (via Hubbard-Stratonovich transformation)

- **The transition $t = t_c$ is claimed to be SUSY.**
  - **Both fields are massless at $t = t_c$, forming an emergent super-multiplet**

Summary

- We studied the system of square-lattice Majorana fermions that may be realized at the TI-SC interface
- Under the neutrality condition (*i.e.*, $\mu_F = 0$), the minimal model can be faithfully mapped to a spin model. The spin representation has no sign problem in the world-line QMC.
- The ground state for $\mu_F = 0$ is a gapped ("Majorana stripe") state, breaking the translational and rotational symmetries.
- The hybridization induces a quantum phase transition, which might belong to a SUSY universality class.

arXiv: 1711.03632