

Quantum Phases in Bose-Hubbard Models with Spin-orbit Interactions

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The plan

1. Introduction to Bose-Hubbard model (BHM)

2. BHM with spin-orbit coupling

- Weak interaction superfluid
- Strong coupling Mott insulator; 1D & 2D magnetic models
- Phase diagram - magnetic structure in strongly interacting superfluid

3. Slave boson theory

- Construction
- Some consequences

4. Conclusions and outlook

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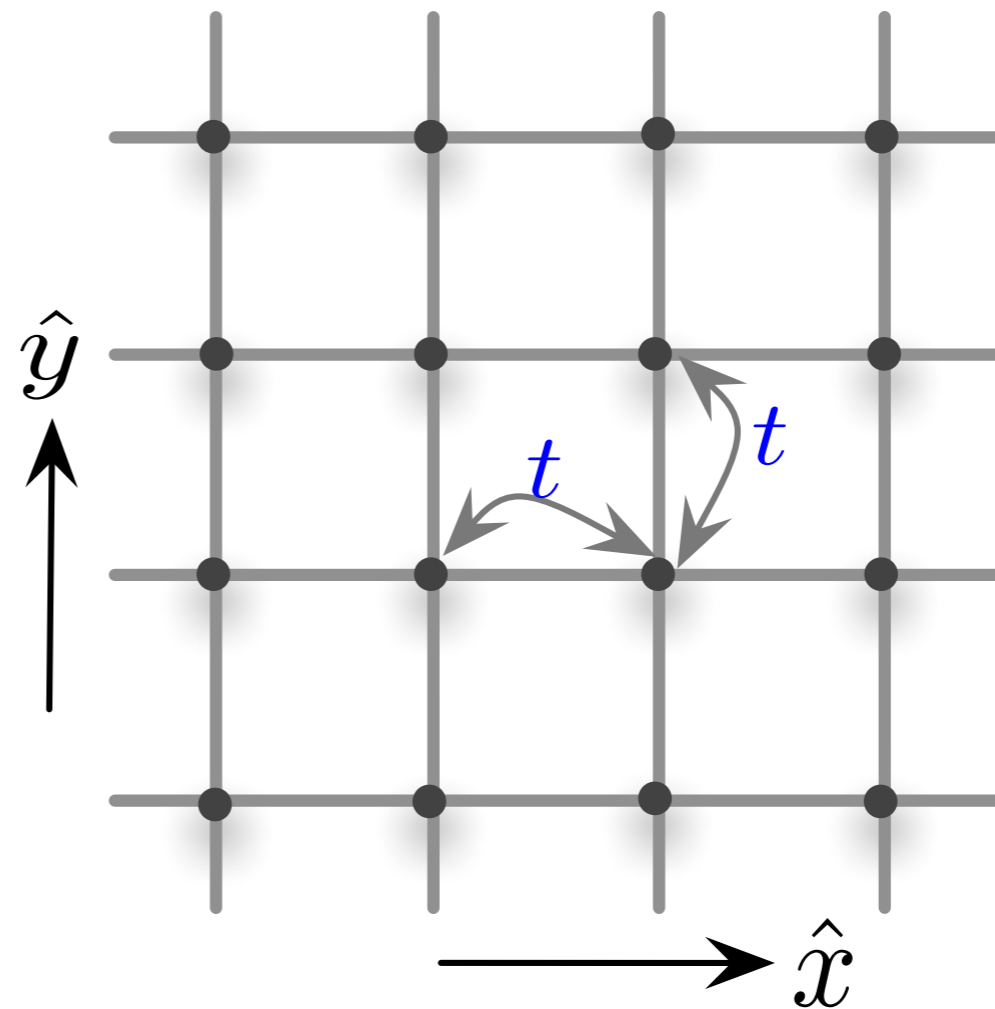
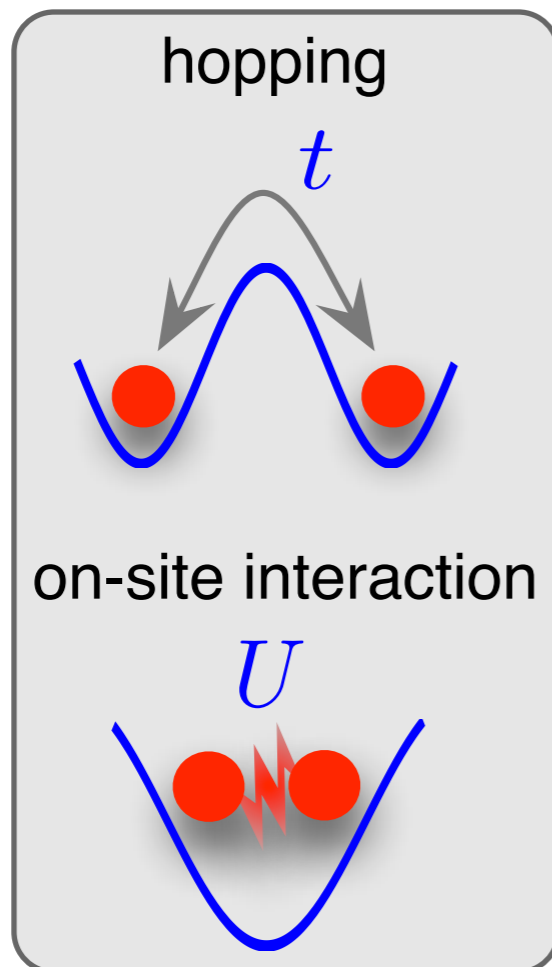
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Optical lattice: Bose-Hubbard model

$$H = -t \sum_{\langle i,j \rangle} (a_i^\dagger a_j + a_j^\dagger a_i) + U \sum_i \frac{n_i(n_i - 1)}{2} - \mu \sum_i n_i$$

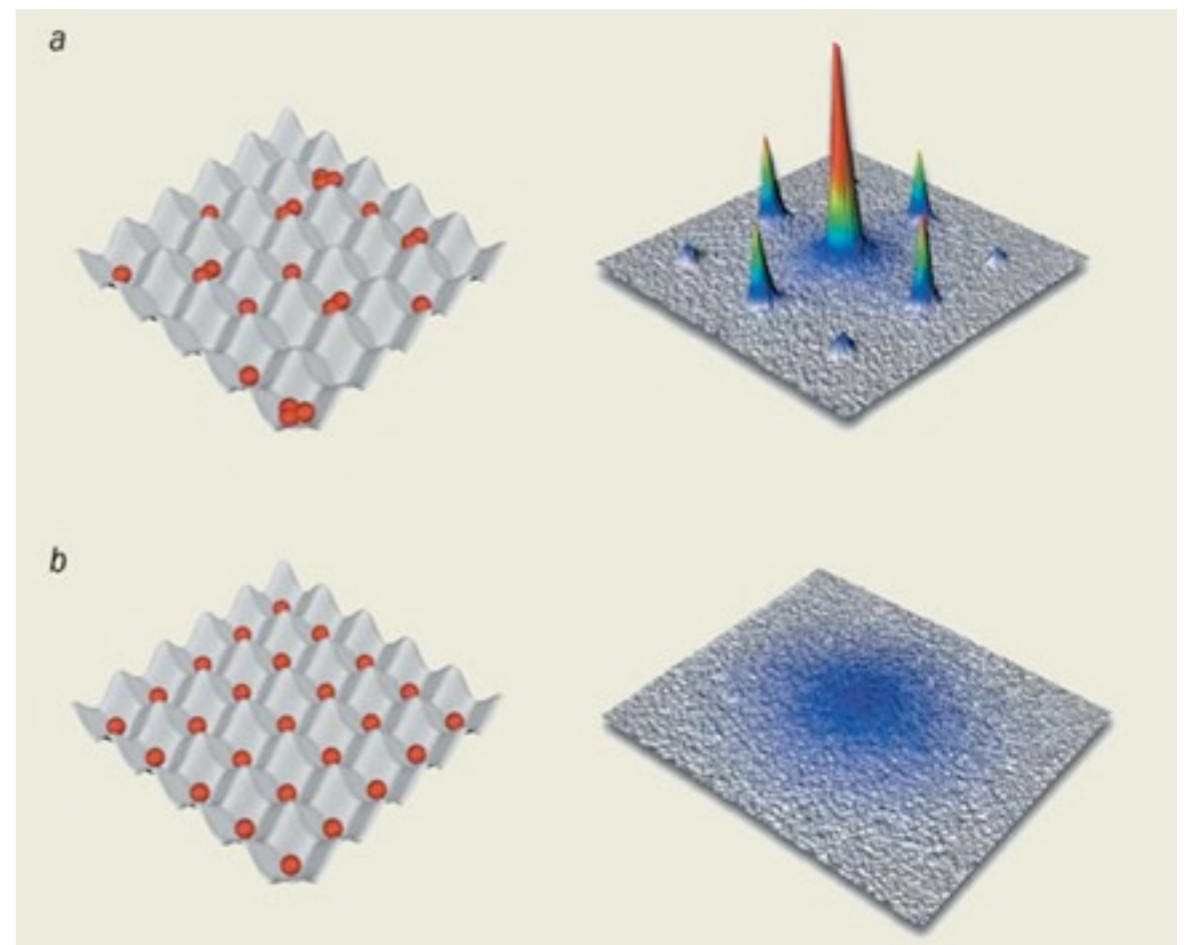
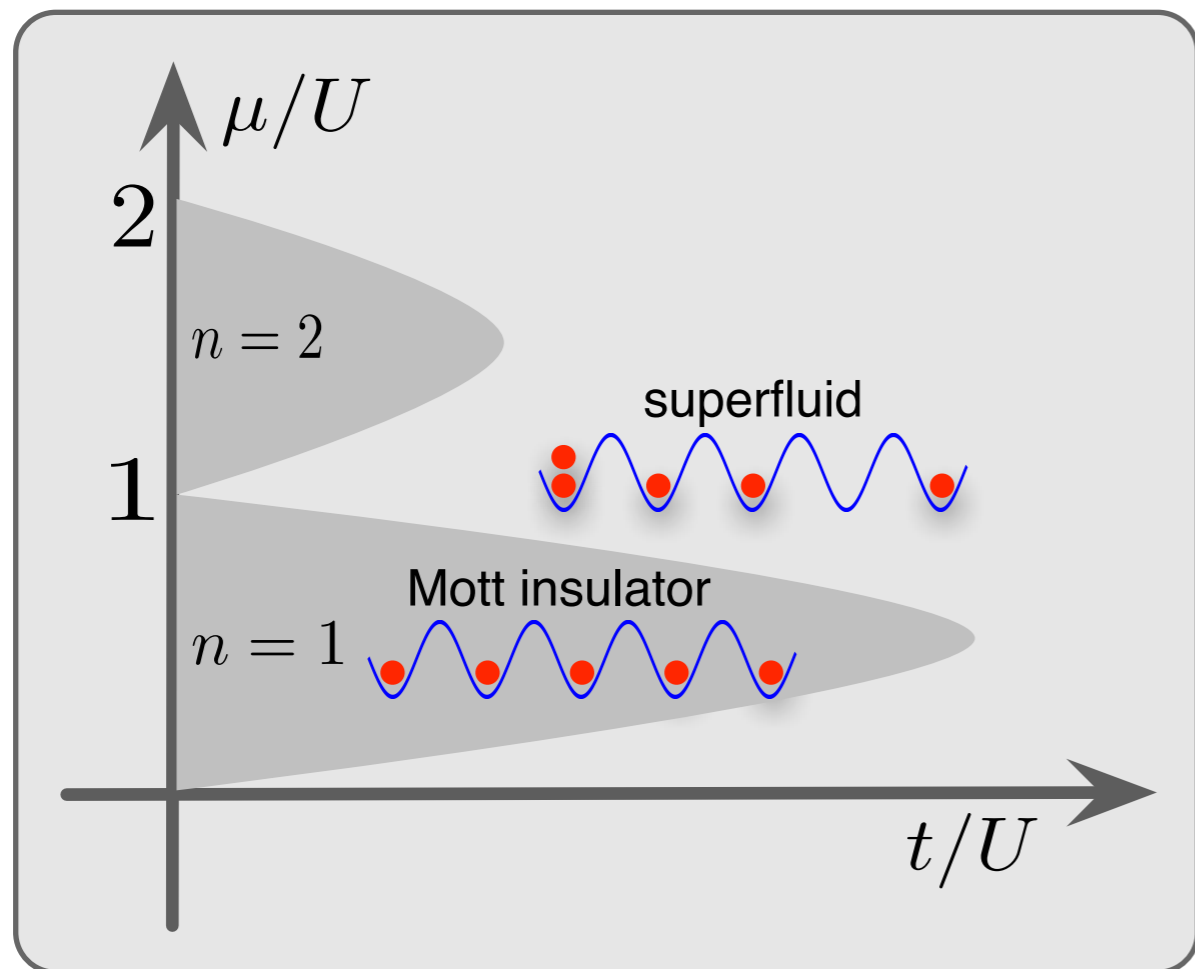


Theory: M. Fisher et al, PRB **40** 546 (1989)
D. Jaksch et al, PRL **81** 3108 (1998)
Experiment: M. Greiner et al., Nature **415** 39 (2002)

Bose-Hubbard Model: mean field theory

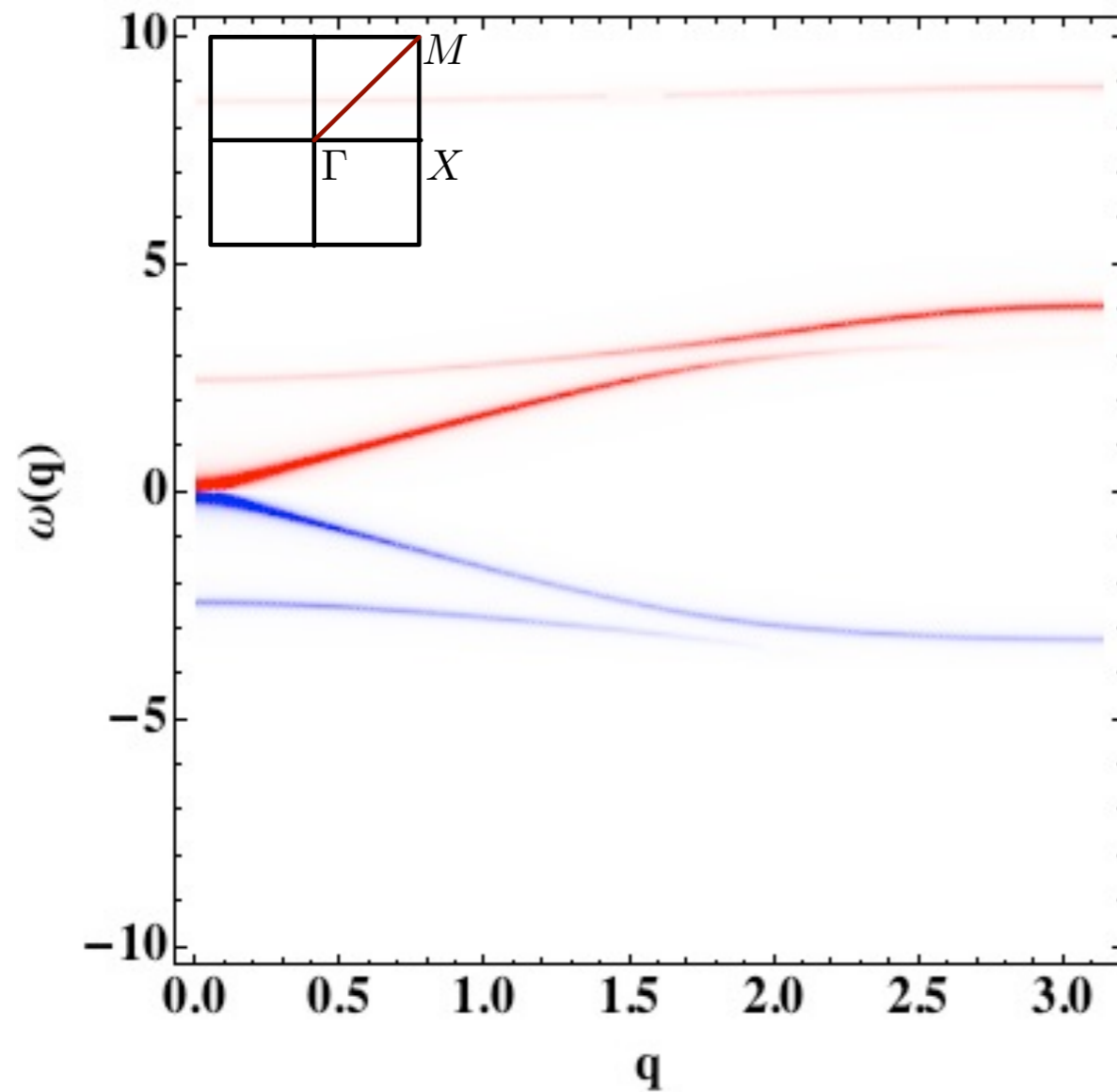
$$a_i^\dagger a_j \rightarrow \langle a_i^\dagger \rangle a_j + a_i^\dagger \langle a_j \rangle - \langle a_i^\dagger \rangle \langle a_j \rangle \quad \text{order parameter}$$

$$H^{\text{mft}} = U \frac{n_i(n_i - 1)}{2} - \mu n_i - t \sum_{j \in \text{nn } i} (\langle a_j \rangle a_i^\dagger + \langle a_j^\dagger \rangle a_i)$$

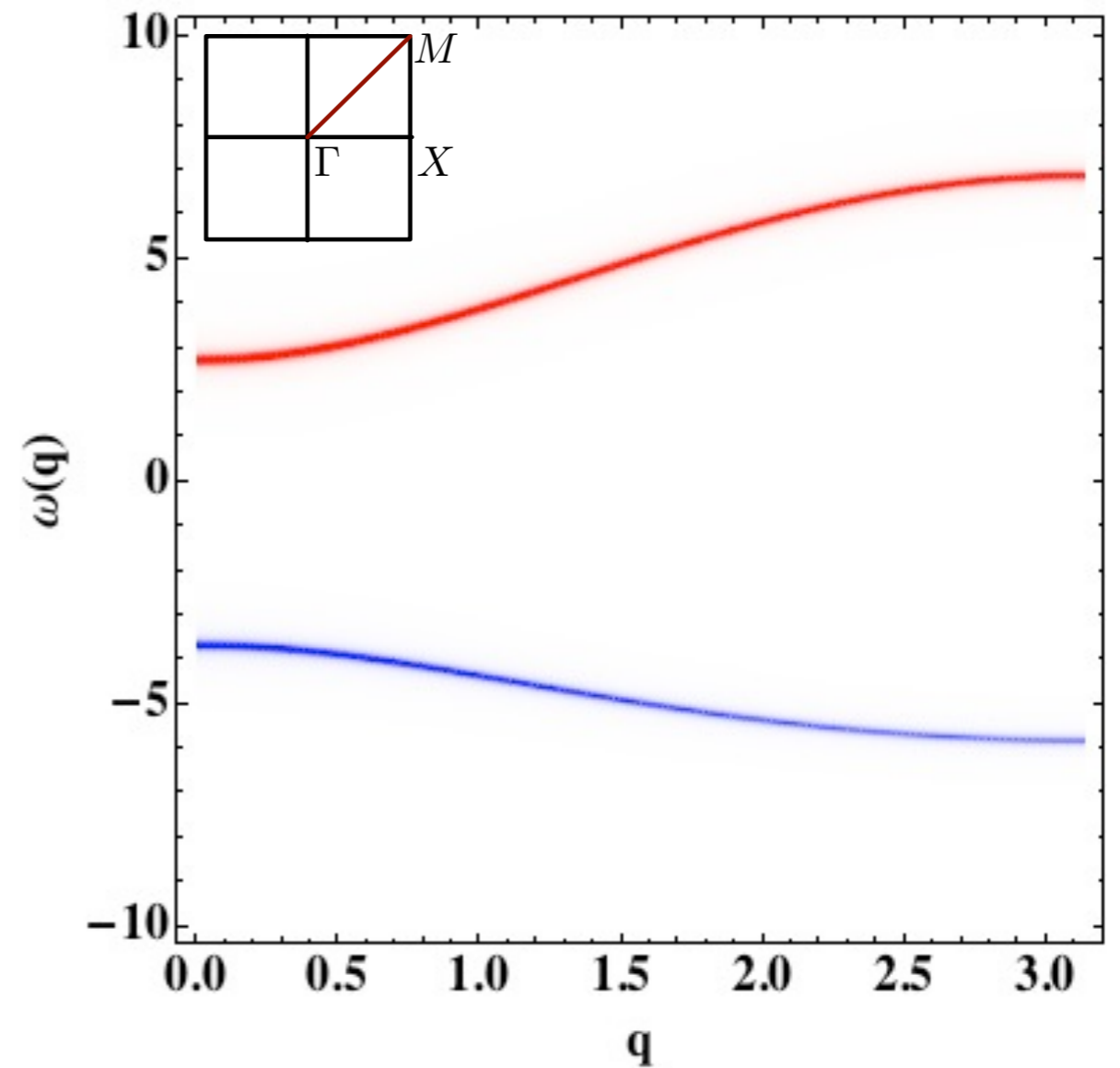


Bose-Hubbard Model: excitations, RPA

Superfluid



Mott insulator



Bose-Hubbard Model: summary

	Mott	Superfluid	Normal
Order Parameters	zero	nonzero (uniform)	zero
Compressibility	zero	nonzero	nonzero
Excitations	gapped	gapless	gapless (?)
Charge Transport (DC...vities)	zero	nonzero + superfluid	nonzero

Considerations in terms of **many-body wave functions** and **density matrices** can be carried out for these different phases (Yang, Kohn, Bloch, Leggett).

What are the effects of spin-orbit couplings in Bose-Hubbard model?

W.Cole et al. PRL **109** 085302 (2012)



William Cole



Arun Paramekanti



Nandini Trivedi

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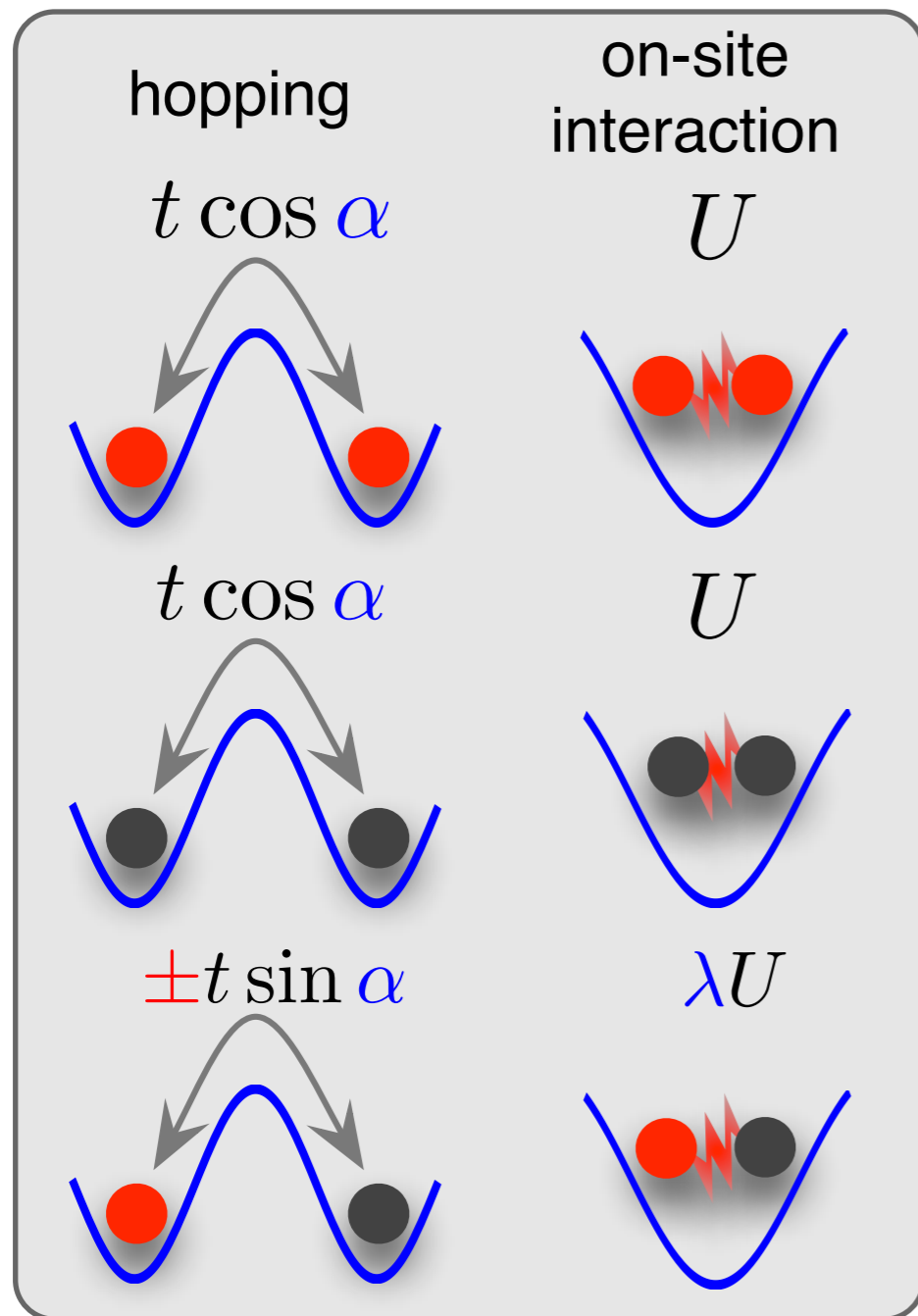
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Bose-Hubbard Model: with spin-orbit interactions

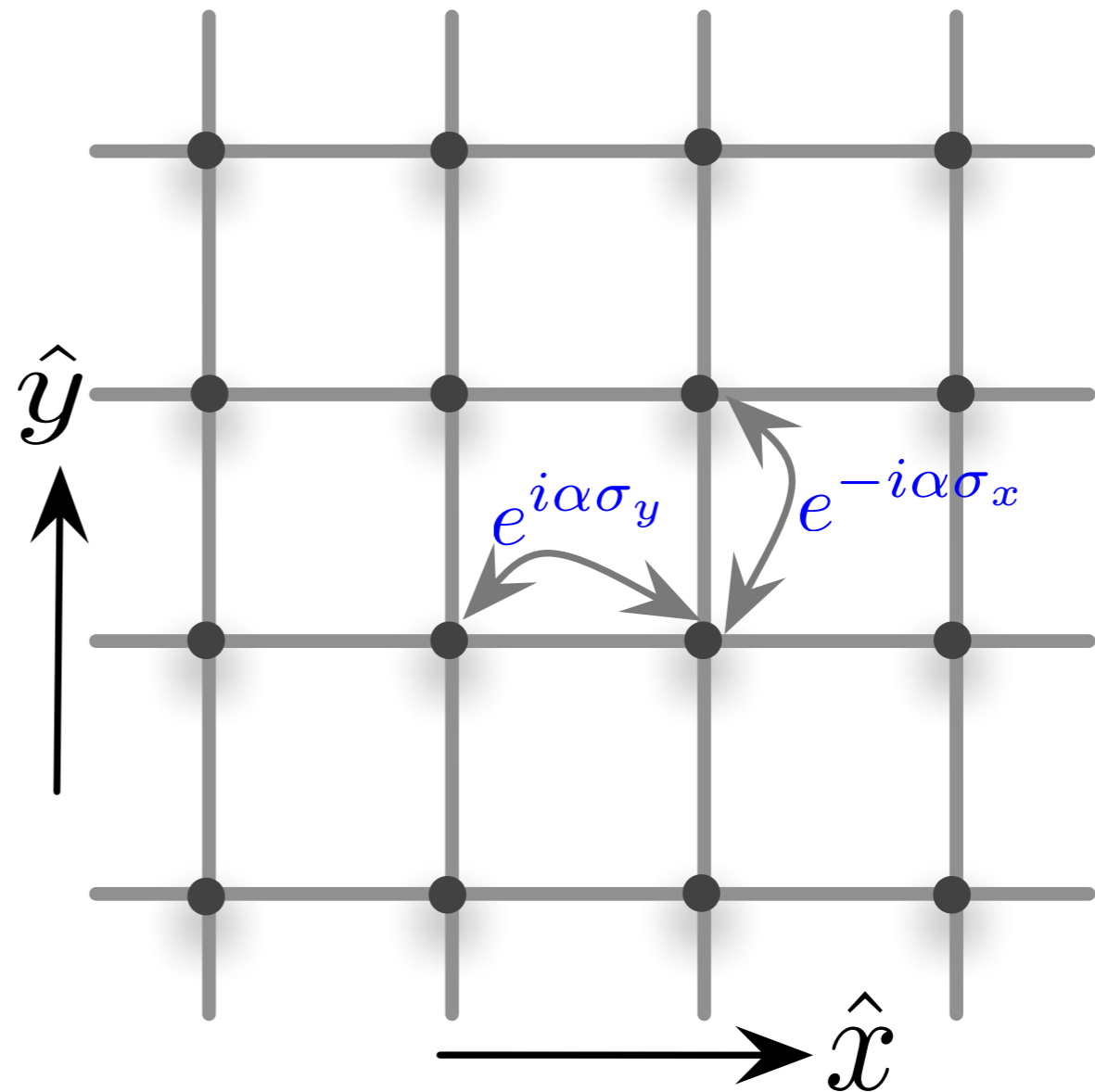
● ● two internal states



$$H_{\text{hop}} = -t a_{i\sigma}^\dagger \mathcal{R}_{\hat{v}}^{\sigma\sigma'} a_{i+\hat{v}\sigma'}$$

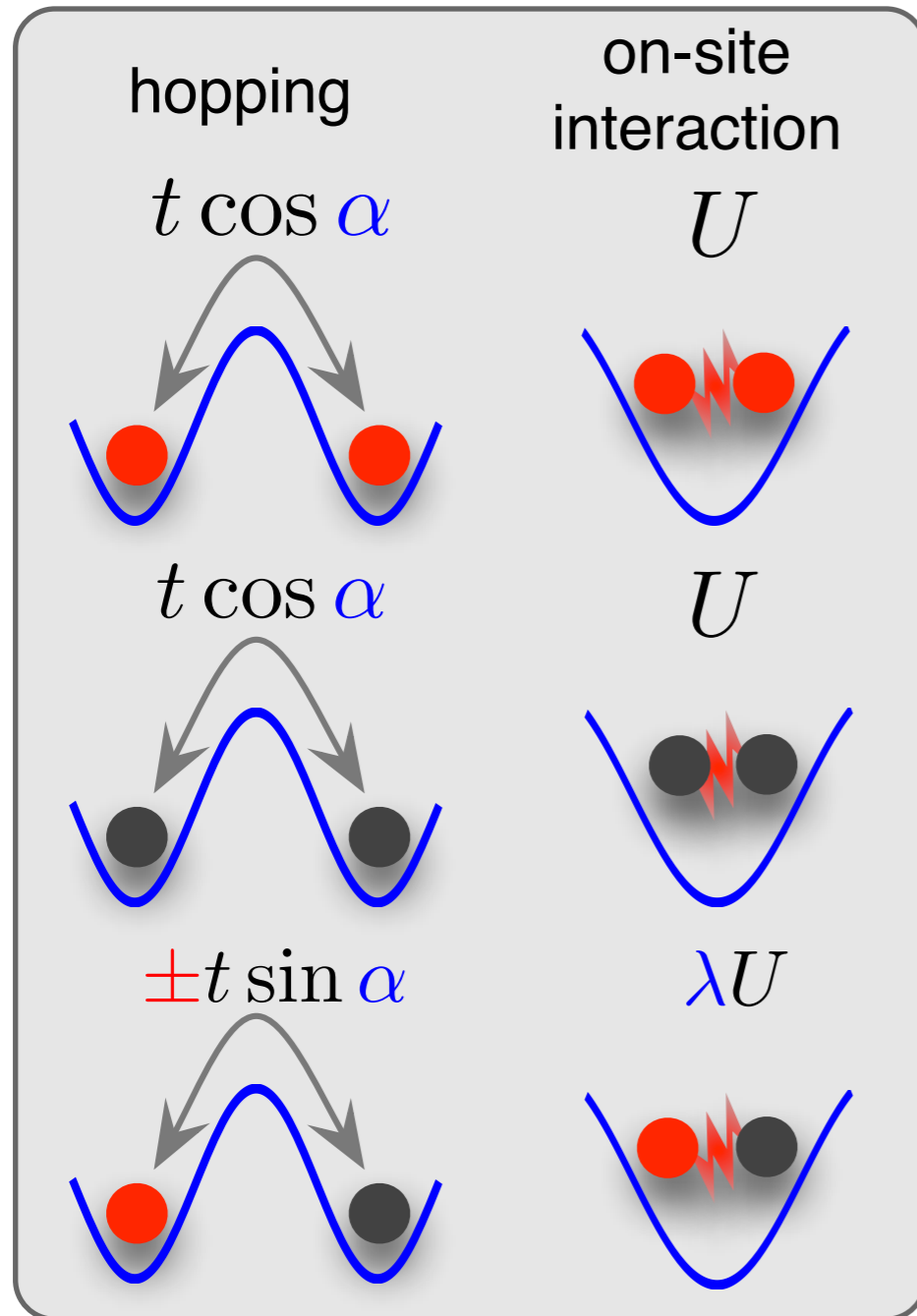
$$\sigma, \sigma' = \uparrow, \downarrow$$

$$\hat{v} = \hat{x}, \hat{y}$$

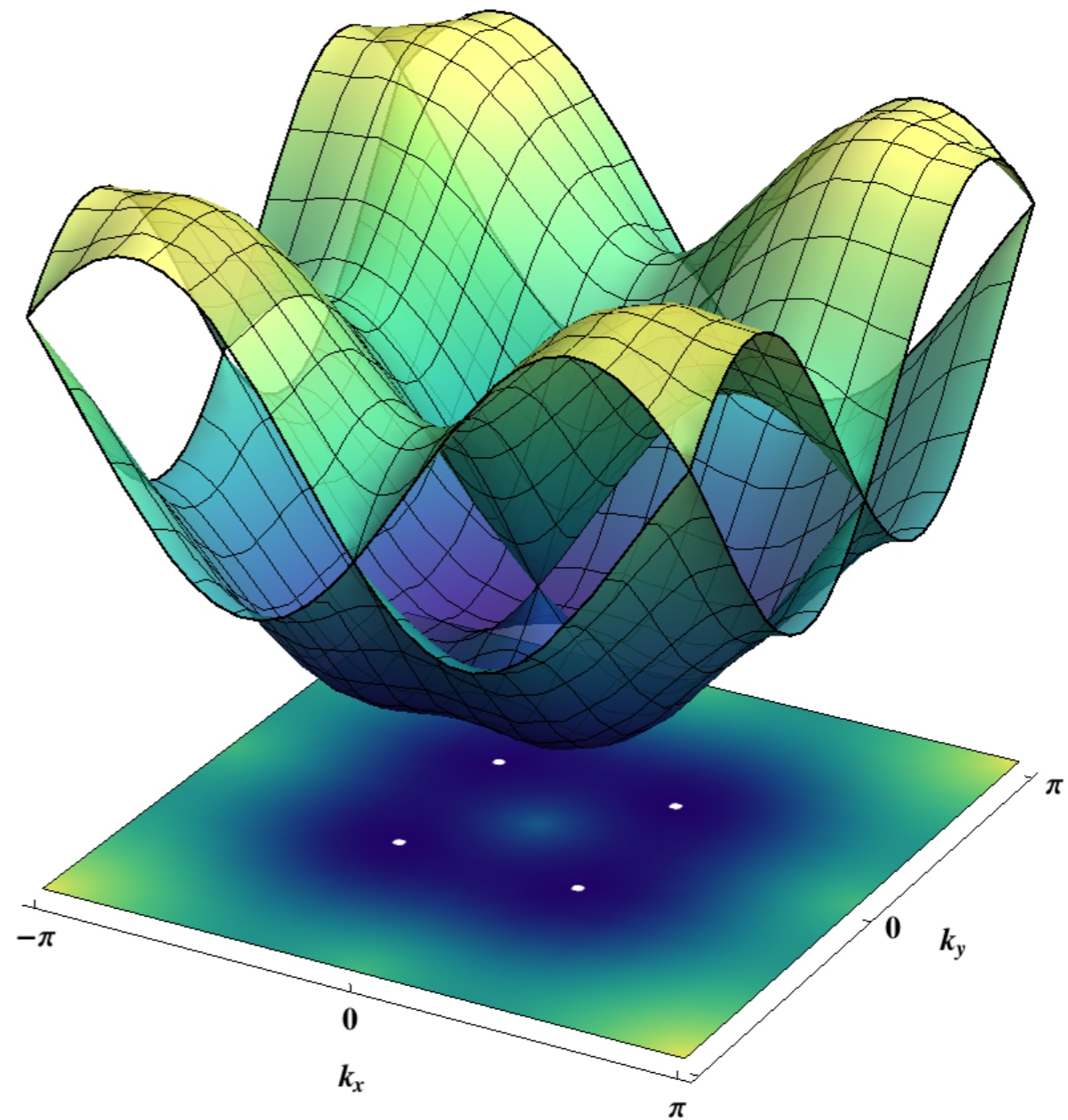


Bose-Hubbard Model: non-interacting band structure

● ● two internal states



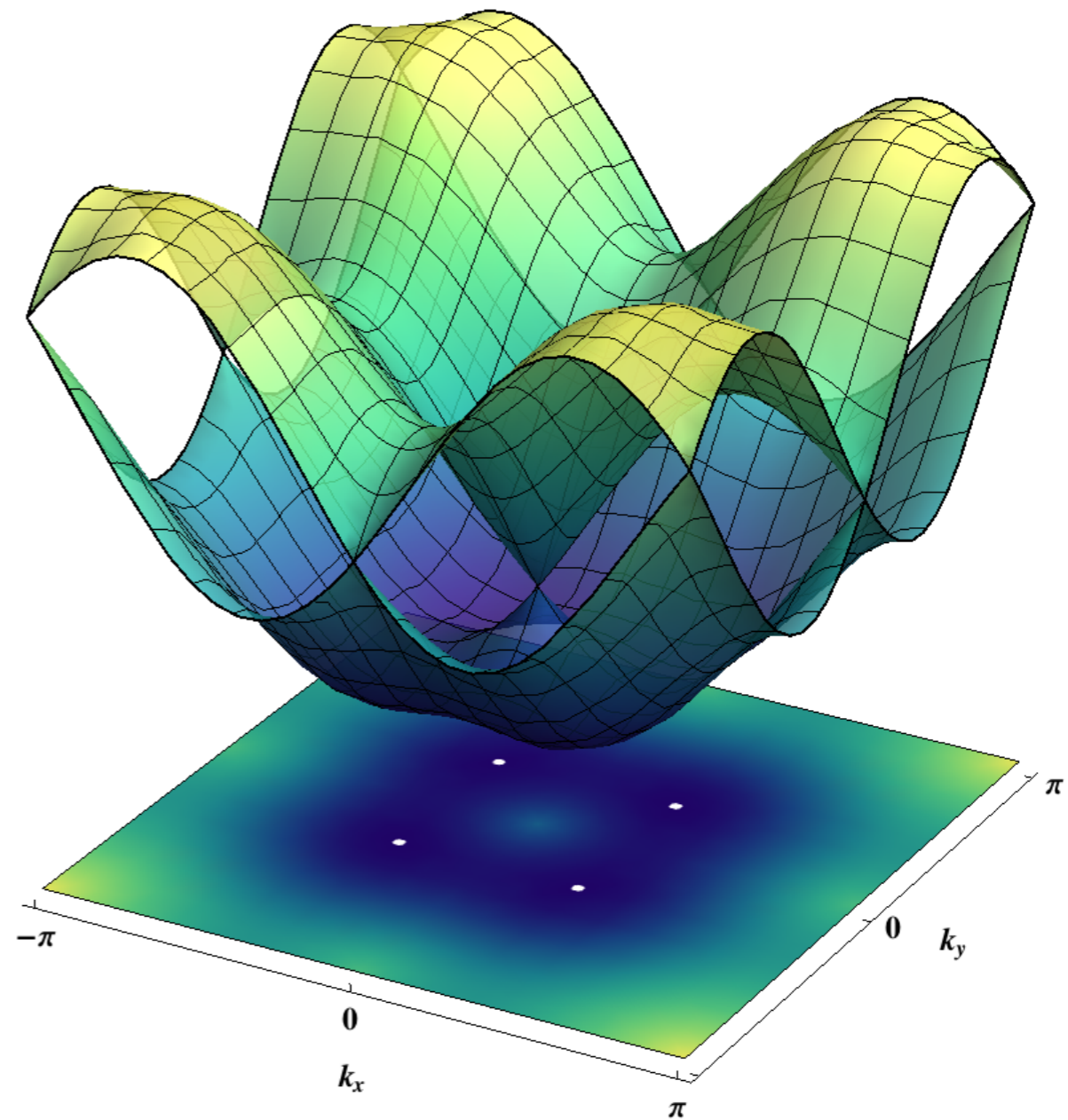
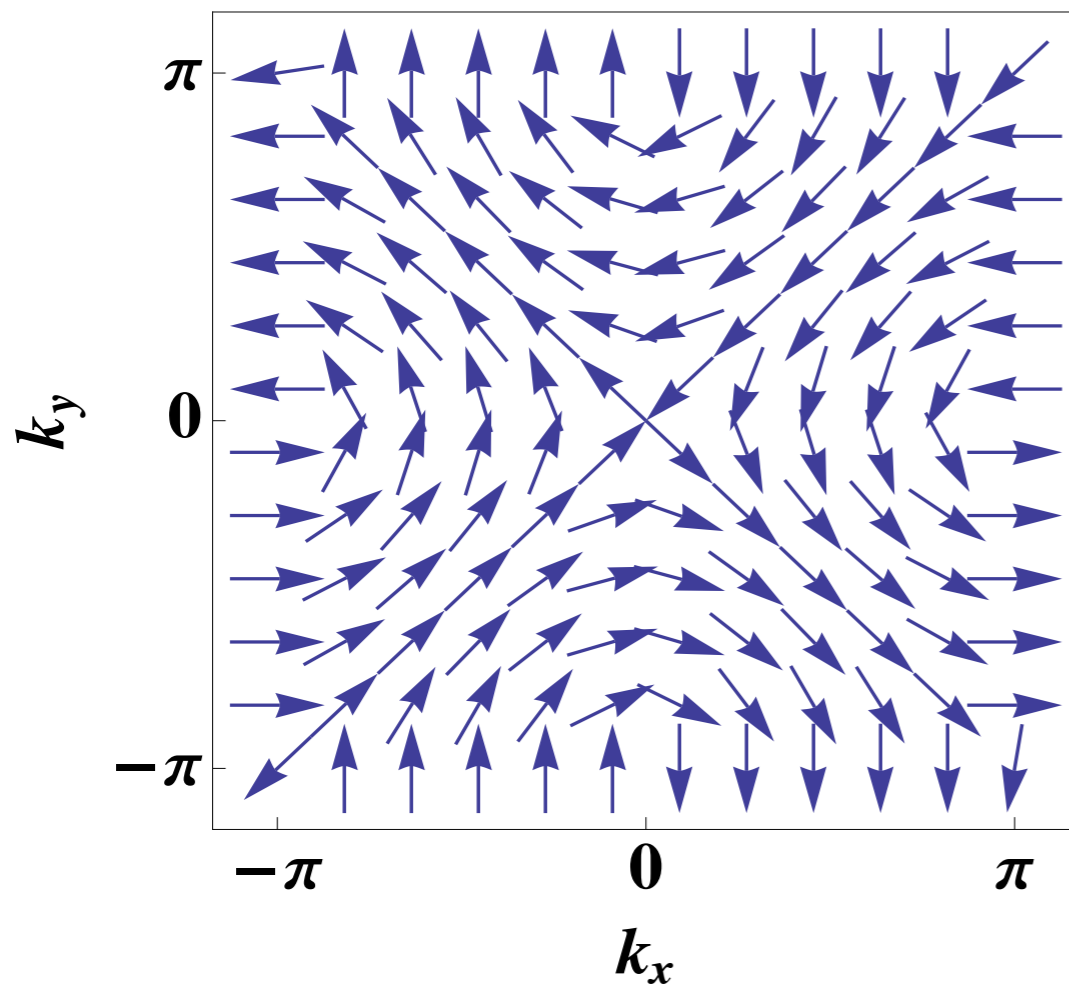
$\alpha = \pi/4$ Lattice version of the Rashba spin-orbit coupling



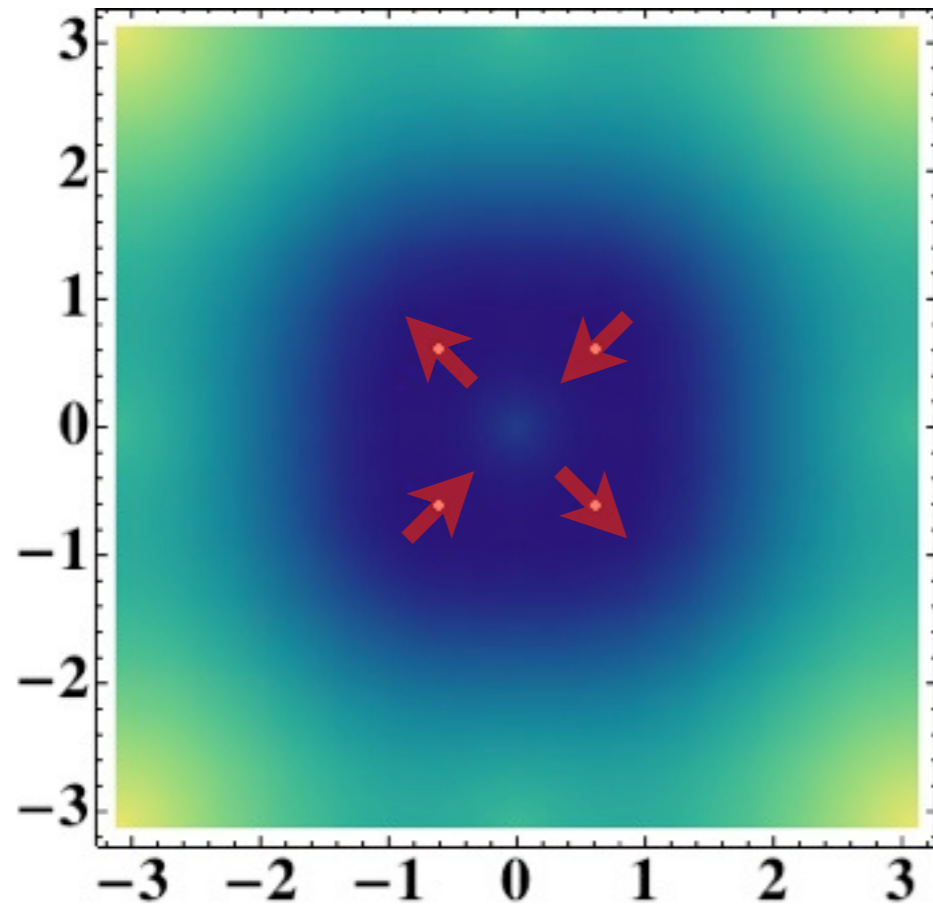
Non-interacting band structure

Non-trivial winding (Chern number) around the Γ point due to existence of Dirac points:

$\alpha = \pi/4$ Lattice version of the Rashba spin-orbit coupling



Weak coupling superfluid



Four degenerate states: $(\pm k_0, \pm k_0)$

$$\sqrt{2} \tan k_0 = \tan \alpha$$

Spins lie in the x-y plane.

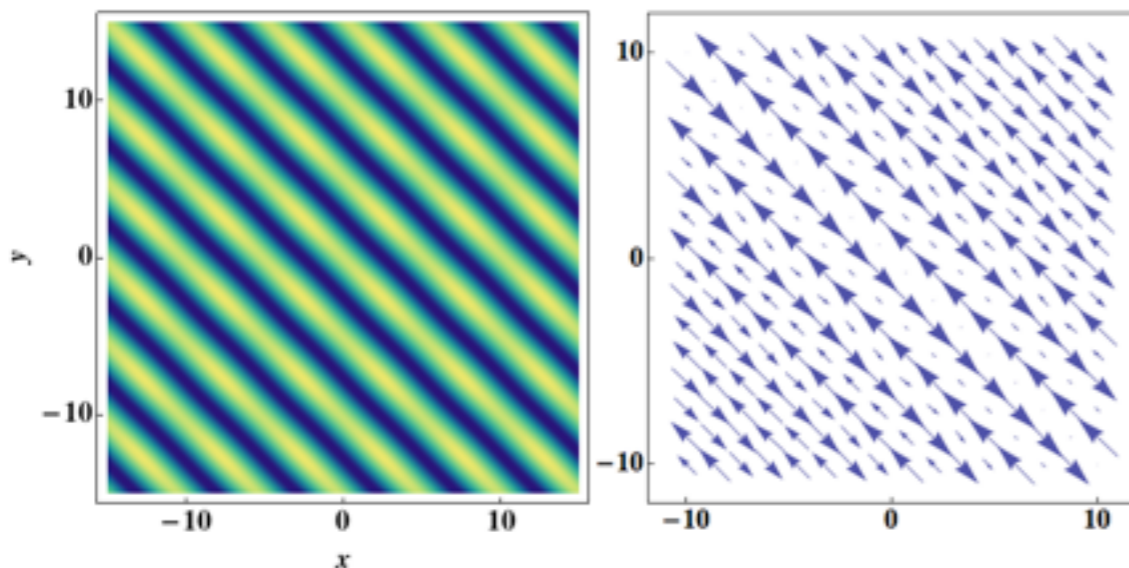
$$U_{\text{int}} \propto \frac{1 + \lambda}{2} (n_{\uparrow} + n_{\downarrow})^2 + \frac{1 - \lambda}{2} (n_{\uparrow} - n_{\downarrow})^2$$

$\lambda < 1$ **no polarization**

only one state is occupied; uniform spin and number density

$\lambda > 1$ **polarization**

two opposite states are occupied; strip spin and uniform number density



Cf. Considerations of Y.Li et al, PRL **108** 225301 (2012)

W.Cole et al. PRL **109** 085302 (2012)

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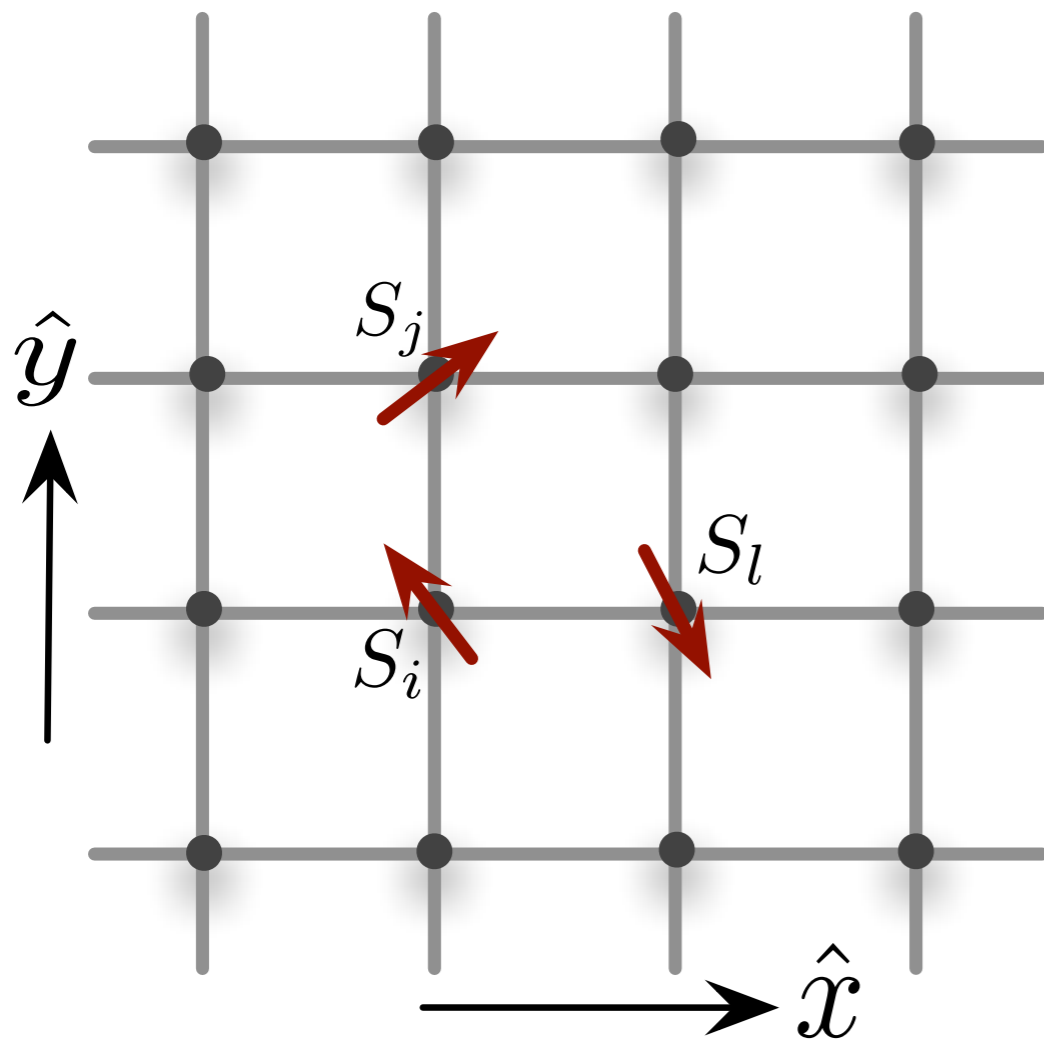
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Strong coupling Mott insulator

Consider the case in which on average, there is one boson per site. Standard perturbation theory gives low energy effective magnetic Hamiltonian



x-direction:

$$-\frac{\cos(2\alpha)}{\lambda} S_i^x S_l^x - \frac{1}{\lambda} S_i^y S_l^y - \frac{2\lambda - 1}{\lambda} \cos(2\alpha) S_i^z S_l^z$$

$$- \sin(2\alpha) \hat{y} \cdot (\mathbf{S}_i \times \mathbf{S}_l)$$

y-direction:

$$-\frac{1}{\lambda} S_i^x S_j^x - \frac{\cos(2\alpha)}{\lambda} S_i^y S_j^y - \frac{2\lambda - 1}{\lambda} \cos(2\alpha) S_i^z S_j^z$$

$$+ \sin(2\alpha) \hat{x} \cdot (\mathbf{S}_i \times \mathbf{S}_j)$$

Dzyaloshinskii-Moriya coupling

Cf. DM term in superfluid, X. Xu and J.Han PRL **108** 185301 (2012)

W.Cole et al. PRL **109** 085302 (2012)

Z.Cai et al. PRA **85** 061606R (2012)

J.Radic et al. PRL **109** 085303 (2012)

M.Gong et al, arXiv:1205.6211

1D magnetic Hamiltonian

For example, 1D Hamiltonian along x-direction. Rotate spins around x by $\pi/2$, such that DM vector is along z

$$-\frac{\cos(2\alpha)}{\lambda} S_i^x S_l^x - \frac{\cos(2\alpha)}{\lambda} (2\lambda - 1) S_i^y S_l^y - \frac{1}{\lambda} S_i^z S_l^z - \sin(2\alpha) (S_i^y S_l^x - S_i^x S_l^y)$$

Some 1D AFM system with DM

System	DM/Exchange
Cooper Benzoate	0.05
Yb ₄ As ₃	?
BaCu ₂ Si ₂ O ₇	0.02?
CsCuCl ₃	0.18

XY-exchange and DM couplings can be tuned by changing α and λ , in particular, DM can be made as large as exchange coupling;

Various limits of the model can be solved exactly.

1D magnetic Hamiltonian: special cases

Case I $\lambda \rightarrow 0$ rotation around x by π
every other site

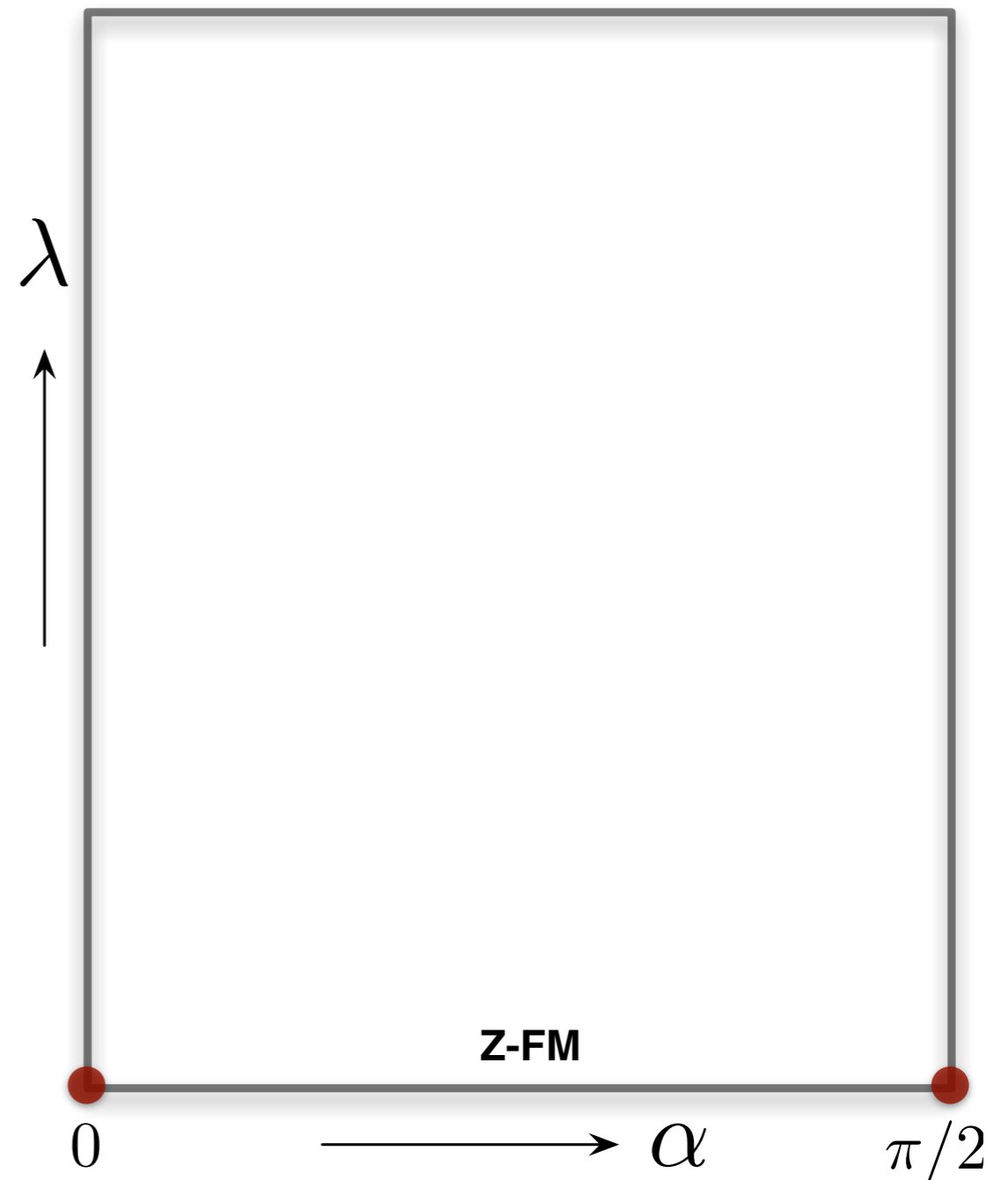
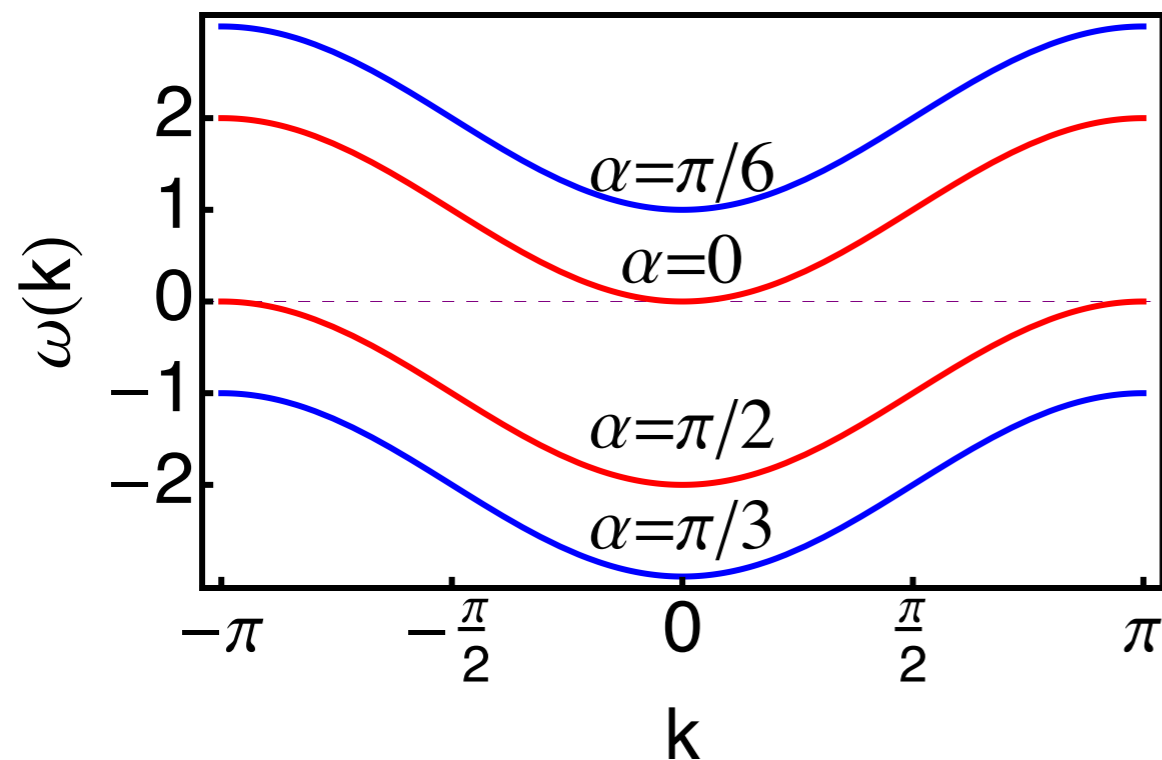
$$-\frac{1}{\lambda} (\cos(2\alpha) S_i^x S_l^x + \cos(2\alpha) S_i^y S_l^y - S_i^z S_l^z)$$

Z-ferromagnetic

$$0 < \alpha < \pi/2; \quad |\cos(2\alpha)| < 1$$

critical points:

$$\alpha = 0, \pi/2; \quad |\cos(2\alpha)| = 1$$

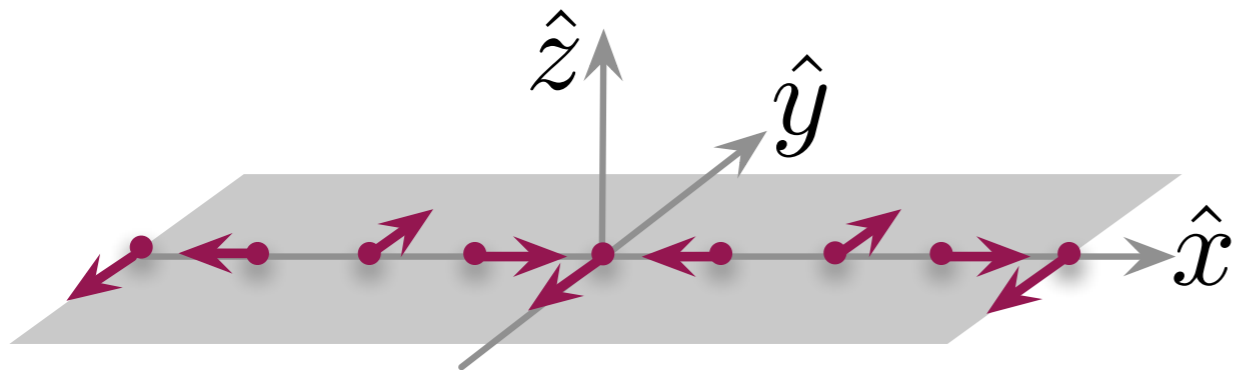


1D magnetic Hamiltonian: special cases

Case II $\lambda = 1$ XXZ+DM

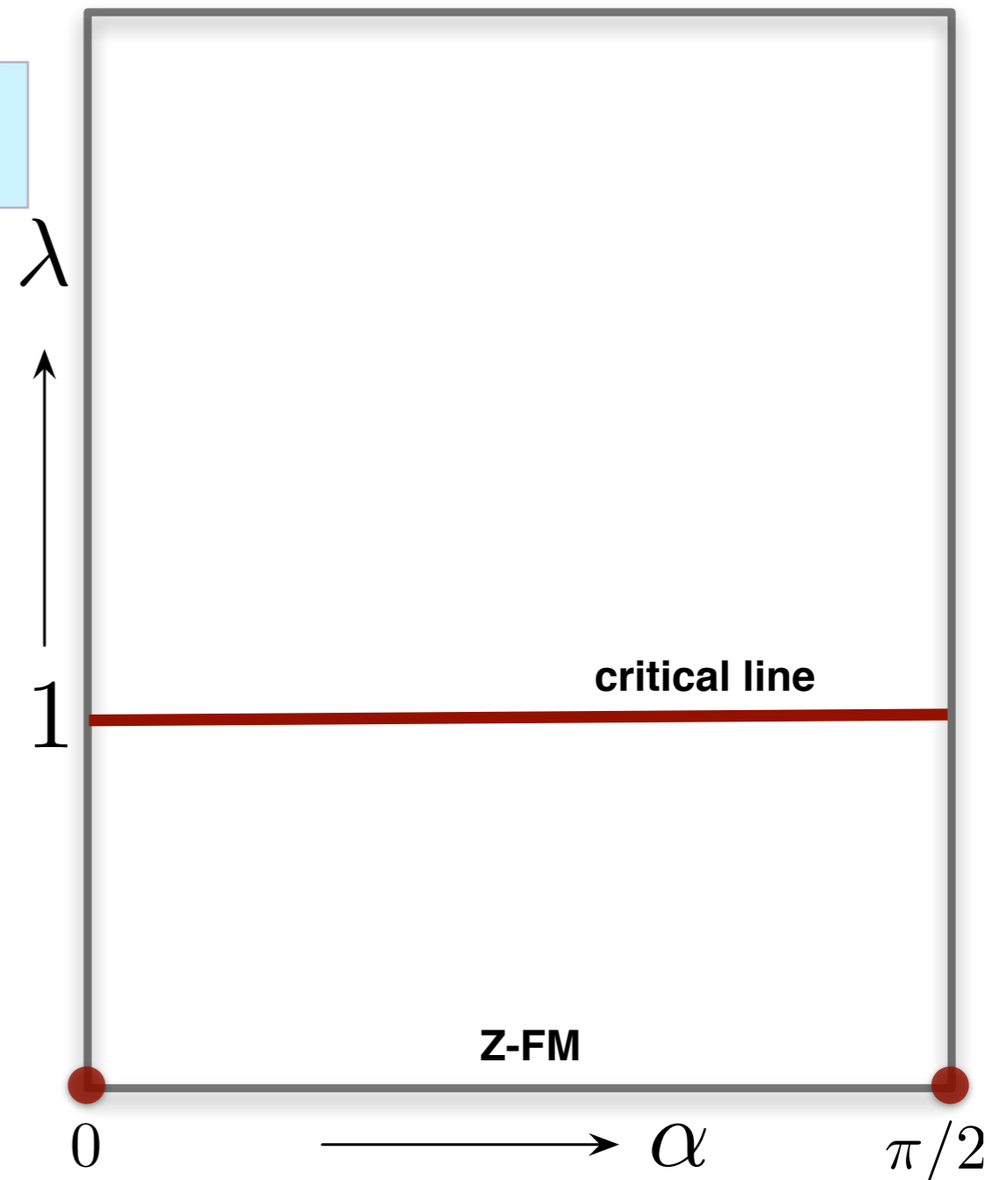
$$-S_i^x S_l^x - S_i^y S_l^y - \frac{1}{\cos(2\alpha)} S_i^z S_l^z - \tan(2\alpha)(S_i^y S_l^x - S_i^x S_l^y)$$

Rotate each spin around z by $\phi=2\alpha$.



Can be mapped to XXZ model with a new twisted boundary condition. It can be solved with Bethe ansatz and turns out to be always critical in bulk.

$$-(\tilde{S}_i^x \tilde{S}_l^x + \tilde{S}_i^y \tilde{S}_l^y + \tilde{S}_i^z \tilde{S}_l^z)$$



1D magnetic Hamiltonian: special cases

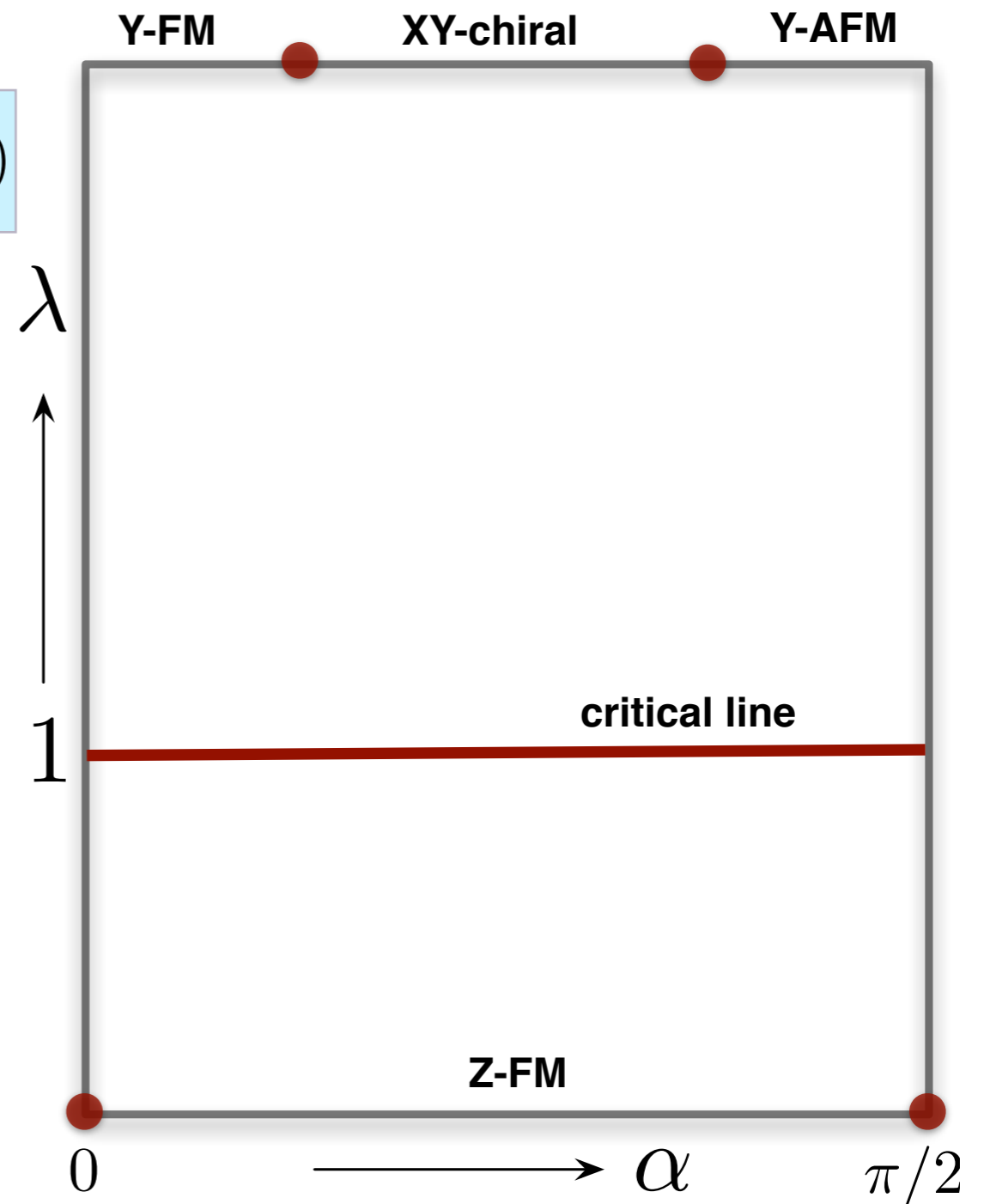
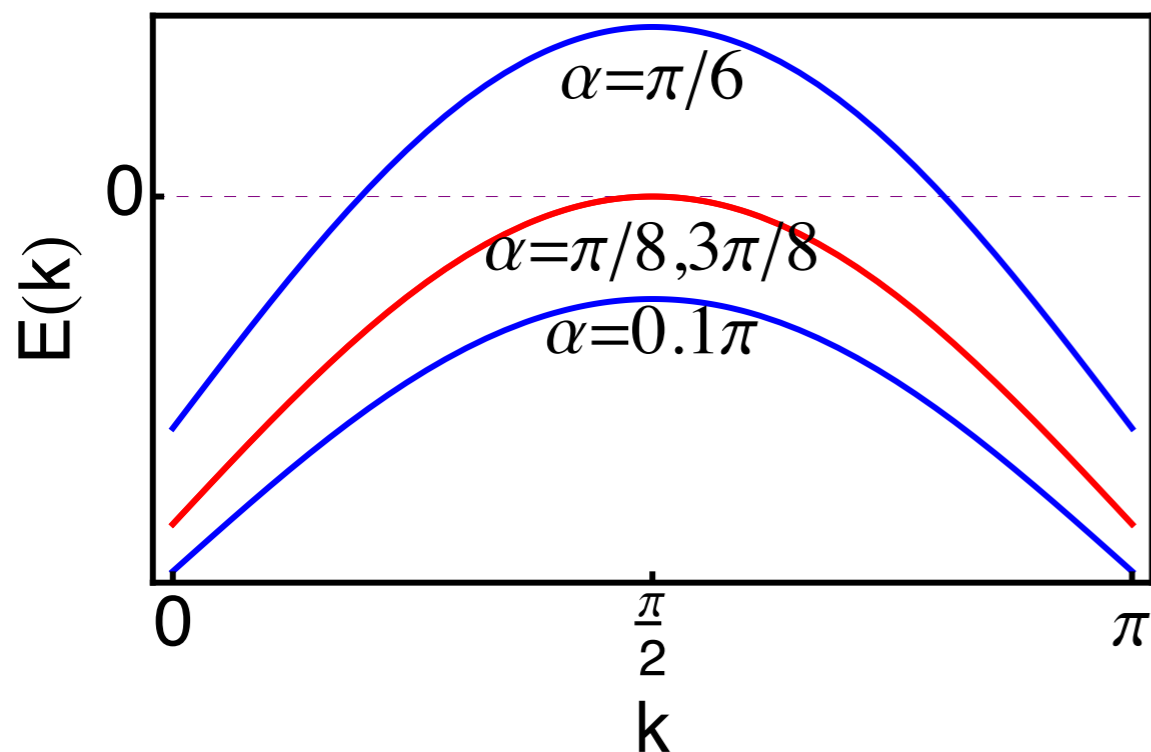
Case III $\lambda \rightarrow \infty$

$$-2 \cos(2\alpha) S_i^y S_l^y - \sin(2\alpha) (S_i^y S_l^x - S_i^x S_l^y)$$

Can be solved using Jordan-Wigner.

$$E_{\pm}(k) = \sin(2\alpha) \sin k \pm |\cos(2\alpha)|$$

Critical points: $\alpha = \pi/8; 3\pi/8$



1D magnetic Hamiltonian: special cases

Case IV $\alpha = \pi/4$

$$-\frac{1}{\lambda} S_i^z S_l^z - (S_i^y S_l^x - S_i^x S_l^y)$$

Ising+DM, can be mapped to XXZ model

$\lambda > 1$ XY-chiral

$\lambda < 1$ Z-Ferromagnetism

Case V XXZ model

$$-\frac{1}{\lambda} (\pm S_i^x S_l^x \pm (2\lambda - 1) S_i^y S_l^y + S_i^z S_l^z)$$

$\alpha = 0$

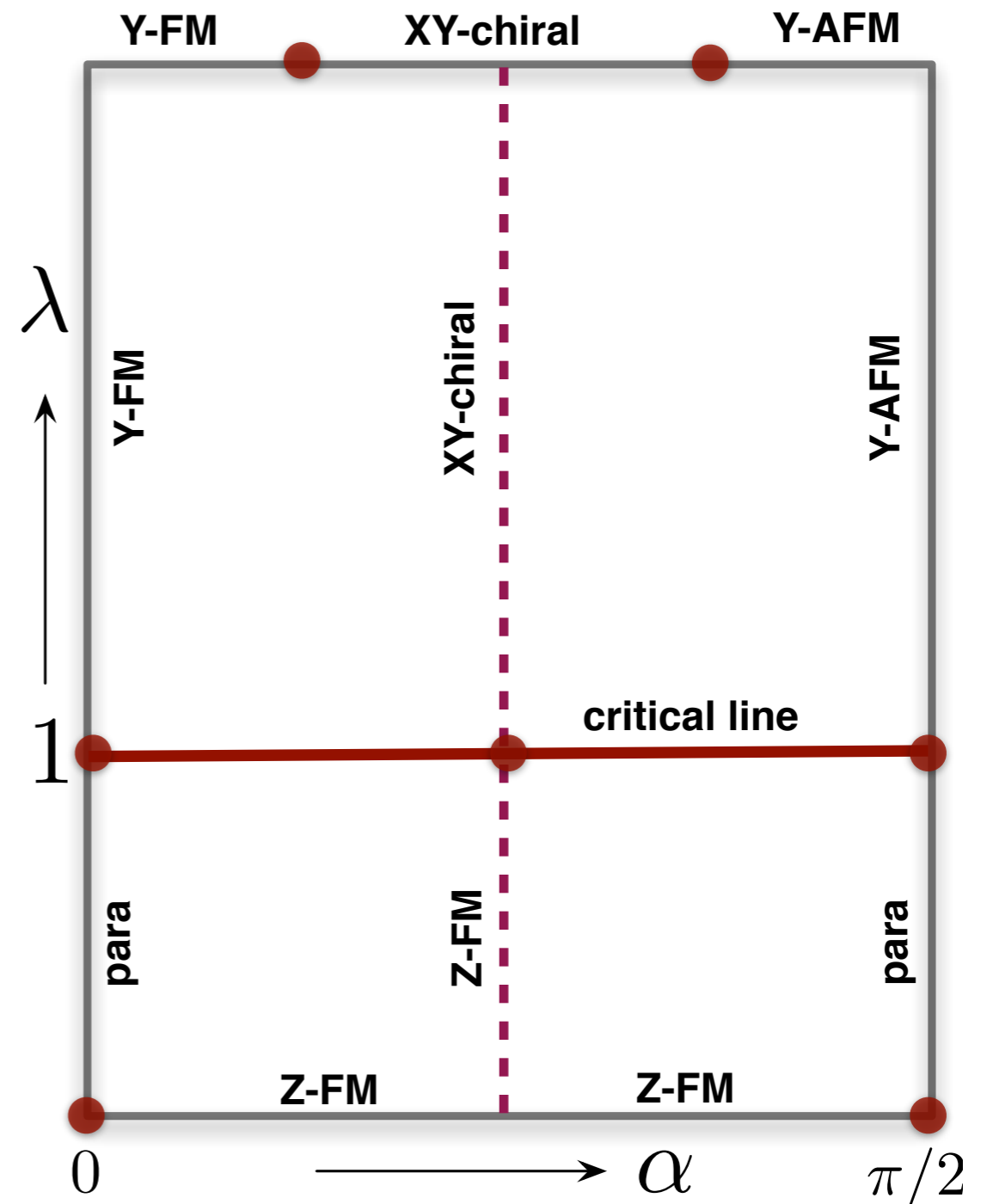
$\alpha = \pi/2$

$\lambda < 1$ Para

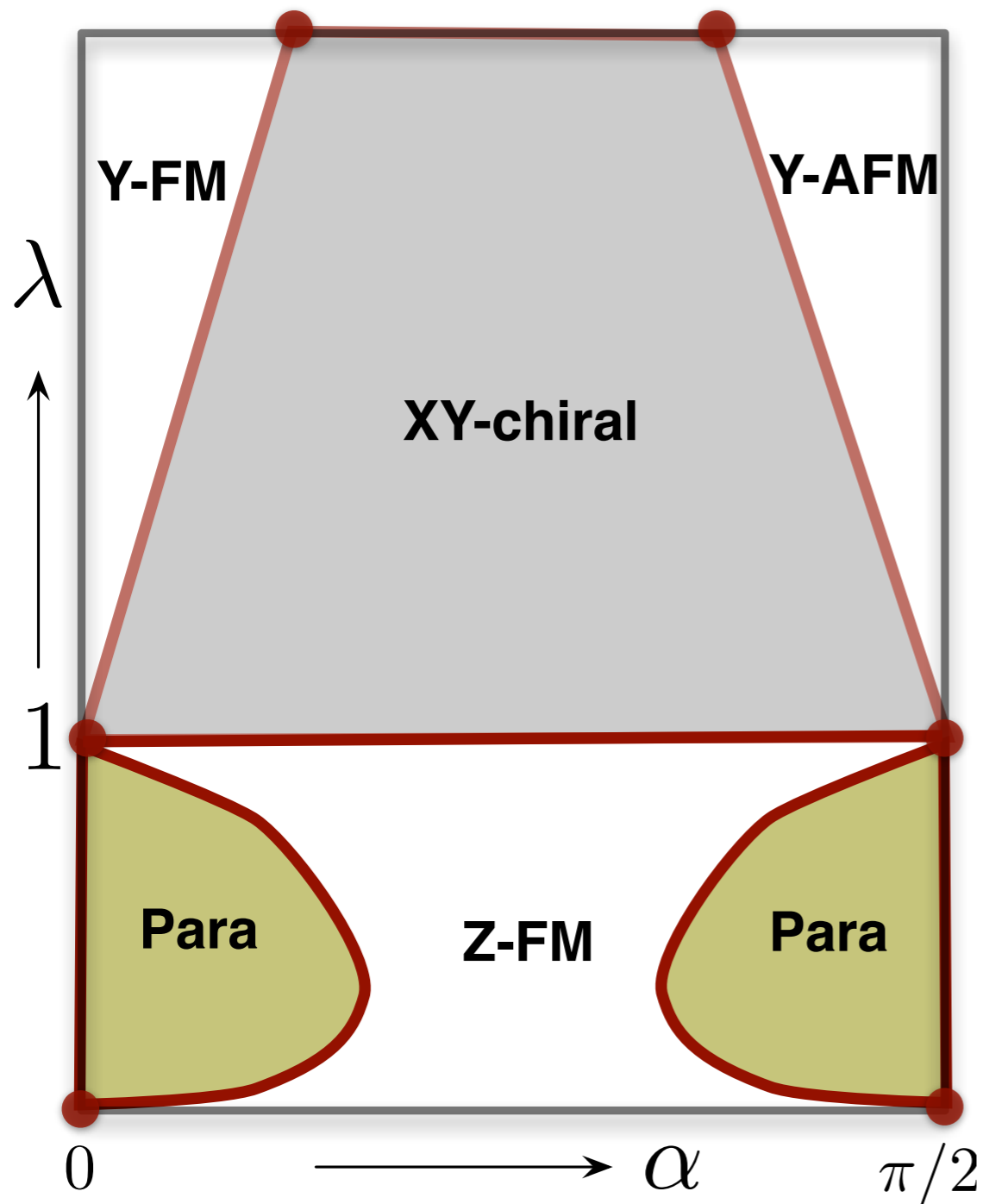
Para

$\lambda > 1$ Y-Ferro

Y-Antiferro



Schematic Phase diagram



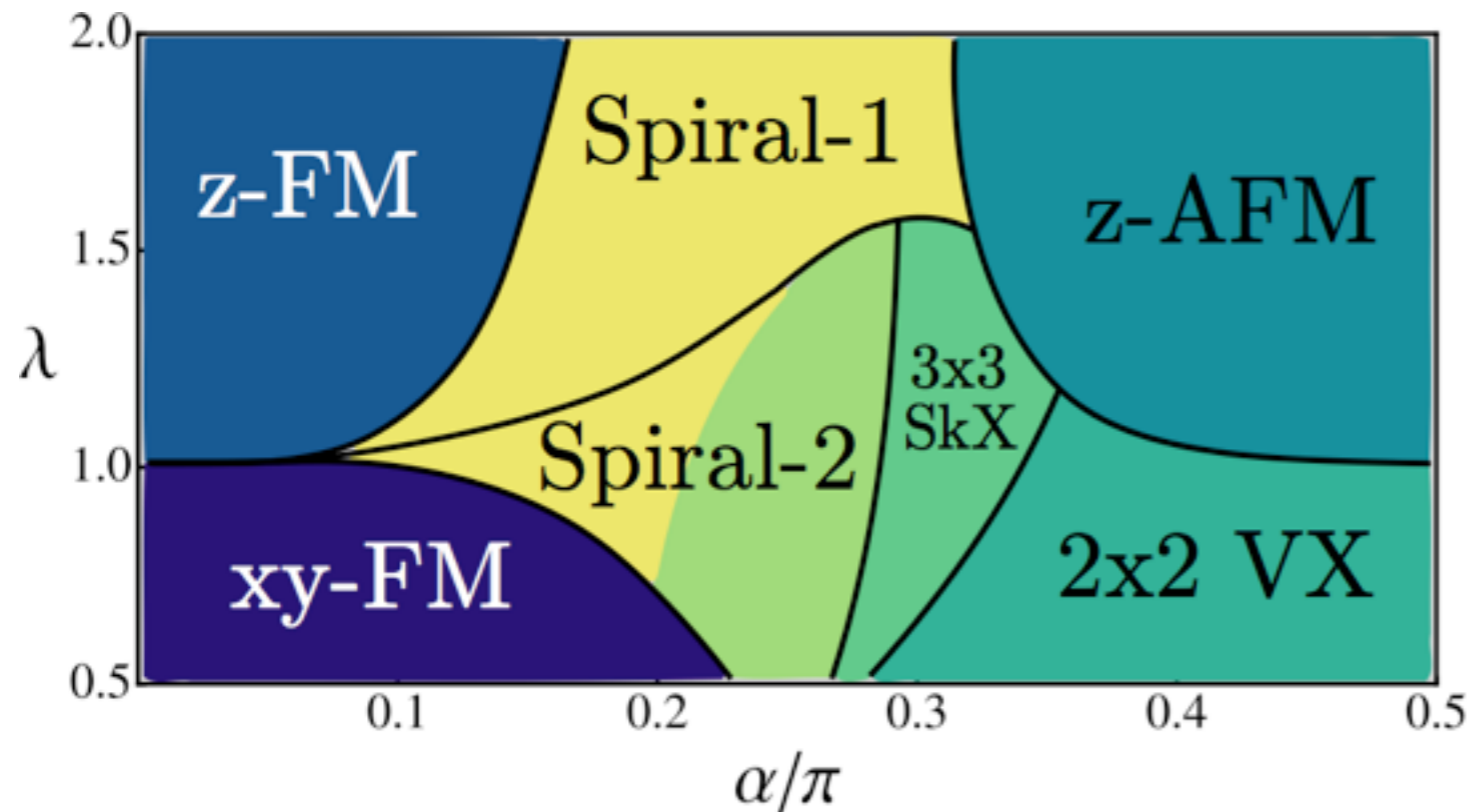
What needs to be done:

Exact Diagonalization (12 sites) suggests phase diagram as shown left. It confirms the part for $\lambda > 1$; but for $\lambda < 1$, not very clear;

Calculate phase diagram with DMRG technique;

Calculate correlation functions and investigate experimental signatures.

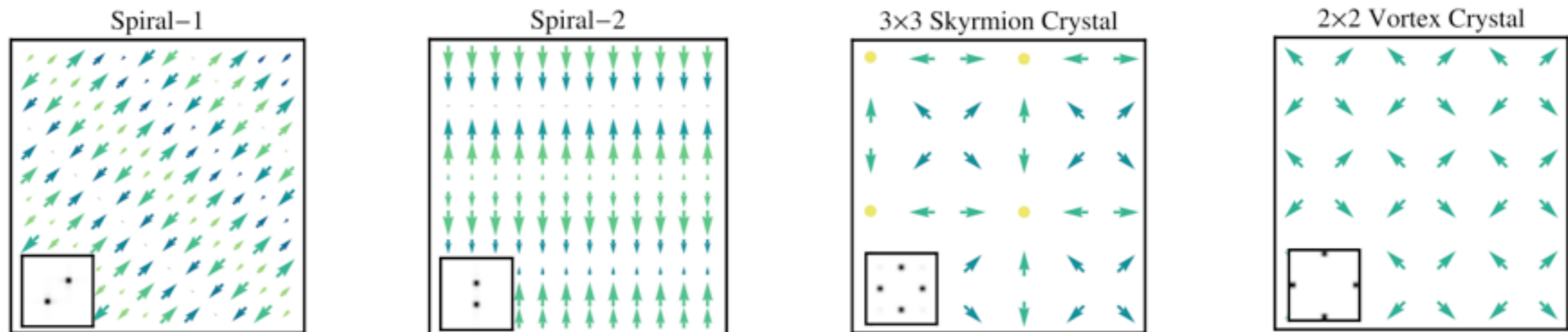
2D classical magnetic phases



Calculated with classical Monte Carlo annealing procedure
+
variational ansatz

Magnetic structure factors:

$$S_{\mathbf{q}} = \left| \sum_i \mathbf{S}_i \exp(i\mathbf{q} \cdot \mathbf{r}_i) \right|^2$$



What are the implications of magnetic ordering
for the superfluid states?

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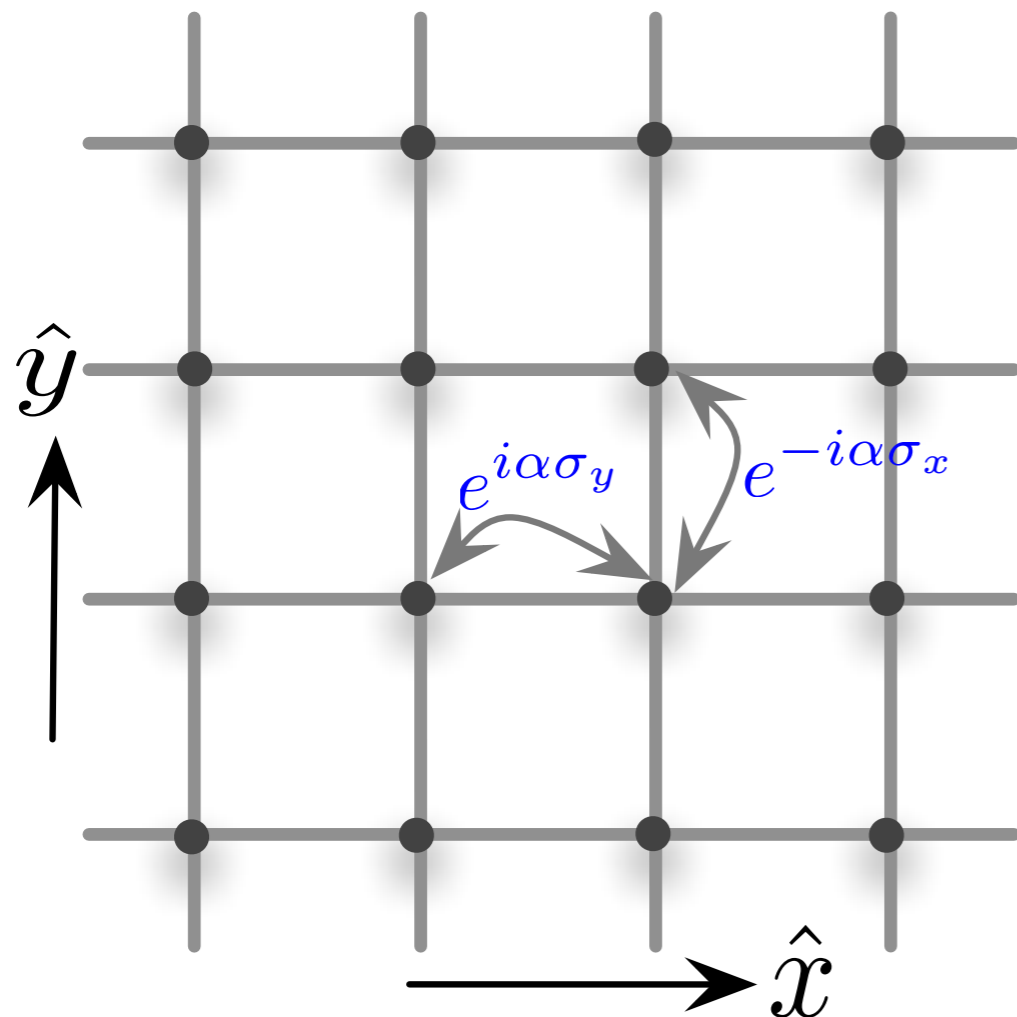
4. Conclusions and outlook

Mean field theory

$$H_{\text{hop}} = -t a_{i\sigma}^\dagger \mathcal{R}_{\hat{\nu}}^{\sigma\sigma'} a_{i+\hat{\nu}\sigma'}$$

$$H_{\text{int}} = \frac{U}{2} (n_{i\uparrow}^2 + n_{i\downarrow}^2 + 2\lambda n_{i\uparrow} n_{i\downarrow})$$

$$H_{\text{hop}}^{\text{mft}} = -t (\langle a_{i\sigma}^\dagger \rangle \mathcal{R}_{\hat{\nu}}^{\sigma\sigma'}) a_{i+\hat{\nu}\sigma'} - t a_{i\sigma}^\dagger (\mathcal{R}_{\hat{\nu}}^{\sigma\sigma'} \langle a_{i+\hat{\nu}\sigma'} \rangle)$$



Due to complicated magnetic ordering, we carry out calculations on a finite cluster (8*8) with periodic boundary conditions to attain self-consistency.

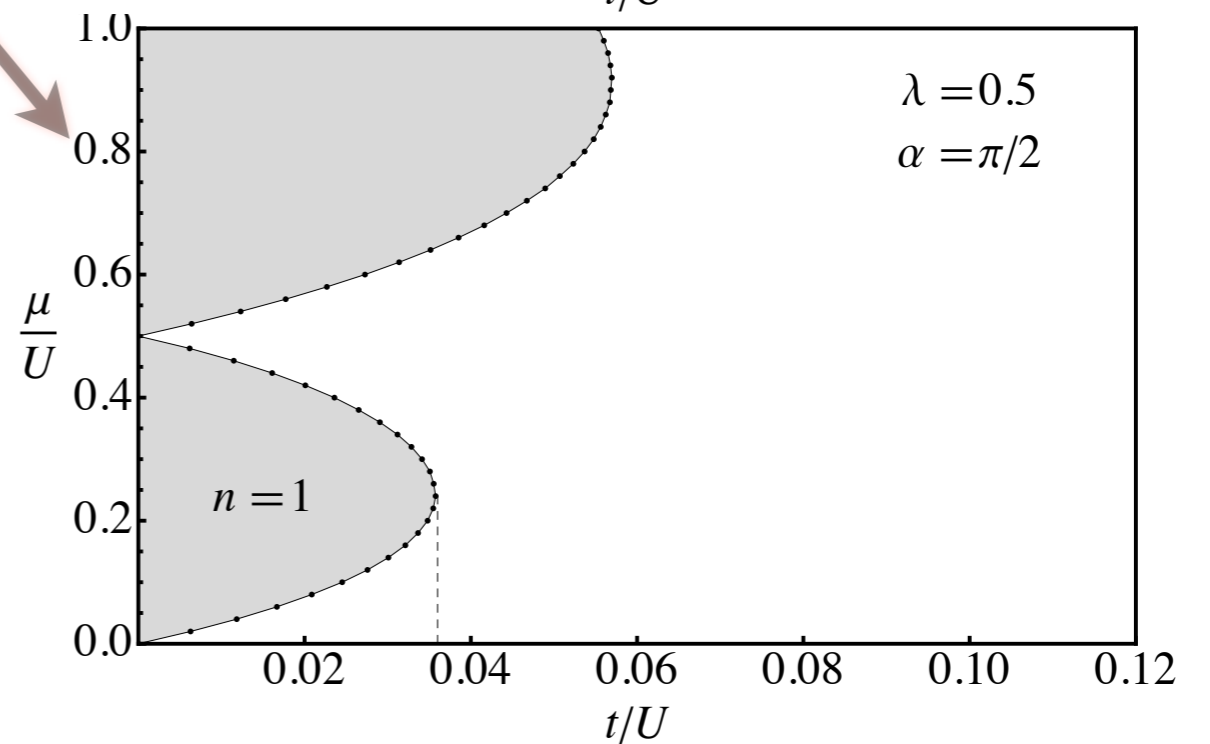
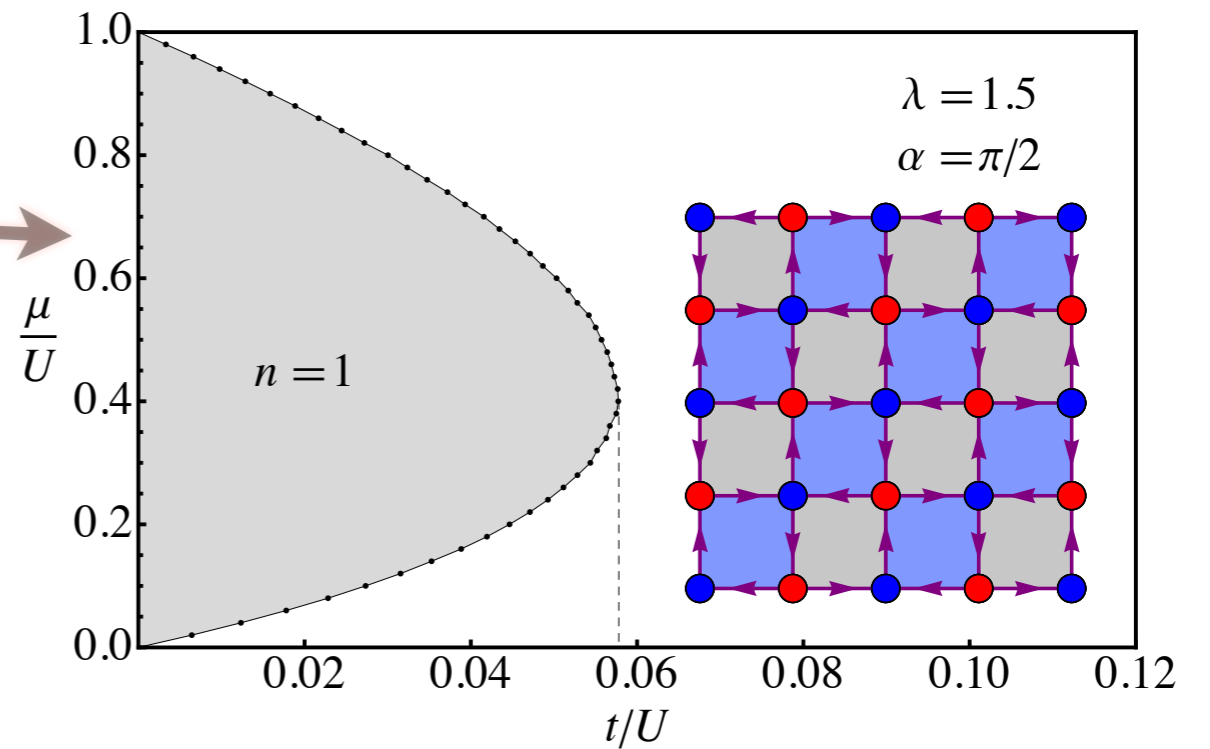
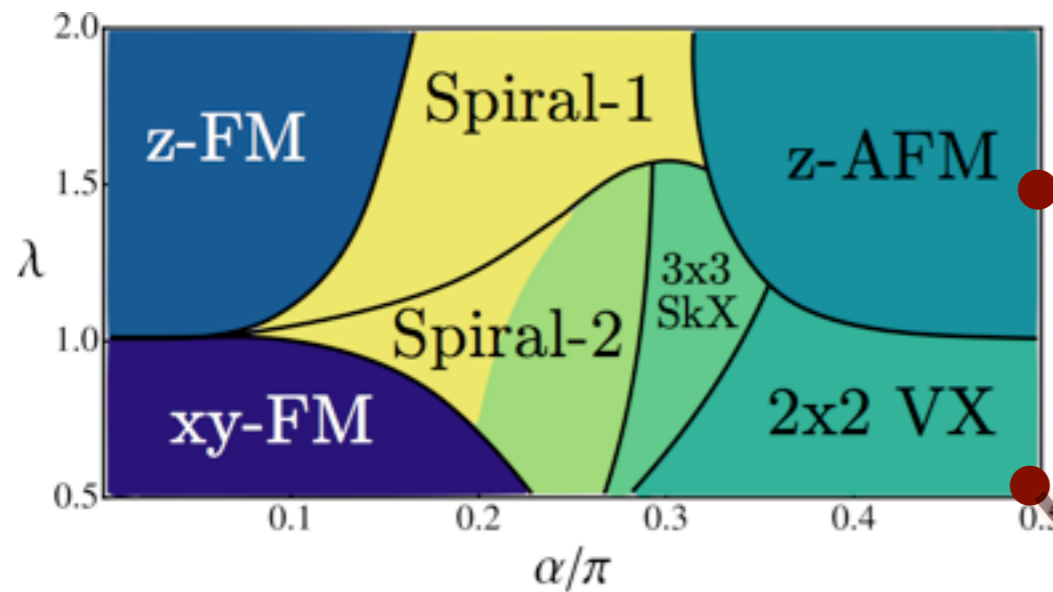
Local magnetization:

$$\mathbf{m}_i = \langle a_{i\sigma}^\dagger \boldsymbol{\tau}_{\sigma\sigma'} a_{i\sigma'} \rangle$$

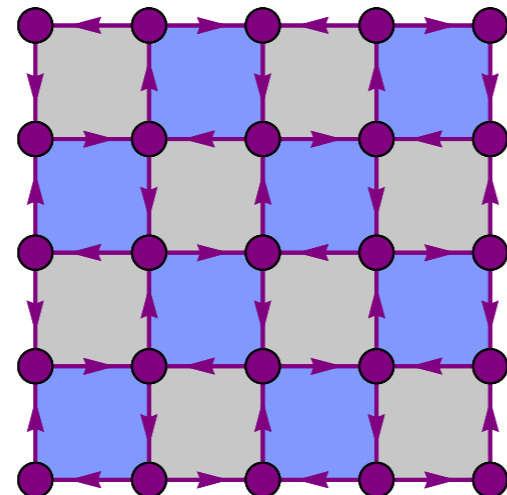
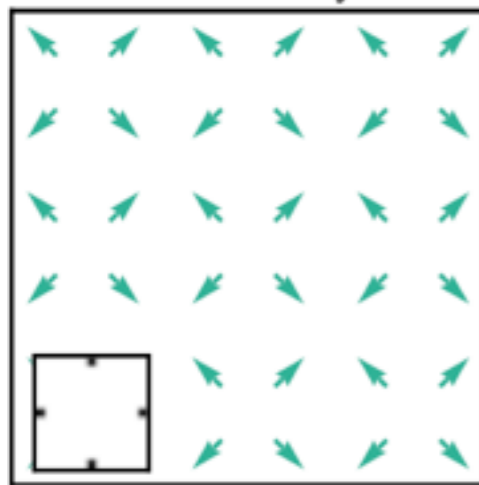
Bond current:

$$\kappa_{\hat{\nu}}^{\sigma\sigma'} = -it (\mathcal{R}_{\hat{\nu}}^{\sigma\sigma'} \langle a_{i\sigma}^\dagger a_{i+\hat{\nu},\sigma'} \rangle - c.c.)$$

Phase diagram



2x2 Vortex Crystal



Smooth evolution of magnetic order from Mott insulator to superfluid!

How are the current patterns related to magnetic ordering?

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Slave boson theory: construction

To describe the interplay between magnetism and superfluidity, introduce

$$a_{\sigma}^{\dagger} = \frac{1}{\sqrt{n_b}} b^{\dagger} f_{\sigma}^{\dagger} \quad n_b = b^{\dagger} b$$

Both b and f_{σ} are bosons operators, satisfying commutation relations

$$[b, b^{\dagger}] = 1; \quad [f_{\sigma}, f_{\sigma'}^{\dagger}] = \delta_{\sigma\sigma'}$$

Local constraint:

$$\sum_{\sigma} f_{\sigma}^{\dagger} f_{\sigma} = b^{\dagger} b$$

Single site Hilbert space: $|m \uparrow, n \downarrow\rangle$

$$|m + n\rangle_b \otimes |m \uparrow, n \downarrow\rangle_f$$

The canonical commutation relations of a-operators are preserved in the physical Hilbert space.

$$H_{\text{hop}} = -t a_{i\sigma}^{\dagger} \mathcal{R}_{\hat{v}}^{\sigma\sigma'} a_{i+\hat{v}\sigma'}$$

$$H_{\text{hop}} = -t \frac{1}{\sqrt{n_{ib}}} f_{i\sigma}^{\dagger} \mathcal{R}_{\hat{v}}^{\sigma\sigma'} f_{i+\hat{v}\sigma'} \frac{1}{\sqrt{n_{i+\hat{v},b}}} b_i^{\dagger} b_{i+\hat{v}}$$

Slave boson mean field theory

Assuming that the magnetic moments are ordered in the ground state, we can then make the classical field approximation and define:

$$z_\sigma = \eta^{-1} \left\langle \frac{f_\sigma}{\sqrt{n_b}} \right\rangle \quad \mathbf{z}^\dagger = (z_\uparrow^*, z_\downarrow^*) \quad \mathbf{z}^\dagger \mathbf{z} = 1$$

Hopping Hamiltonian within mean field becomes:

$$H_{\text{hop}}^{\text{mft}} = -t \left[|\eta|^2 z_{i\sigma}^* \mathcal{R}_{\hat{v}}^{\sigma\sigma'} z_{i+\hat{v}\sigma'} \right] b_i^\dagger b_{i+\hat{v}}$$

Thus, the original spin-orbit couplings for a-bosons become abelian gauge fields for the charge degrees of freedom b, **within slave boson mean field and if spinons (f) are condensed.**

The constraint is implemented with U(1) gauge fields, which will be gapped through Higgs mechanism, **if spinons are condensed.** The suppressed gauge fluctuations may ensure the validity of the slave boson mean field theory.

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Slave boson theory: understand current patterns

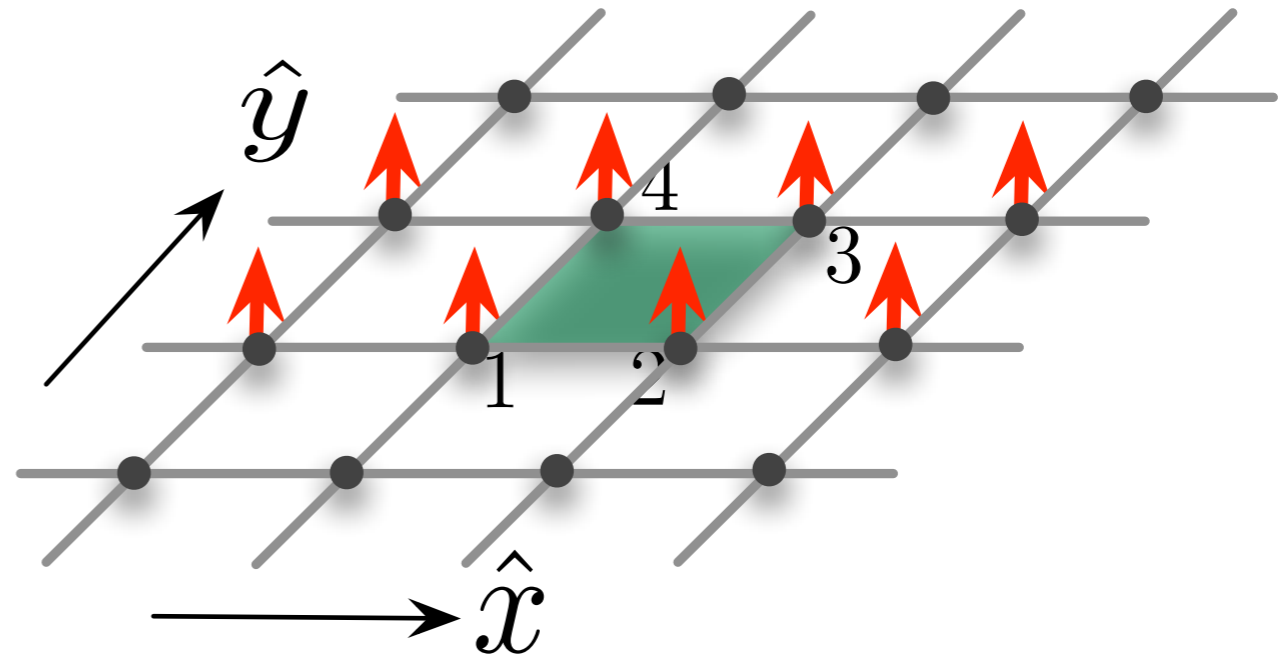
Case I: Ferromagnetic background

$$\mathbf{z}_i = (1, 0), \quad \forall i$$

$$H_{\text{hop}}^{\text{mf}} = -(t \cos \alpha) b_i^\dagger b_{i+\hat{v}}$$

renormalized hopping.

$$U_c^{\text{fm}} = U_c \cos \alpha$$



Case II: Anti-ferromagnetic background

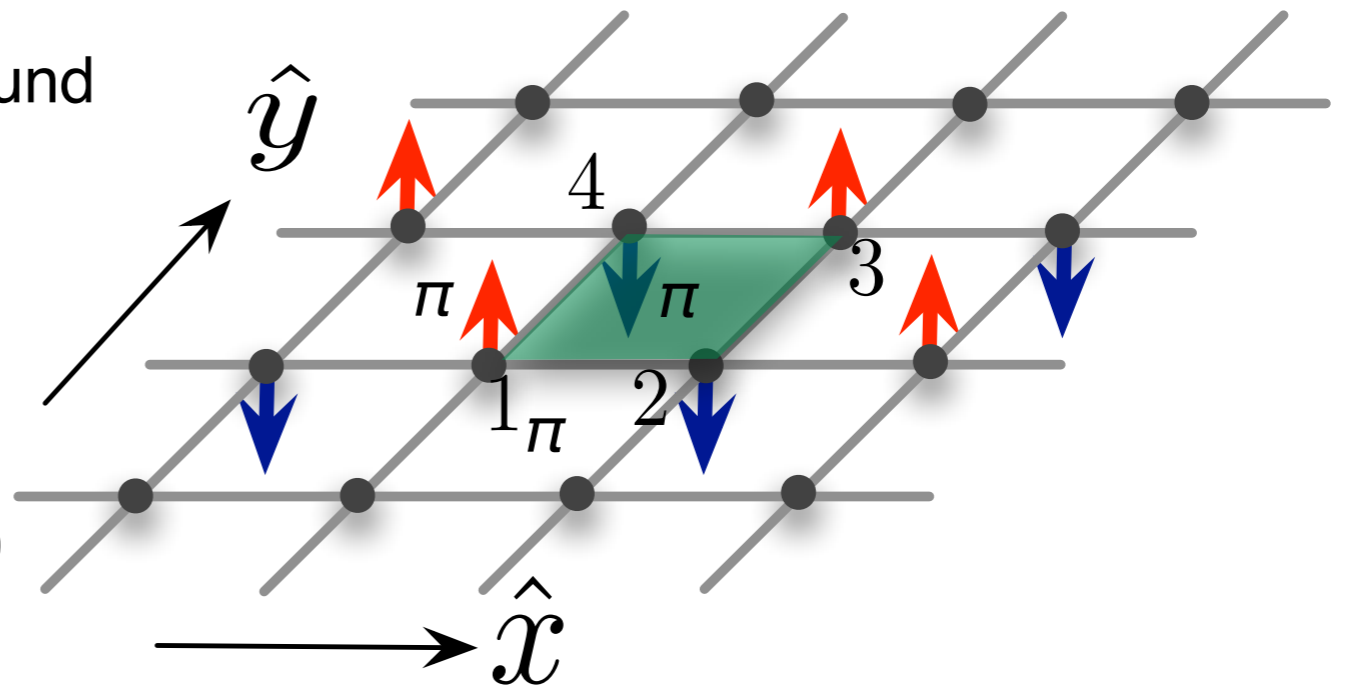
$$\mathbf{z}_i = (1, 0); \quad \text{Sublattice A}$$

$$\mathbf{z}_i = (0, 1); \quad \text{Sublattice B}$$

$$\prod t_{12} t_{23} t_{34} t_{41} = -t^4 \sin^4 \alpha < 0$$

π -flux lattice, Dirac points at $(0, \pm\pi/2)$

Two-fold degeneracy of current patterns!



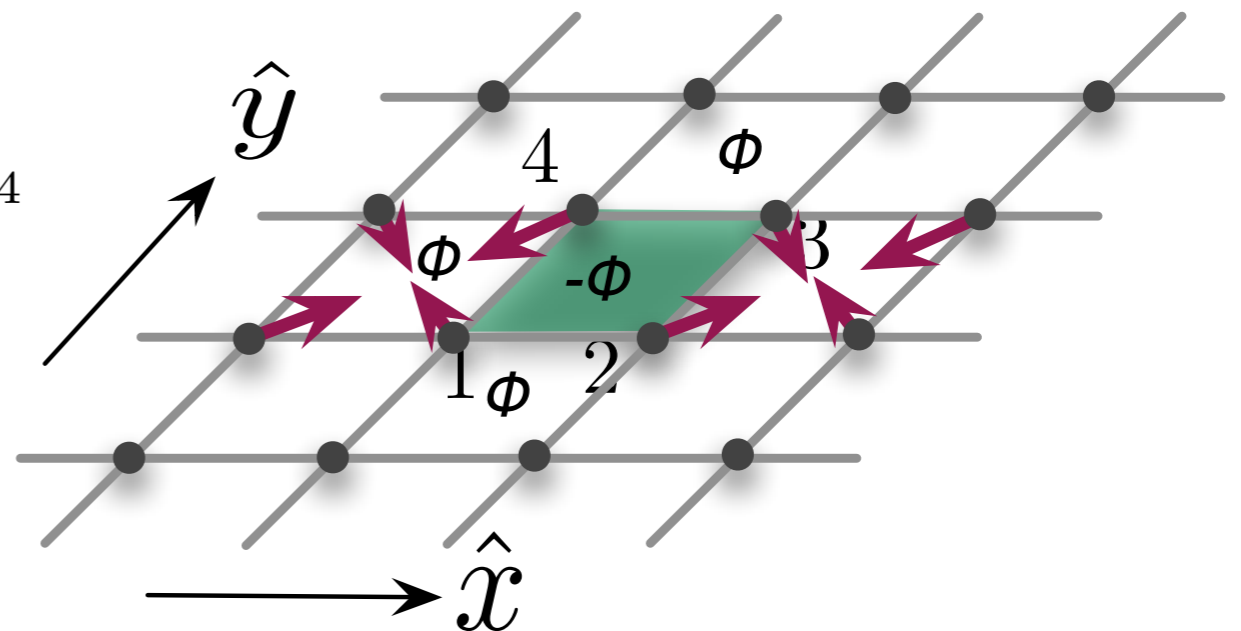
Slave boson theory: understand current patterns

Case III: Spin crystal background

$$\prod t_{12}t_{23}t_{34}t_{41} = -\frac{1}{4}(\cos \alpha - i\sqrt{2} \sin \alpha)^4$$

Alternating flux Φ in each plaquette.

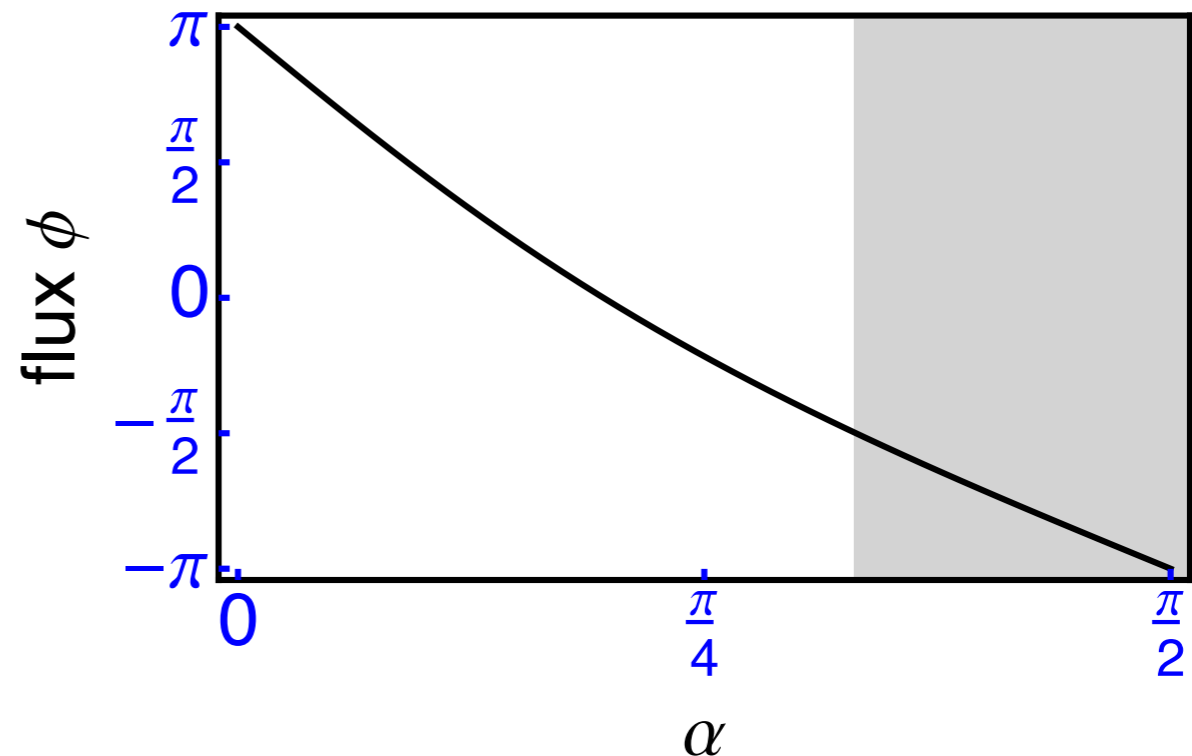
Fixed current patterns!



What needs to be done:

Self-consistent determination of the spinon fields z (full slave boson mean field theory);

Possibility of an “exotic” Mott insulator in BHM with spin-orbit coupling;



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We have studied Bose-Hubbard Model with spin-orbit interactions and established its **weak coupling superfluid states**, **magnetic structure in the Mott insulating states** and determined the **phase diagram** using mean field theory.

We proposed a new **slave boson theory** and argued that it was helpful for us to understand certain features of the strongly interacting superfluids close to the Mott transition.

Magnetic models in either 1D or 2D are worth investigating in detail. In particular, for 1D, the complete phase diagram with **exact diagonalization** or **density matrix renormalization group** calculation; possibility of experimental implementation. For 2D, **collective excitations** and **order from disorder** calculations.

Understand the phase diagram with slave boson theory. In particular, investigate the possibility of **“exotic” Mott insulating states** (e.g. disordered magnetic states close to the Mott boundary).

Thank you!