

Effects of Geometric Frustration in Itinerant Electron Systems

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I am indebted to many with whom I've worked and many more who have shared their wisdom.

Overview

- Frustration
 - General description
 - Magnetism as the paradigm
 - Ising & Continuous symmetry
 - Itinerant Fermi systems
- Materials - brief comments
- Hubbard model
- Select results and future plans

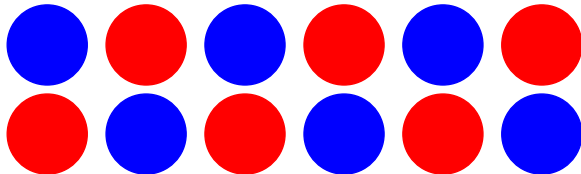
Research interest: What are the low temperature phases of correlated magnetic/charge systems in and how does frustration affect those phases? Tune the frustration.

Frustration - a toy model

You have two balls, red and blue Rule: stack rows of balls, nearest neighbors must be of opposite color

The rule is satisfied for all balls

in a direct stacking

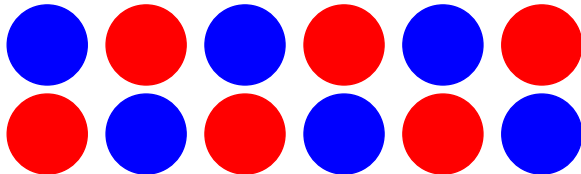


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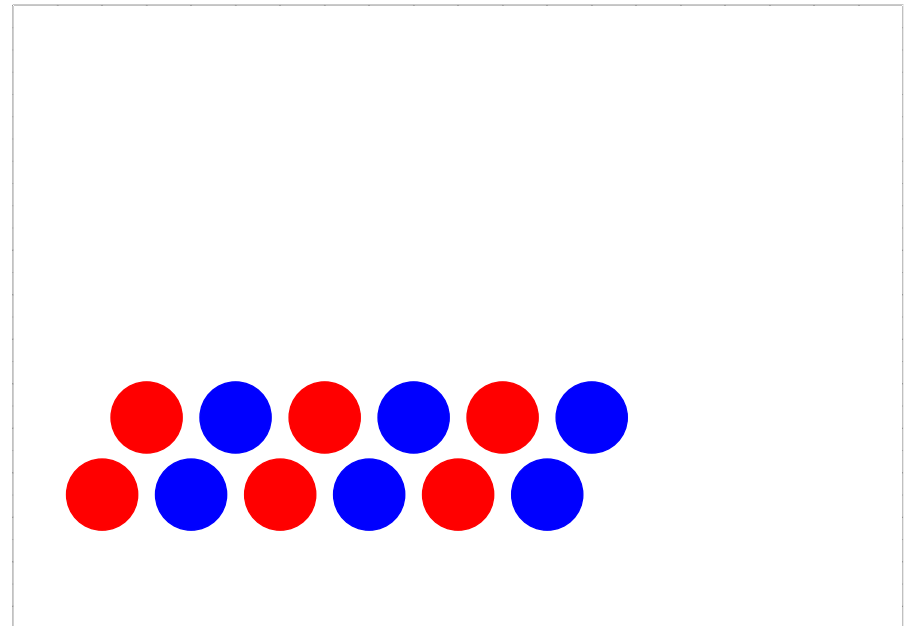
The rule is satisfied for all balls.

in a direct stacking



The rule is not satisfied for a
closed packed stacking.

Frustrated



A simple model of magnetism: Ising

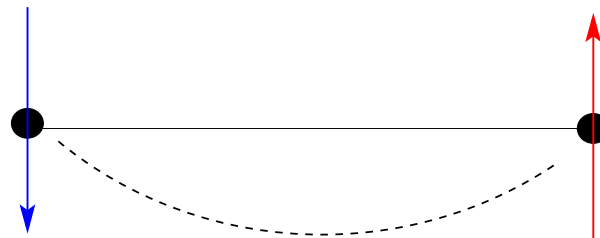
$$H = J \sum_{\langle i,j \rangle} \sigma_i \sigma_j \quad \sigma_i = \pm 1 = \text{up/down} \quad J > 0 \text{ AFM}$$

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spin down, -1

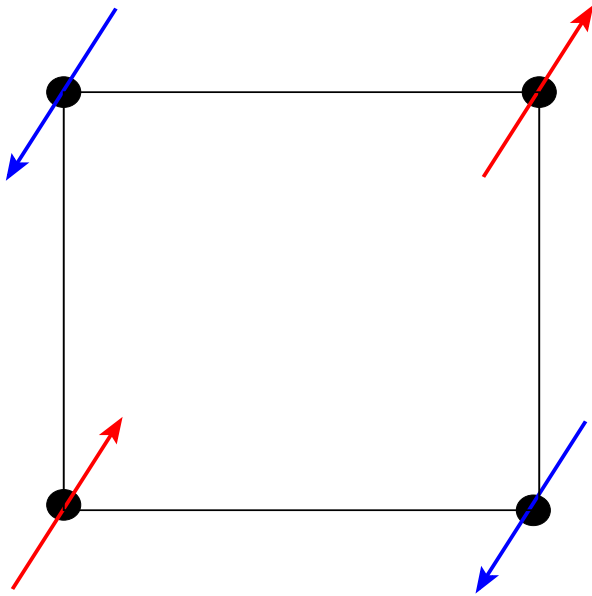
spin up, +1



antiferromagnetic coupling

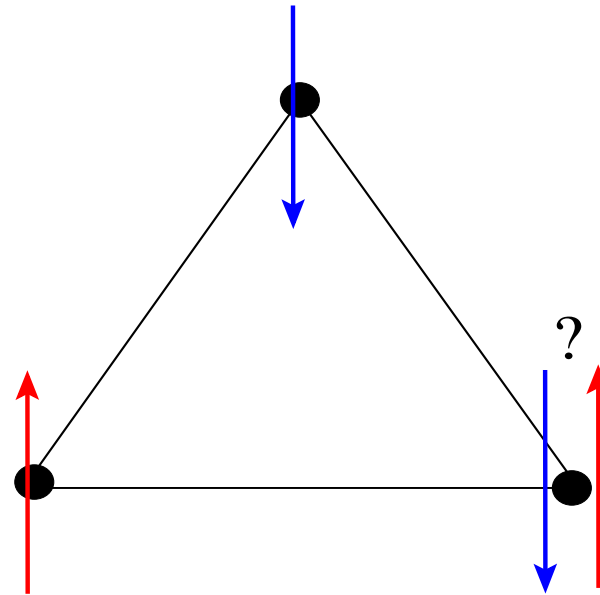
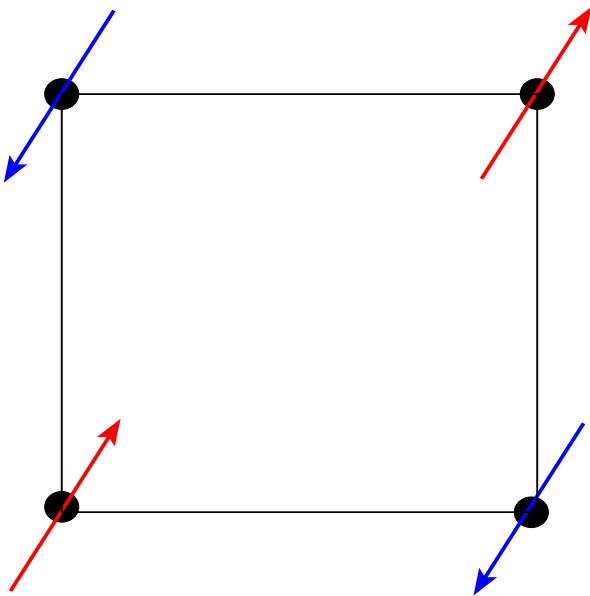
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Triangular motif induces competition among interactions, **geometry** induced frustration.

$J_1 - J_2$ *Ising model*

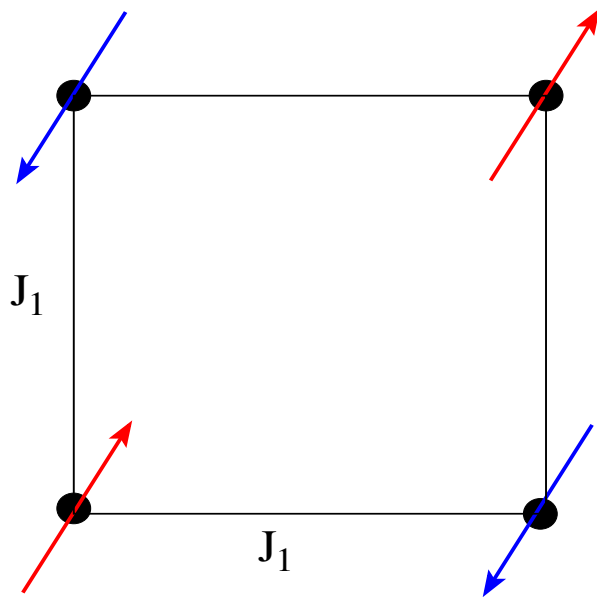
Include 2nd nearest neighbor interactions: J_2

$$H = J_1 \sum_{\langle i,j \rangle} \sigma_i \sigma_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \sigma_i \sigma_j$$

$J_1 - J_2$ Ising model

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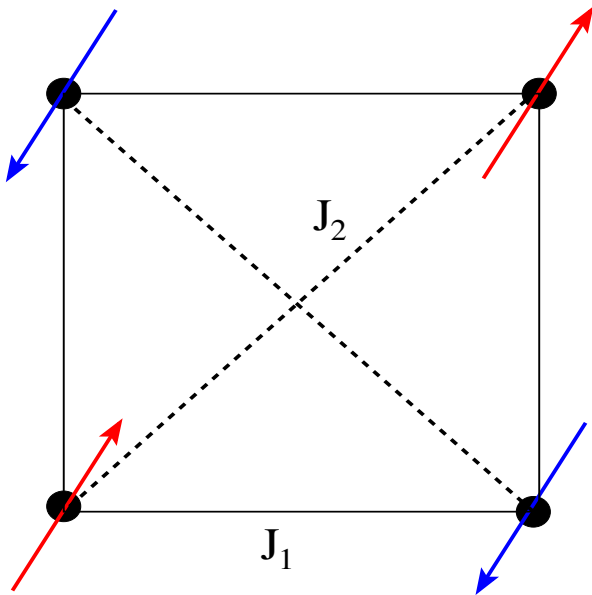


For $J_1 = 1$, $J_2 = 0$,
square lattice AFM

$J_1 - J_2$ Ising model

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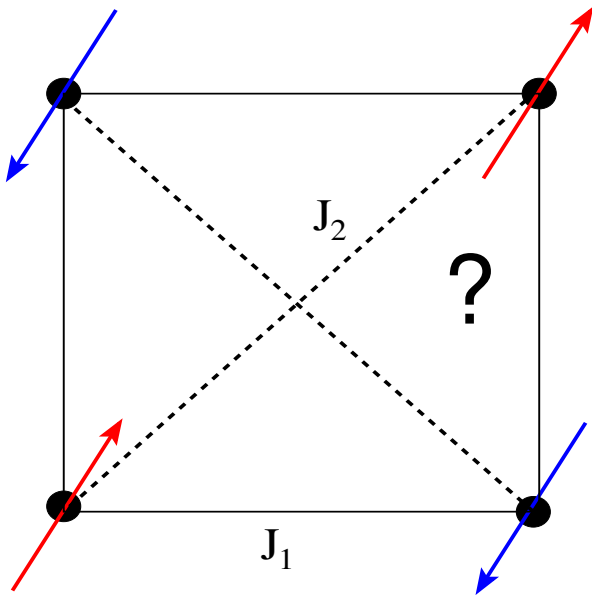


With $J_1 = 1$, $J_2 > 0$, frustration

$J_1 - J_2$ Ising model

Include 2nd nearest neighbor interactions: J_2

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With $J_1 = 1$, $J_2 > 0$, frustration
Competing interactions
engender frustration.

Mean-field phases

Fourier transform the interaction

$$J(\mathbf{q}) = \sum_{i,j} J(\mathbf{r}_{ij}) e^{-i\mathbf{q}\cdot\mathbf{r}_{ij}}$$

The minimum of $J(\mathbf{q})$ occurs at ordering wave vector, \mathbf{q}_{ord} .

Mean-field phases

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What happens to q_{ord} as frustration is **tuned**?

Mean-field phases

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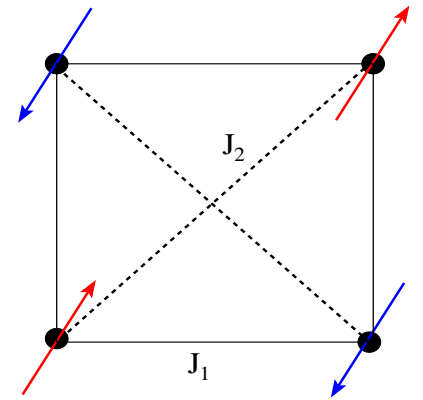
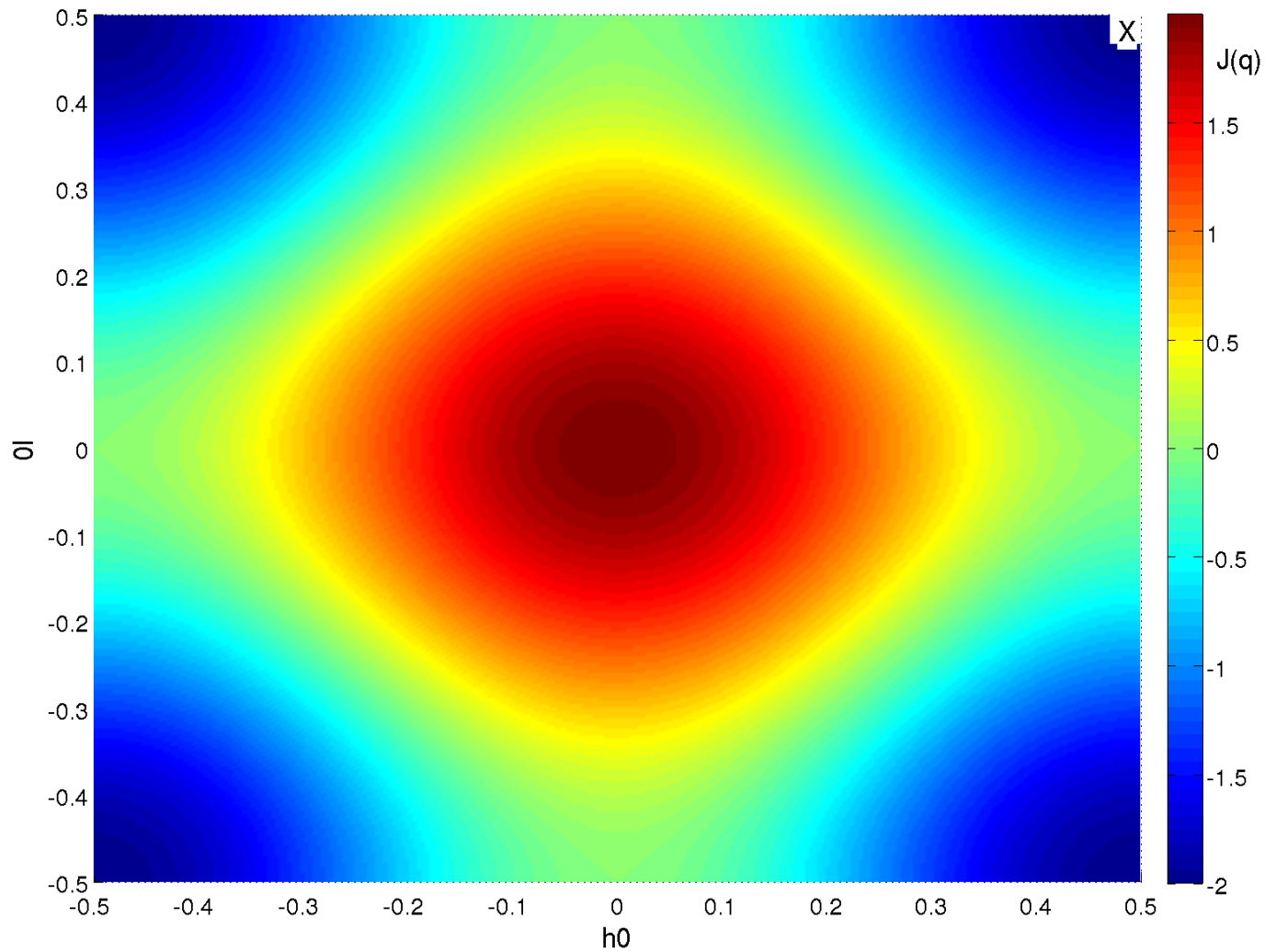
The minimum of $J(\mathbf{q})$ occurs at ordering wave vector, \mathbf{q}_{ord} .
What happens to q_{ord} as frustration is **tuned**?

- $J_1 - J_2$ model on the square lattice
- Nearest neighbor model on the anisotropic triangular lattice

$J_1 - J_2$ model

$$J_1 = 1, J_2 = 0$$

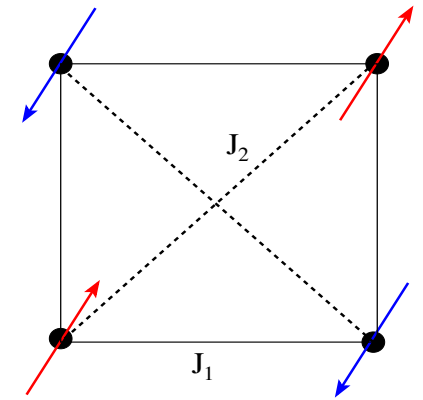
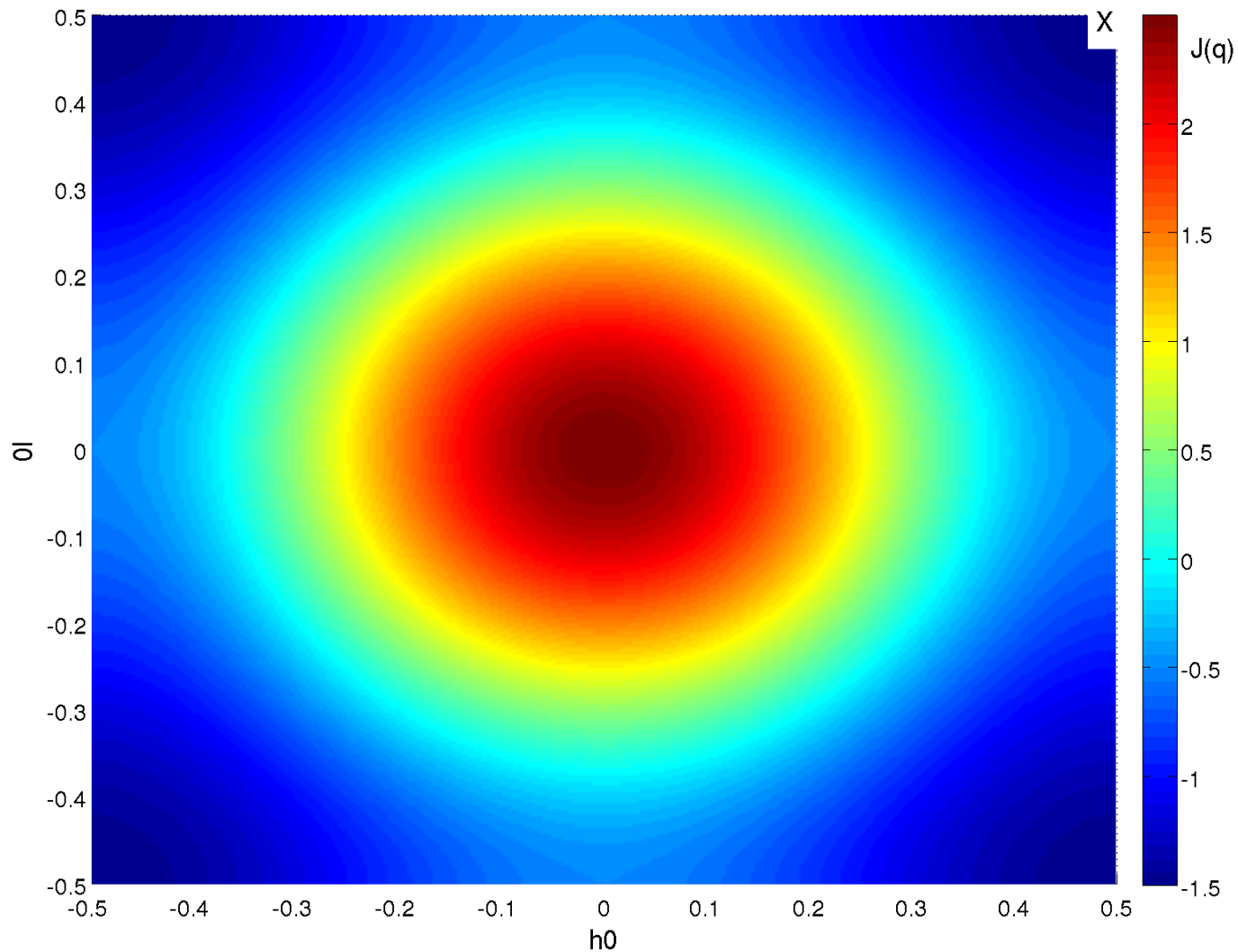
$$\mathbf{q}_{\text{ord}} = (\pi, \pi)$$



$J_1 - J_2$ model

$$J_1 = 1, J_2 = 0.25$$

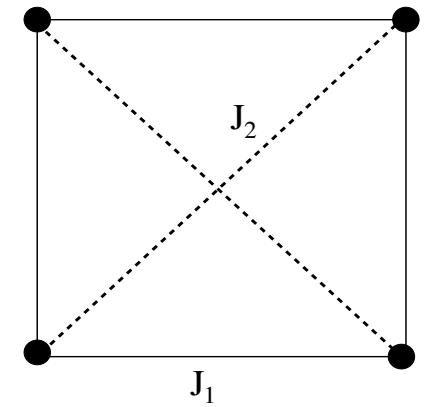
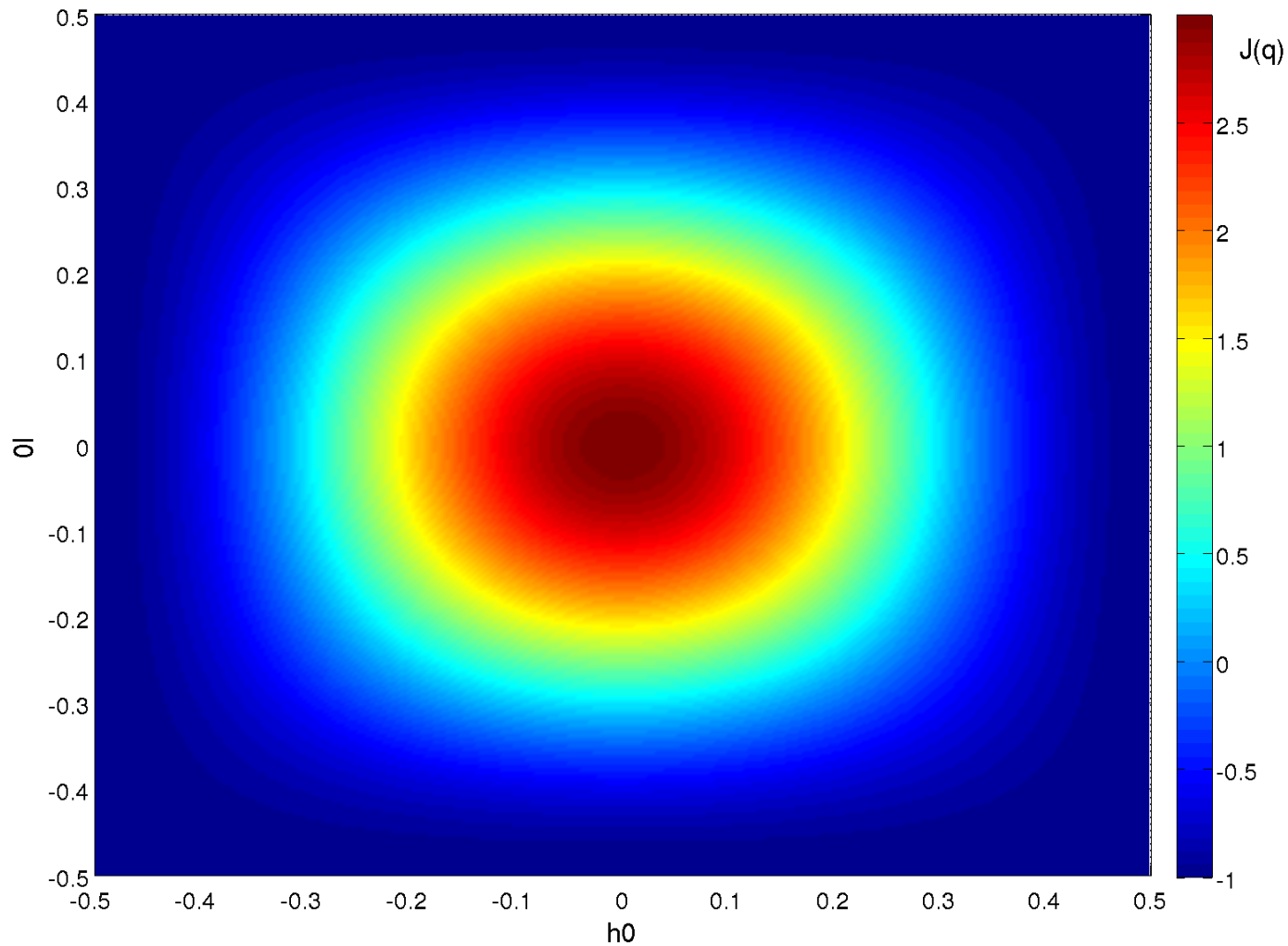
$$\mathbf{q}_{\text{ord}} = (\pi, \pi)$$



$J_1 - J_2$ model

$$J_1 = 1, J_2 = 0.50$$

$$\mathbf{q}_{\text{ord}} = (q, q)$$

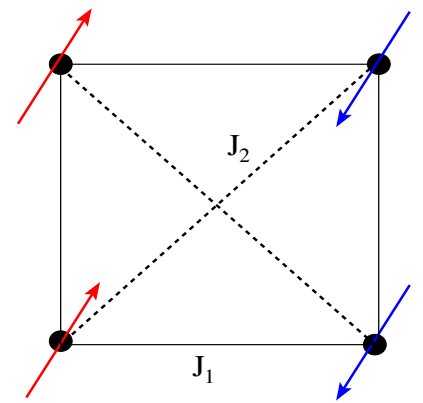
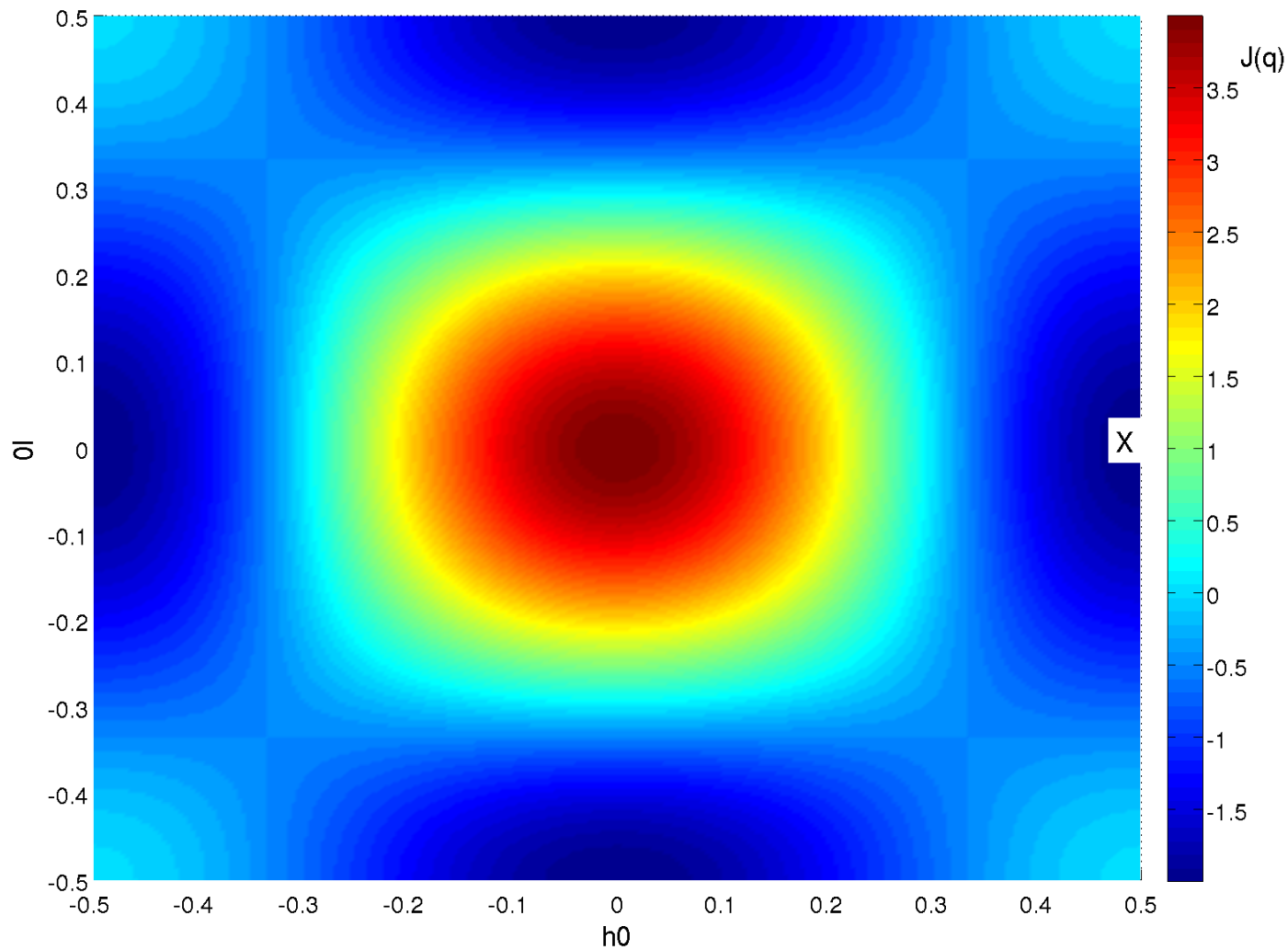


Disordered

$J_1 - J_2$ model

$$J_1 = 1, J_2 = 1.00$$

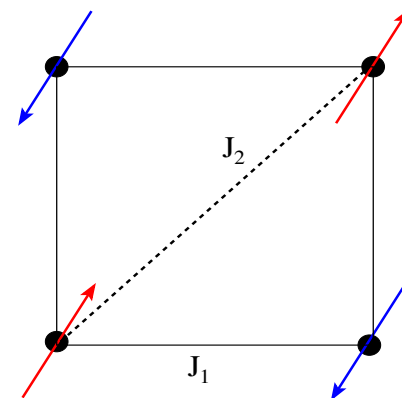
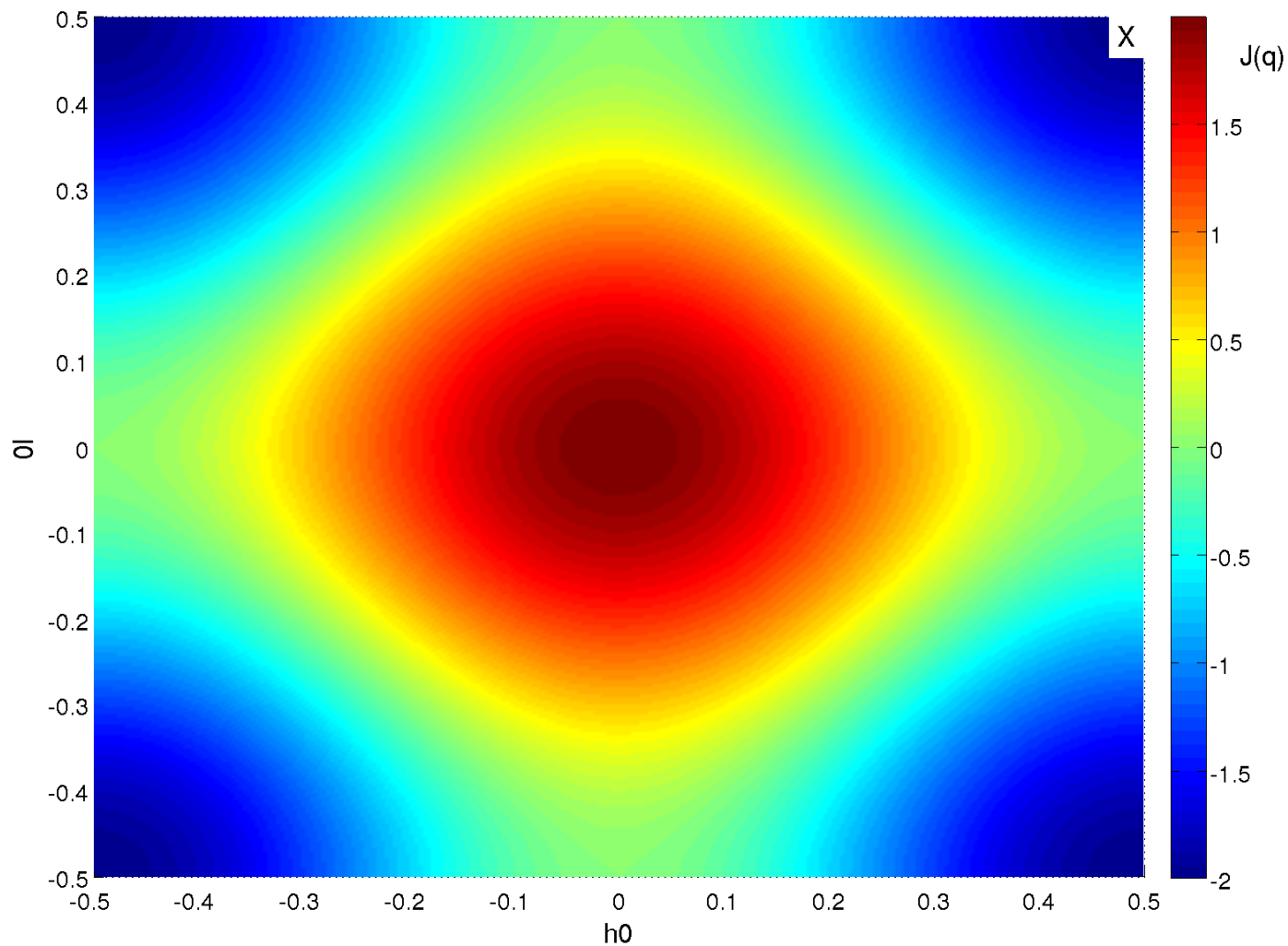
$$\mathbf{q}_{\text{ord}} = (\pi, 0)$$



Anisotropic triangular lattice

$$J_1 = 1, J_2 = 0$$

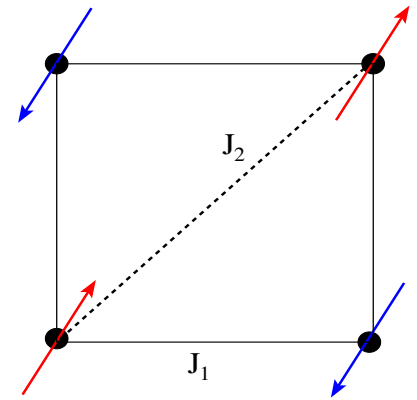
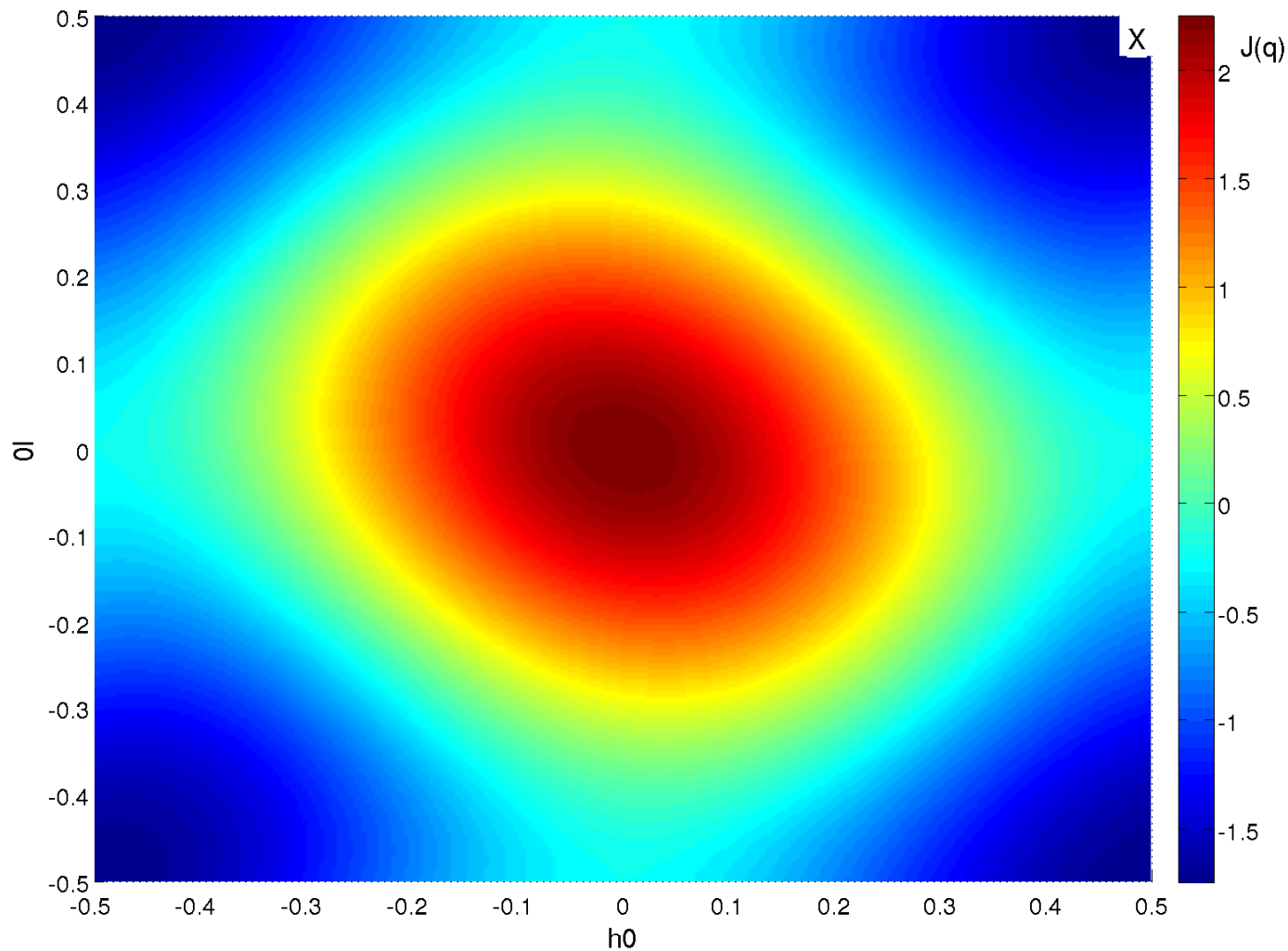
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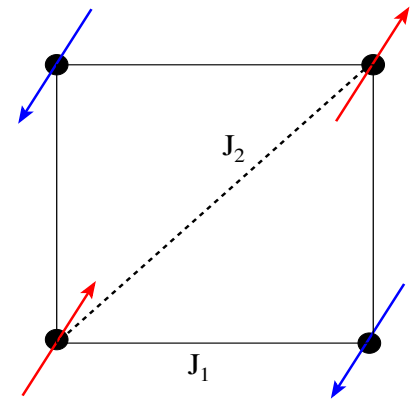
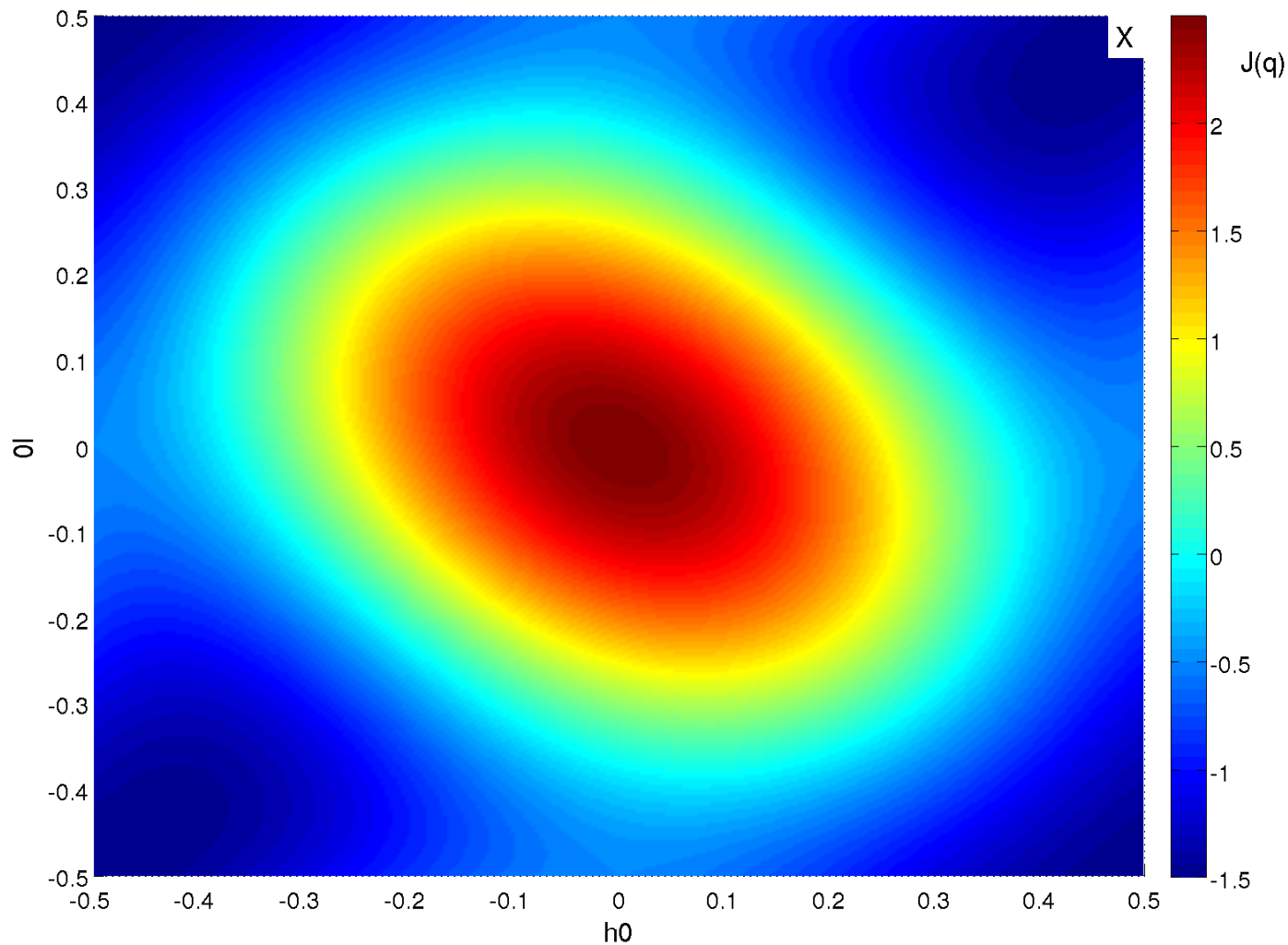
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Anisotropic triangular lattice

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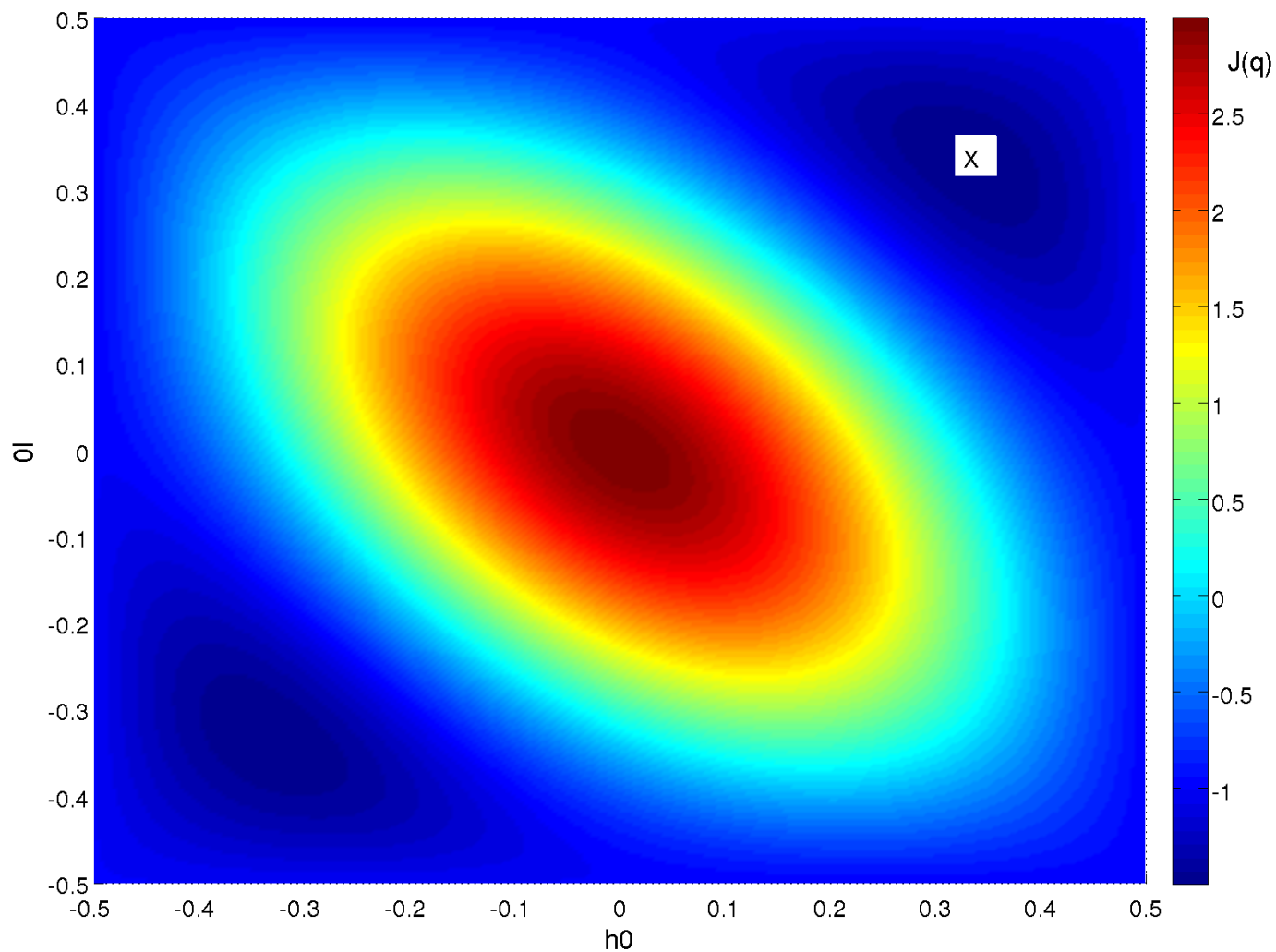
$$\mathbf{q}_{\text{ord}} = (\pi, \pi)$$



Anisotropic triangular lattice

$$J_1 = 1, J_2 = 1.00$$

$$\mathbf{q}_{\text{ord}} \approx (2\pi/3, 2\pi/3)$$

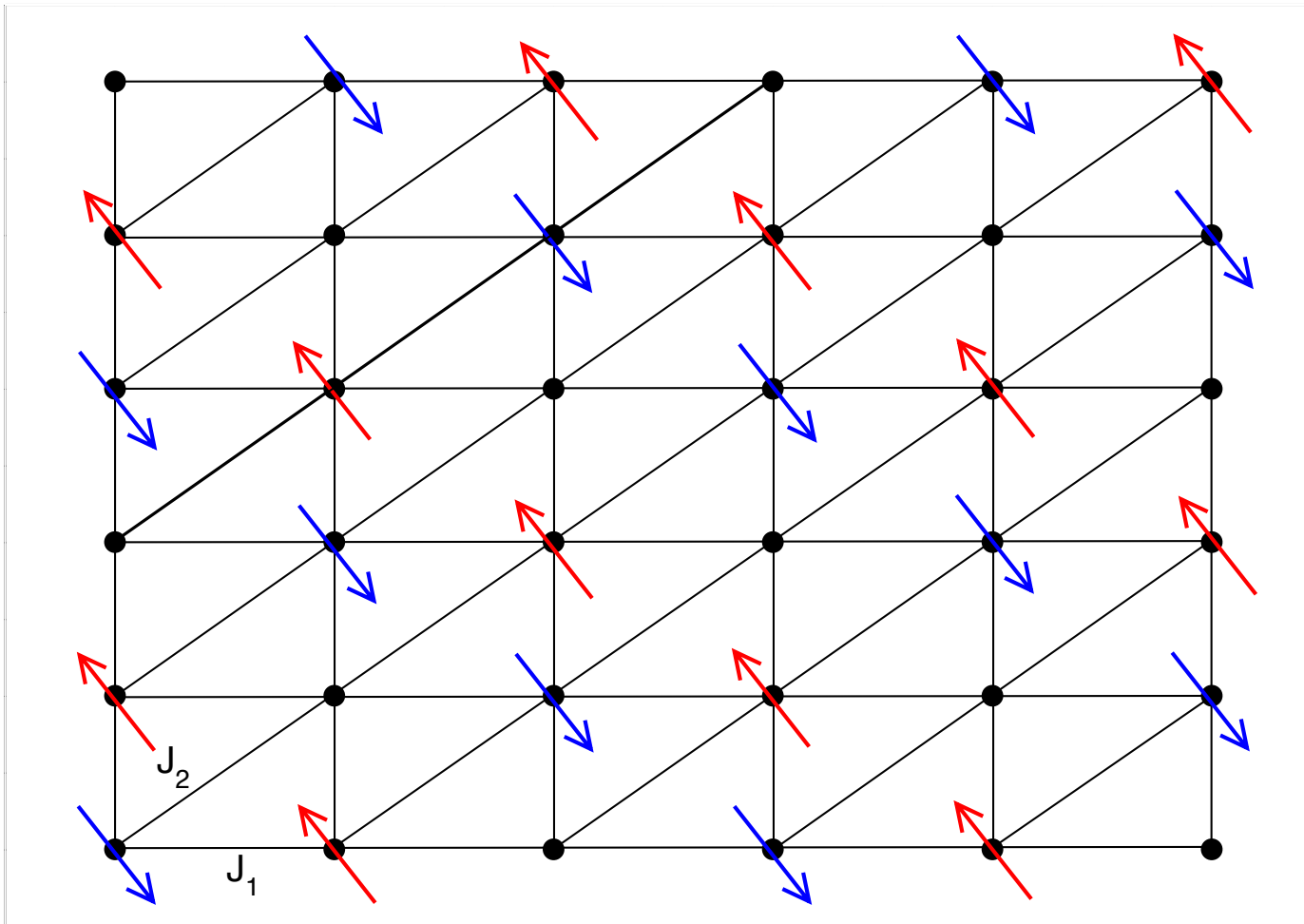


But partial
ordering

Anisotropic triangular lattice

$$J_1 = 1, J_2 = 1$$

$$\mathbf{q}_{\text{ord}} \approx (2\pi/3, 2\pi/3)$$



One possible configuration
Dots are random up/down

Residual entropy

$$S/N = 0.32306$$

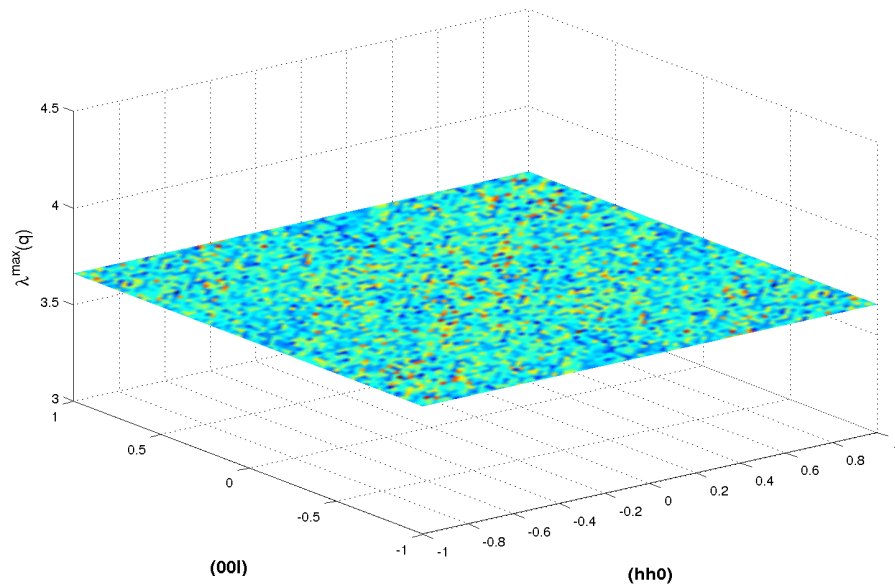
Wannier, *Phy. Rev.* **79** 1950

Houtappel, *Physica* **16** 1950

Complicated Ising systems

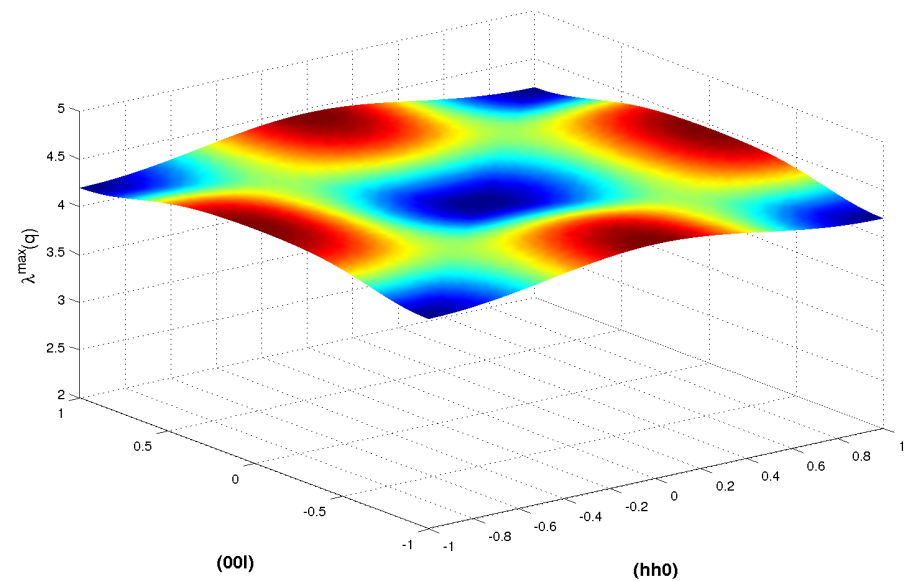
Spin ice: $\text{Ho}_2\text{Ti}_2\text{O}_7$ & $\text{Dy}_2\text{Ti}_2\text{O}_7$

Nearest neighbor model



Dipolar model

Quasi-degeneracy
yields interesting physics



Continuous spin + frustration

$$H = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \quad J > 0 \text{ AFM}$$

$$\mathbf{S}_i \rightarrow \text{SO}(n) \text{ or } \text{SU}(N)$$

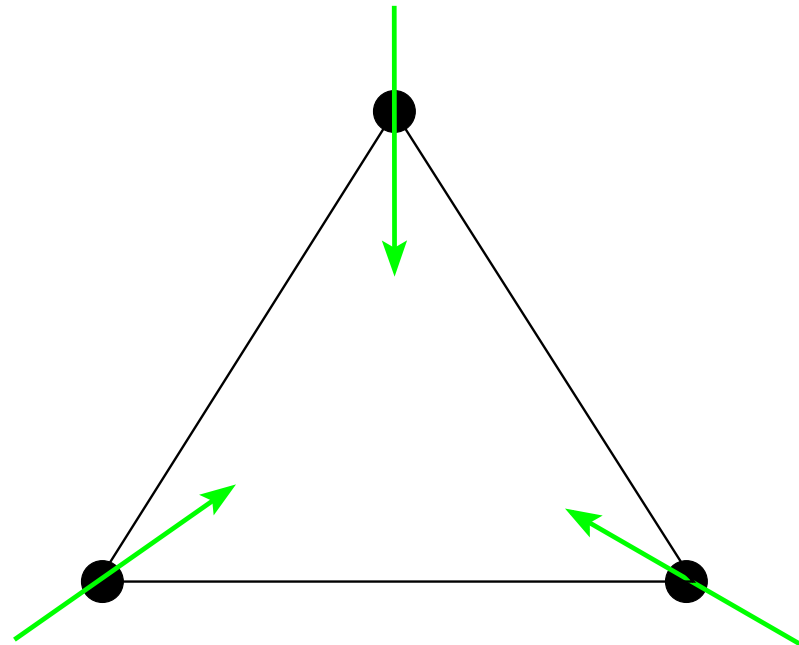
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Non-collinear states

Rich spin textures emerge



Itinerant electrons

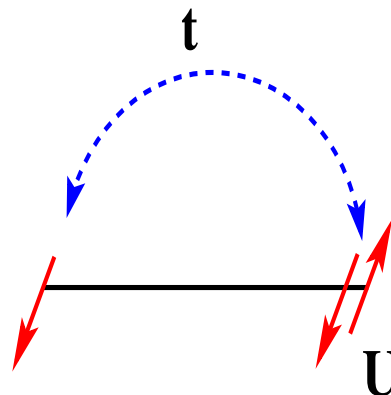
- Relative to quantum magnets, the Hilbert space expands to include charge, orbital, and spin dof
- Consider the simplest model, single band & on-site interactions: charge and spin dof only.
- **Hubbard model** - single band

$$H = - \sum_{\langle i,j \rangle, \sigma} t_{ij} (\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \hat{c}_{j\sigma}^\dagger \hat{c}_{i\sigma}) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} - \mu \sum_{i,\sigma} \hat{n}_{i\sigma}$$

t_{ij} nn hopping

U on site repulsion

μ chemical potential

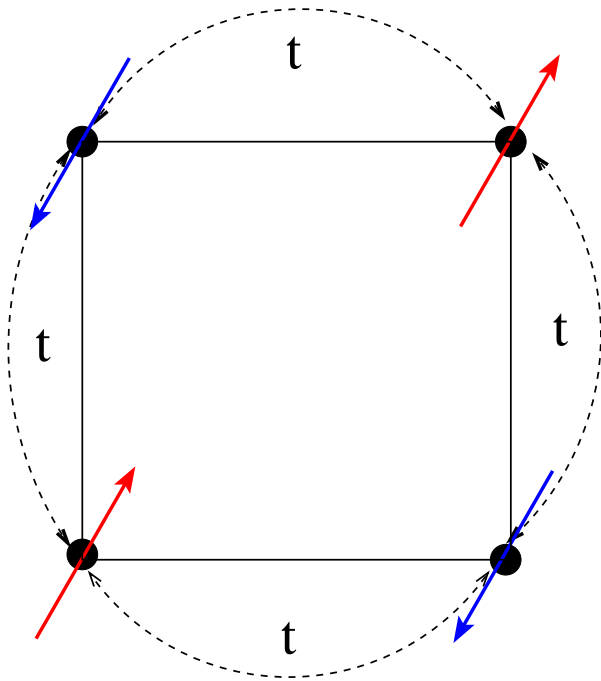


Itinerant electrons & frustration

- Frustration enters via hopping, kinetic energy, term
- Virtual fluctuations reduce energy if neighboring spins are anti-aligned.

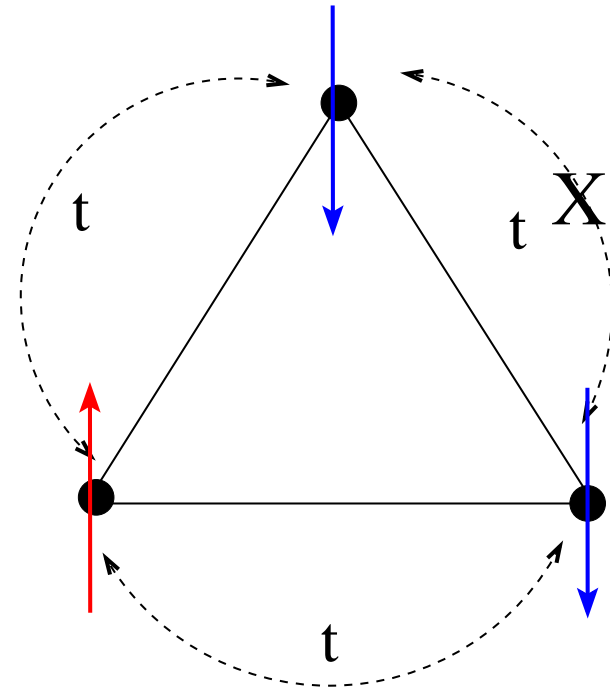
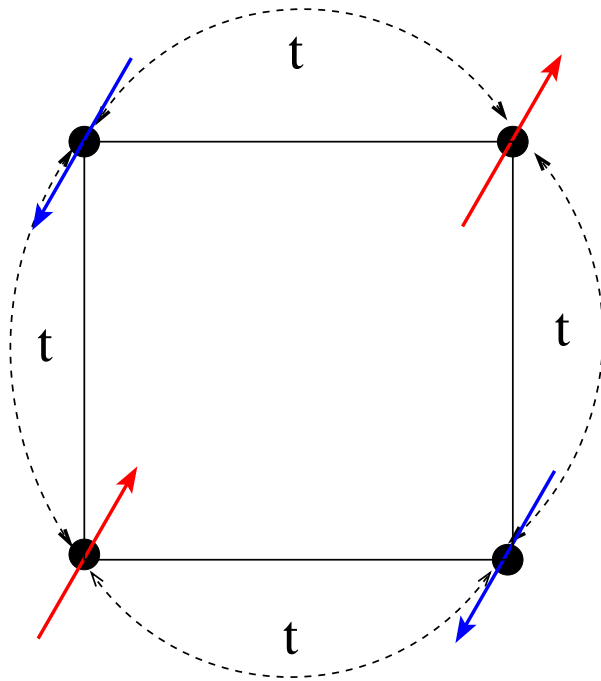
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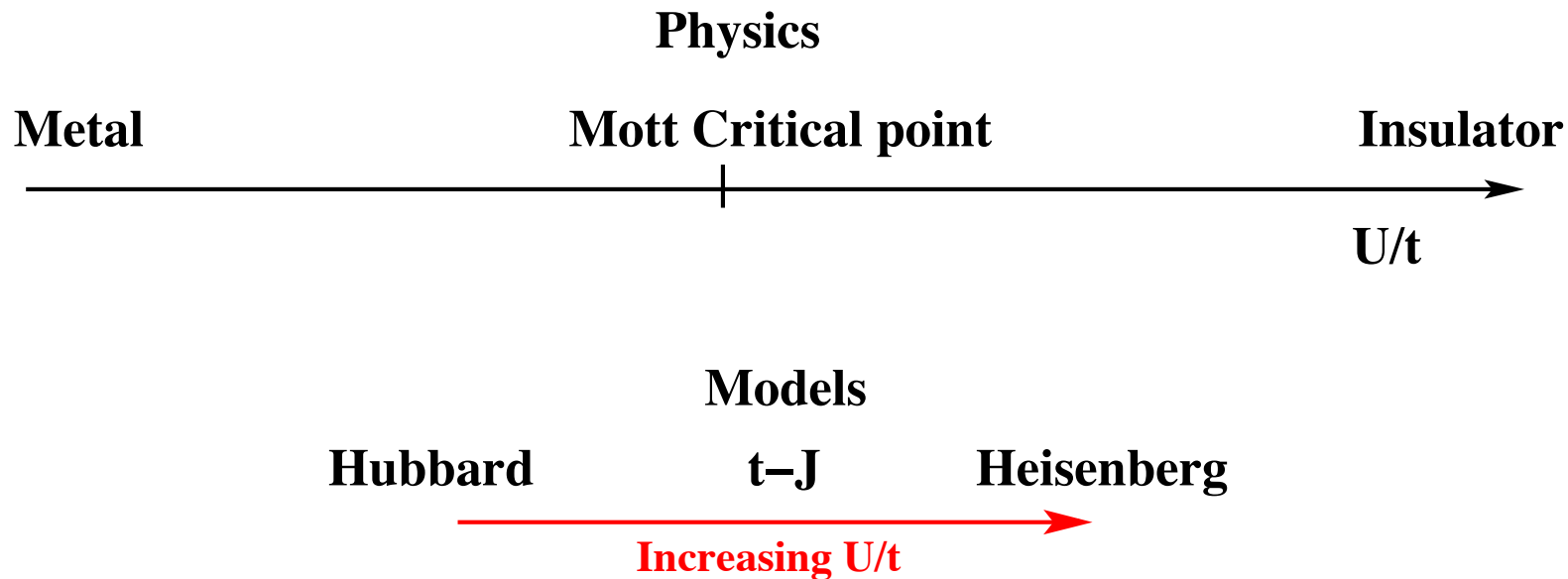
Itinerant electrons & frustration

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Hubbard to quantum magnets

- In the large U limit the 2nd OPT
 - $t - J$ model and Heisenberg model
- Capacity to tune from metal to insulator.



Materials - motivation

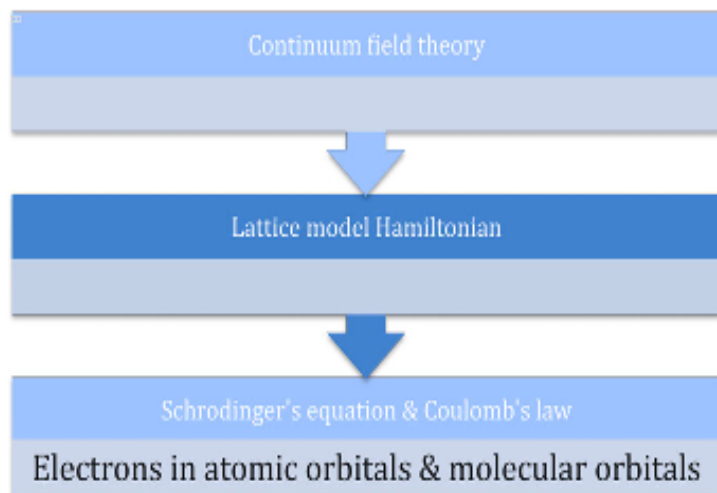
$S = 1/2$ magnets

- Triangular lattice
 - Cs_2CuCl_4
 - Cs_2CuBr_4
- Kagome lattice
 - $\text{ZnCu}_3(\text{OH})_6\text{Cl}_2$ herbertsmithite
 - $\text{Cu}_3\text{Zn}(\text{OH})_6\text{Cl}_2$ kapellasite (polymorph)

Itinerant systems

- Triangular lattice
 - $\text{k}-(\text{ET})_2\text{Cu}_2(\text{CN})_3$
 - $\text{k}-(\text{ET})_2\text{Cu}_2(\text{SCN})_3$
 - Na_xCoO_2

Links to field theory



A question of length scales.

Long lengths - QFT, continuum

Electrons on crystal - microscopic hamiltonian

Molecules - Schrödinger equation

Figure 1. The hierarchy of objects and descriptions associated with theories of organic charge transfer salts. The arrows point in the direction of decreasing length scales, increasing energy scales and increasing numbers of degrees of freedom. At the level of quantum chemistry (Schrödinger's equation and Coulomb's law) one can describe the electronic states of single (or pairs of) molecules in terms of molecular orbitals (which can be approximately viewed as superpositions of atomic orbitals). Just a few of these molecular orbitals interact significantly with those of neighbouring molecules in the solid. Low-lying electronic states of the solid can be described in terms of itinerant fermions on a lattice and an effective Hamiltonian such as a Hubbard model (see section 6.2). In the Mott insulating phase the electrons are localized on single lattice sites and can be described by a Heisenberg spin model (see section 6.1). The low-lying excitations of these lattice Hamiltonians and long-wavelength properties of the system may have a natural description in terms of quasi-particles which can be described by a continuum field theory such as a nonlinear sigma model. At this level unexpected objects may emerge such as gauge fields and quasi-particles with fractional statistics (see section 7).

Powell & McKenzie, Rep. Prog. Phys. **74** (2011)
Review on organic Mott insulators.

Methods to study Hubbard model

- Field theoretic techniques
- Numerics to study the model directly - numerous
- Mean field approximations of hamiltonian
- Perturbative methods - series expansions
- I have used quantum Monte Carlo (QMC), mean-field theory, exact diagonalization
- In QMC, the issue is with the interaction: $U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$

Hubbard-Stratonovich transformation

$$e^{-\Delta\tau U \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}} = e^{-\Delta\tau(\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow})} \sum_{x_i = \pm 1} P(x_i) e^{\gamma x_i (\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})}$$

QMC - quick comments

detQMC* - finite T, sign problem with fermions and frustration

$$\langle \hat{O} \rangle = \frac{\text{Tr} \text{Tr}_x \{ \hat{O} e^{\beta H[x]} \}}{\text{Tr} \text{Tr}_x \{ e^{\beta H[x]} \}}$$

CP/ Φ QMC** - T=0, project $|\Psi_o\rangle$, importance sampled RW

$$|\Psi_o\rangle = \lim_{n \rightarrow \infty} e^{-n \Delta \tau H[x]} |\Psi_T\rangle \rightarrow |\Psi^{(n)}\rangle \propto \sum_k O_T(\phi_k^{(n)}) |\phi_k^{(n)}\rangle$$

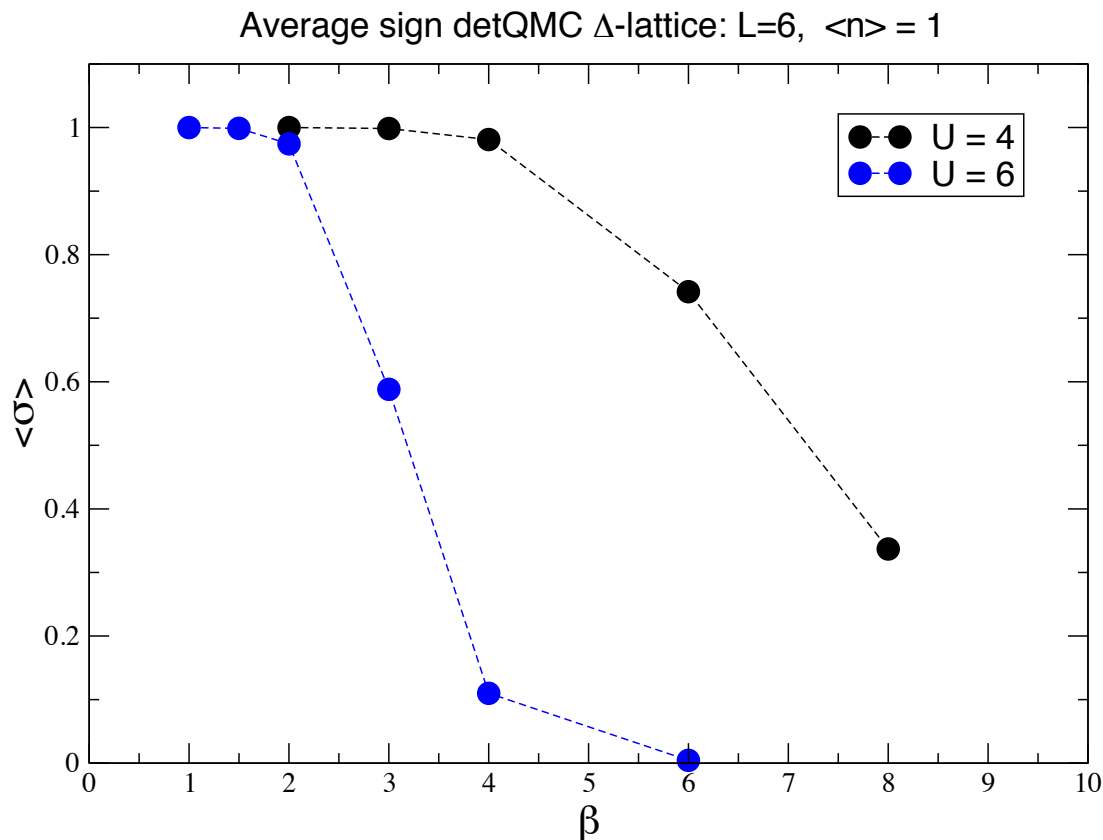
Importance function: $O_T(\phi_k^{(n)}) = \langle \Psi_T | \phi_k^{(n)} \rangle$

Constraint: $O_T(\phi_k^{(n)}) > 0$ PBC; $\text{Re} \left\{ \frac{O_T(\phi_k^{(n+1)})}{O_T(\phi_k^{(n)})} \right\} > 0$ TABC

* PRD **24** 2278; ** PRL **74** 3652, PRL **90** 136401

The sign problem in QMC

- Origins of sign problem are method depend.
- In essence the signal-to-noise vanishes in your measurements.
- In detQMC the weights (probabilities) can be negative



The sign is included in calculation of observables

Frustration makes sign problem worse

Mean-field theory

In MFT you ignore fluctuations in the charge and spin dof. Think of it as the next lowest order approximation, non-interacting being the lowest. **No sign problem.**

$$H = - \sum_{\langle i,j \rangle, \sigma} t_{ij} (\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \hat{c}_{j\sigma}^\dagger \hat{c}_{i\sigma}) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} - \mu \sum_{i,\sigma} \hat{n}_{i\sigma}$$

Hartree-Fock treatment of on-site interaction:

$$\begin{aligned} U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} &\rightarrow U(\hat{n}_{i\uparrow} \langle \hat{n}_{i\downarrow} \rangle + \hat{n}_{i\downarrow} \langle \hat{n}_{i\uparrow} \rangle - \langle \hat{n}_{i\uparrow} \rangle \langle \hat{n}_{i\downarrow} \rangle) \\ &- U(\hat{S}_i^+ \langle \hat{S}_i^- \rangle - \hat{S}_i^- \langle \hat{S}_i^+ \rangle - \langle \hat{S}_i^+ \rangle \langle \hat{S}_i^- \rangle) \end{aligned}$$

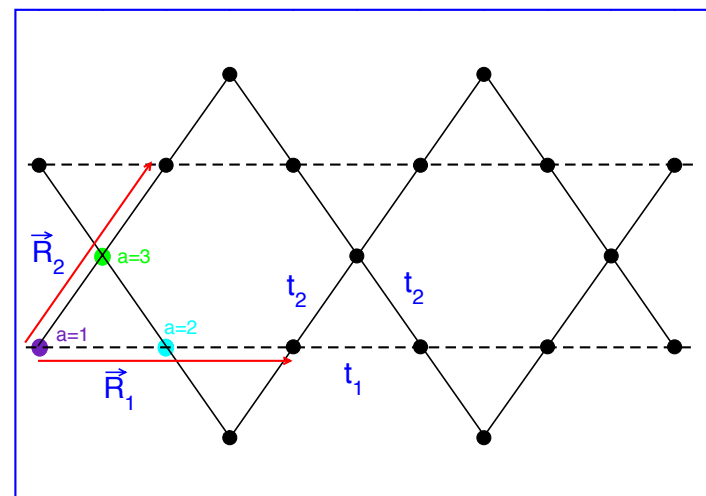
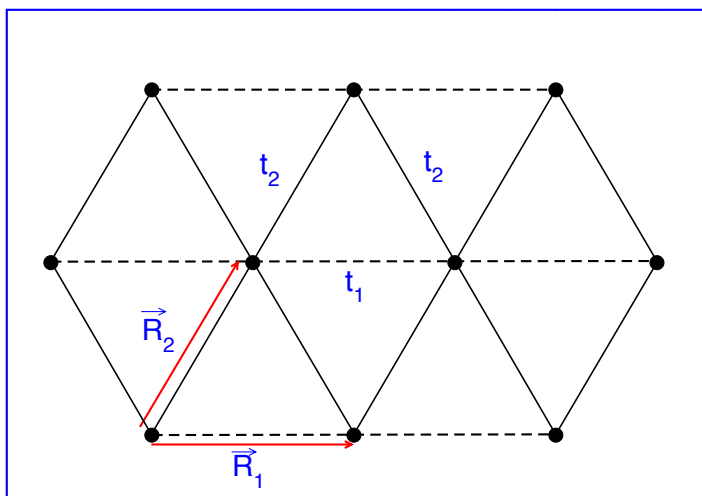
Self consistent MF equations: $\partial F / \partial \langle \hat{O} \rangle = 0 \rightarrow \langle \hat{n}_{i\uparrow} \rangle, \langle \hat{n}_{i\downarrow} \rangle, \langle \hat{S}_i^+ \rangle, \langle \hat{S}_i^- \rangle$

Our work, done a real-space lattice of N sites, in GCE and CE

Lattice systems of interest

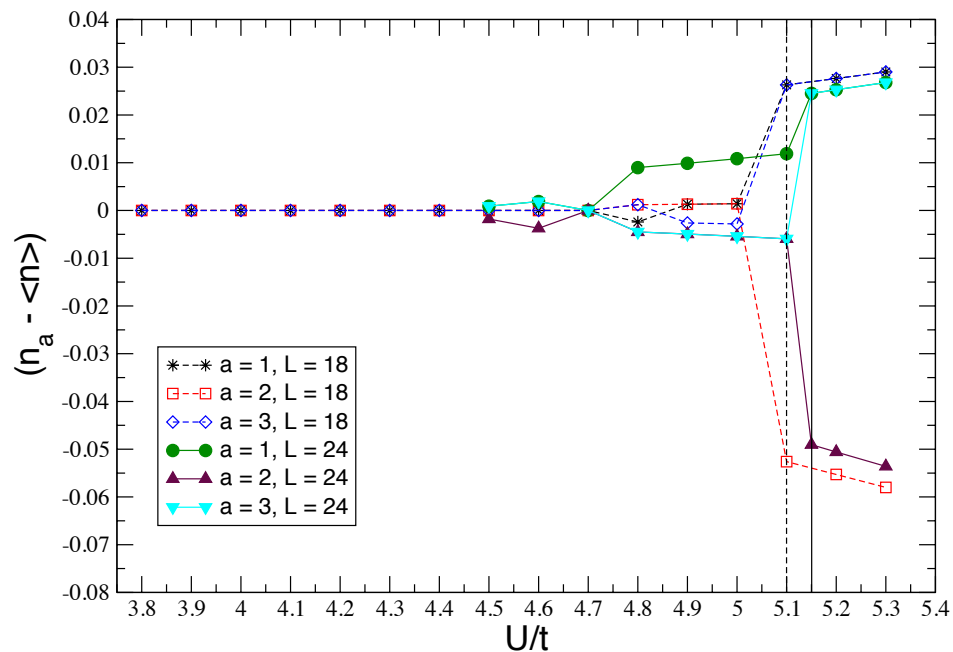
2D lattice with geometric frustration

- Triangular lattice
 - Isotropic lattice at $\langle n \rangle = 2/3$
 - Anisotropic lattice at $\langle n \rangle = 1$
- Kagome lattice
 - Anisotropic lattice at $\langle n \rangle = 1$

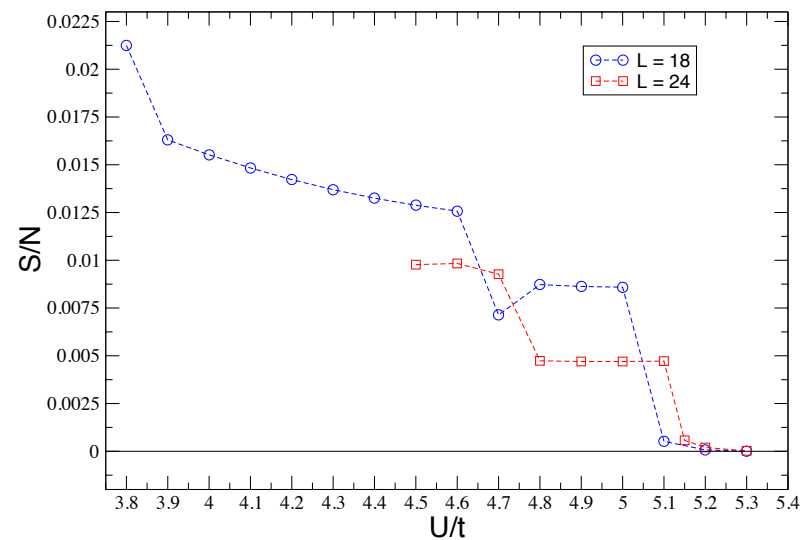
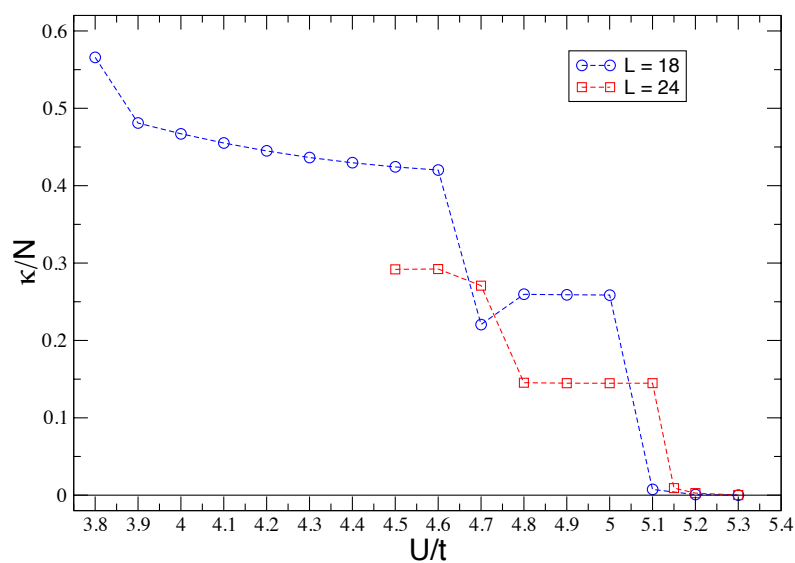
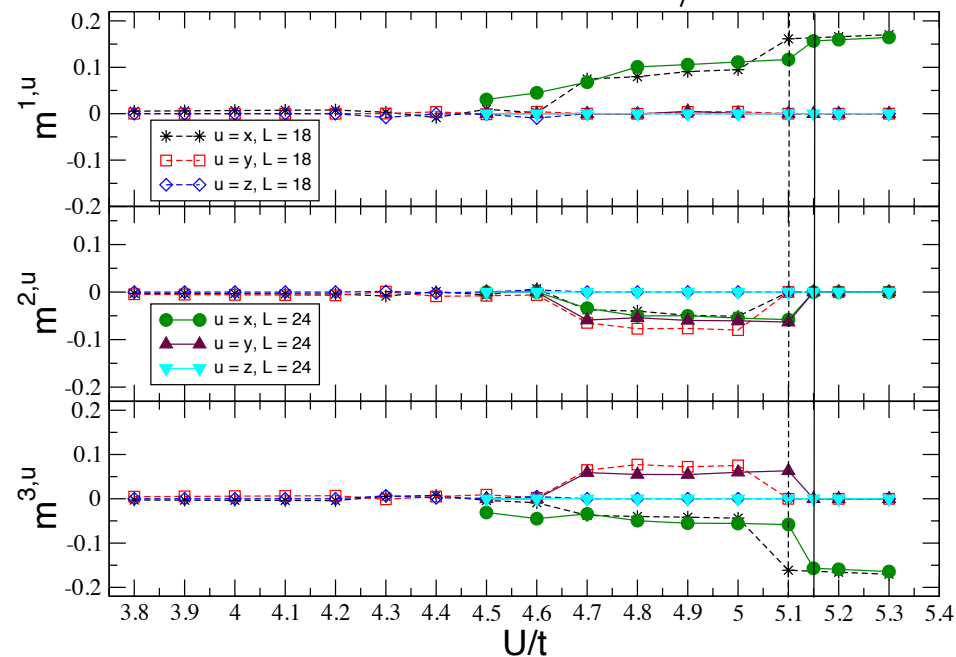


1/3-filling in ground state

Work with Richard Scalettar

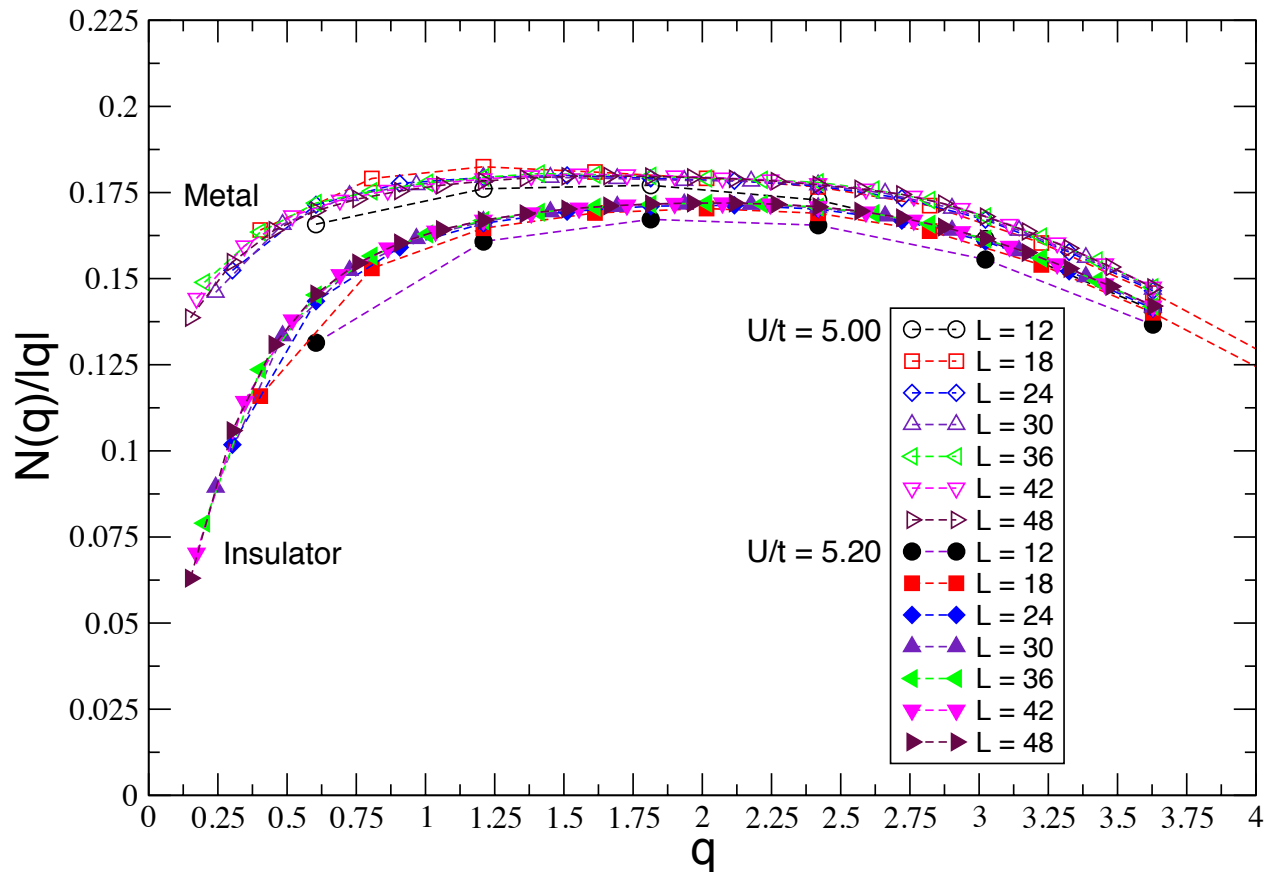


GCE at $T/t = 0.01$



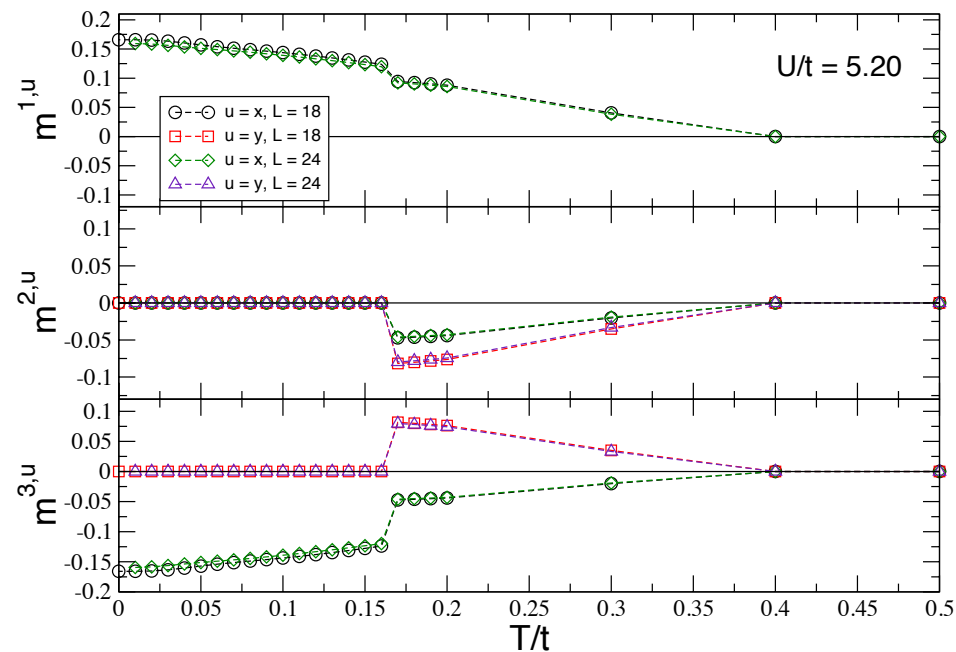
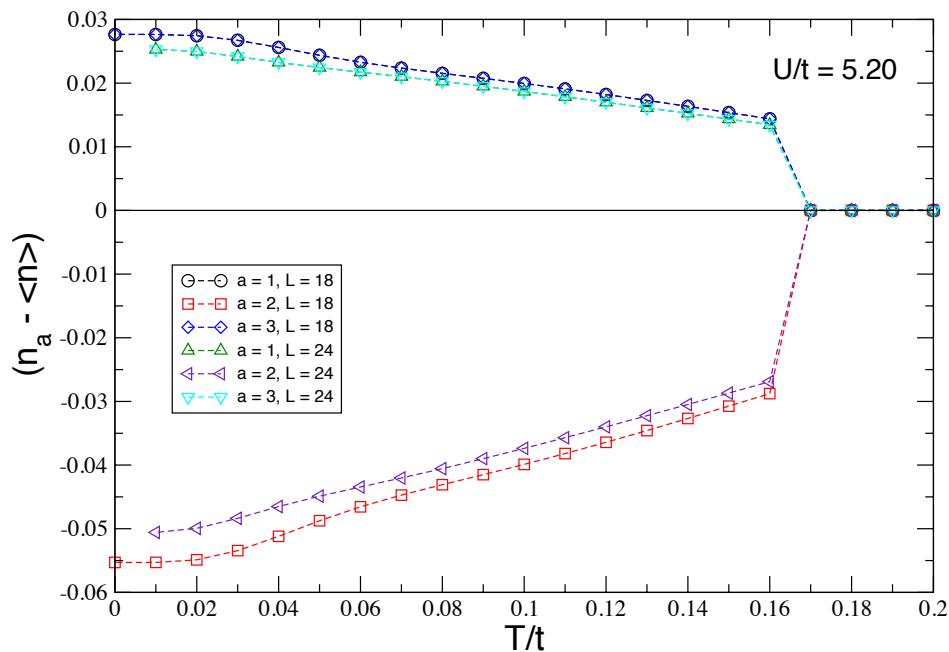
1/3-filling in ground state

Fourier transform of charge-charge correlations

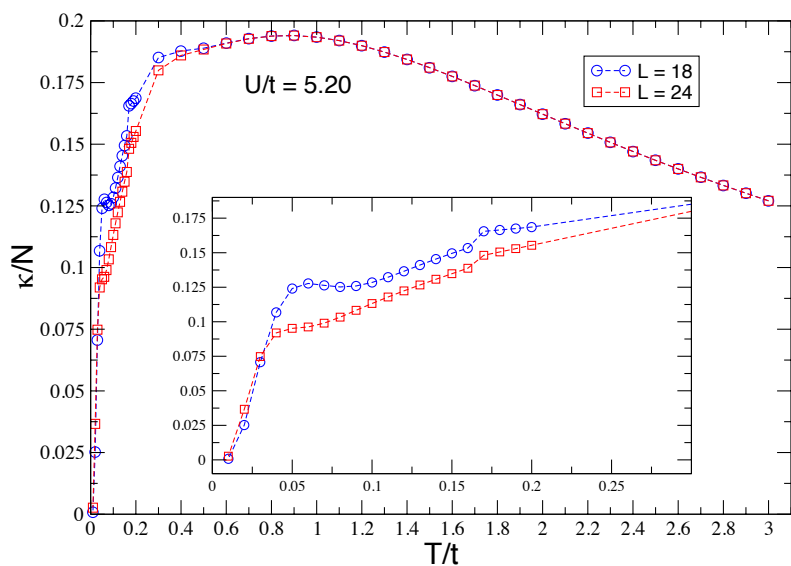


Metal-Insulator transition at
 $U_c/t \approx 5.15$

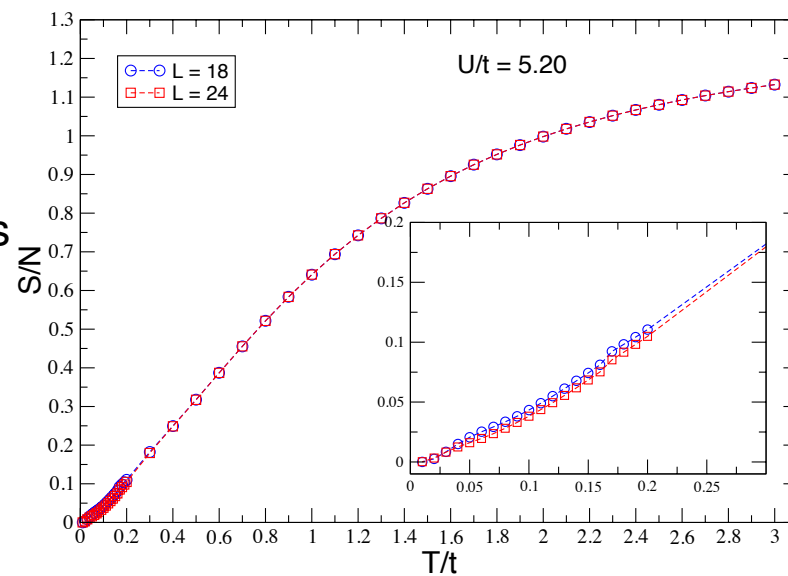
1/3-filling at finite T



Broken discrete symmetry of lattice, MW theorem does not apply.

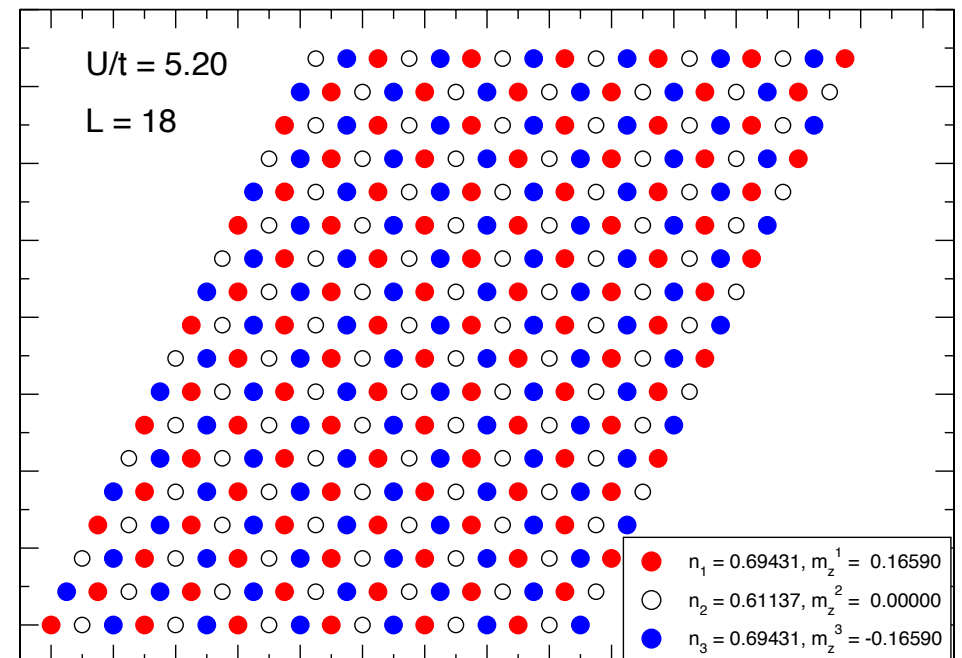
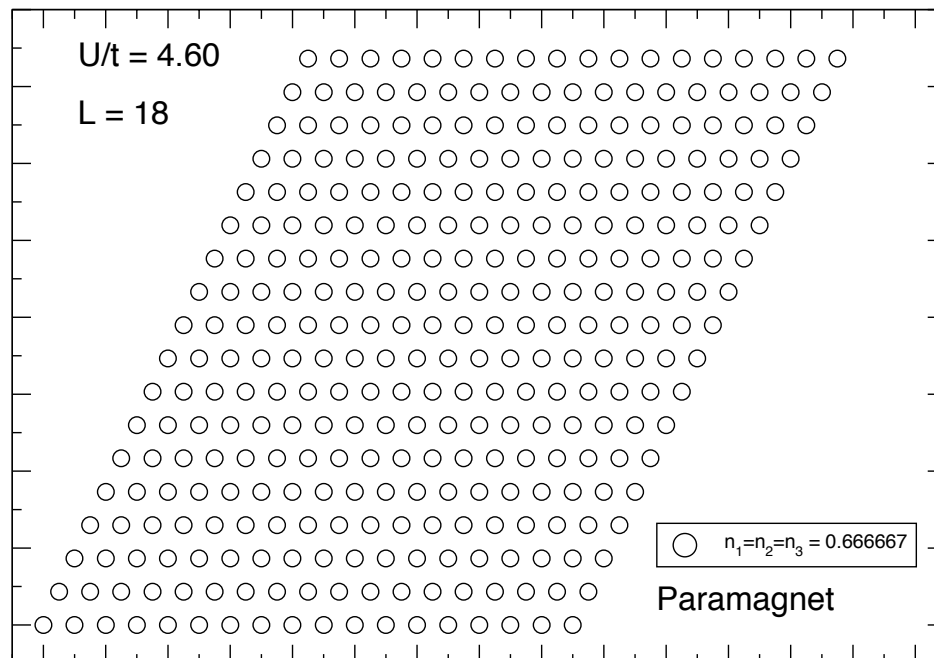


Transition looks
1st order



1/3-filling in ground state

- Charge order with partial magnetic order.
- Magnetic order on honeycomb substructure - no frustration.
- Frustration driven MIT



Final comments

- Complete the HF work on the triangular and kagome lattices
- Beyond Hartree-Fock MFT - make stronger connections to materials
 - CP/ Φ QMC ?
 - Include Onsager reaction field in the MFT
 - Thouless - Anderson - Palmer (TAP) applied to the Hubbard model
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Thanks!