Mean-Field Studies of the hole-doped $J-K-\Gamma$ Model

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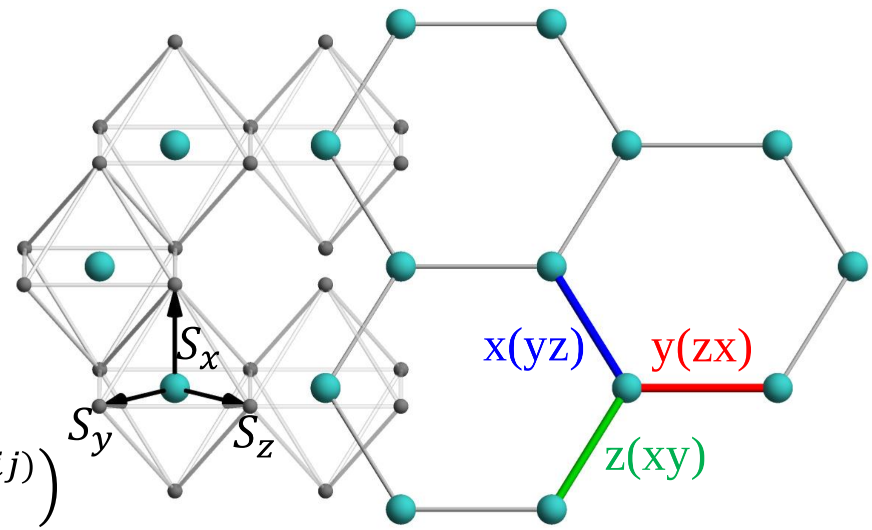
Outline

- Recent mean-field results on the honeycomb lattice
- Some results on the triangular lattice

Model and Method

Johann Schmidt et al., Phys. Rev. B **97,** 014504 (2018)

$$
\begin{aligned}
H &= H_k + H_{JK\Gamma} \\
H_{JK\Gamma} &= J\sum_{\langle ij\rangle}\left(\boldsymbol{S}_i\cdot\boldsymbol{S}_j-\frac{1}{4}n_in_j\right) \\
&+ K\sum_{\langle ij\rangle} S_i^{\gamma(ij)}S_j^{\gamma(ij)} \\
&+ \Gamma\sum_{\langle ij\rangle}\left(S_i^{\alpha(ij)}S_j^{\beta(ij)}+S_i^{\beta(ij)}S_j^{\alpha(ij)}\right)
\end{aligned}
$$



- For a quantum spin system, it is hard to solve exactly except for some simple cases.
- The general approach for understanding its physical properties is mean-field approximation.
- For ordered spin states, we can simply replace the spin operator S_i^α by its quantum averages $\langle S_i^\alpha\rangle$ and obtain a mean-field Hamiltonian.
- For spin-liquid states, this approach is invalid, because the local moment is zero.
- To obtain the mean-field ground state of the spin-liquids, a strange trick: the slave boson approach was introduced.

Schwinger Fermion Representation

Introducing the spinon operators $f_{i\sigma}$, $\sigma = \uparrow, \downarrow$, which are spin-1/2 charge-neutral operators. The spin operators are represented by:

$$S_i^\alpha = \frac{1}{2}\begin{bmatrix} f_{i\uparrow}^\dagger & f_{i\downarrow}^\dagger \end{bmatrix} \sigma^\alpha \begin{bmatrix} f_{i\uparrow} \\ f_{i\downarrow} \end{bmatrix} \quad \alpha = x, y, z \quad \left\{ f_{i\sigma}, f_{j\sigma'}^\dagger \right\} = \delta_{ij}\delta_{\sigma\sigma'} \quad \left\{ f_{i\sigma}, f_{j\sigma'} \right\} = 0$$

For the original spin model, there are two spin states per site, i.e. $|\uparrow\rangle$ and $|\downarrow\rangle$.
Adopting the above representation, there are four states per site, i.e. $|\ 0\rangle$, $|\uparrow\rangle$, $|\downarrow\rangle$ and $|\uparrow\downarrow\rangle$.
The equivalence between the original and the rewritten Hamiltonian is valid only in the subspace where there is exactly one fermion per site:

$$f_{i\uparrow}^\dagger f_{i\uparrow} + f_{i\downarrow}^\dagger f_{i\downarrow} = 1$$

To understand the $SU(2)$ gauge structure, we introduce a doublet: $\psi_i = \left(f_{i\uparrow}, f_{i\downarrow}^\dagger\right)^T$
For a general $SU(2)$ transformation between the spinons:

$$\begin{bmatrix} f_{i\uparrow} \\ f_{i\downarrow}^\dagger \end{bmatrix} \to \begin{bmatrix} a & b \\ -b^* & a^* \end{bmatrix} \begin{bmatrix} f_{i\uparrow} \\ f_{i\downarrow}^\dagger \end{bmatrix}$$

We can verify that the physical spin operators are unchanged.
The $SU(2)$ gauge transformation means that: two mean-field Hamiltonian related by a $SU(2)$ gauge transformation correspond to the same physical spin wave function.

Xiao-Gang Wen, Phys. Rev. B **65,** 165113 (2002)

Spin-singlet and triplet pairing operators

To study the possible superconducting pairing in the spin model, we introducing spin-singlet and triplet pairing operators defined on the nearest-neighbor bonds:

$$s_{ij}^{\dagger} = \frac{1}{\sqrt{2}}\begin{bmatrix} f_{i\uparrow}^{\dagger} & f_{i\downarrow}^{\dagger} \end{bmatrix} i\sigma_y\sigma_0 \begin{bmatrix} f_{j\uparrow}^{\dagger} \\ f_{j\downarrow}^{\dagger} \end{bmatrix} \qquad t_{ij}^{\alpha\dagger} = \frac{1}{\sqrt{2}}\begin{bmatrix} f_{i\uparrow}^{\dagger} & f_{i\downarrow}^{\dagger} \end{bmatrix} i\sigma_y\sigma_\alpha \begin{bmatrix} f_{j\uparrow}^{\dagger} \\ f_{j\downarrow}^{\dagger} \end{bmatrix}$$

where $\alpha = x, y, z$, and σ are the Pauli matrices acting on spin space, with σ_0 sbeing the 2×2 identity matrix.

$$c_{i\uparrow}^{\dagger}c_{j\uparrow}^{\dagger} = \frac{1}{\sqrt{2}}\left(t_{ij}^{x\dagger} - it_{ij}^{y\dagger}\right) \qquad c_{i\downarrow}^{\dagger}c_{j\downarrow}^{\dagger} = -\frac{1}{\sqrt{2}}\left(t_{ij}^{x\dagger} + it_{ij}^{y\dagger}\right)$$

$$c_{i\uparrow}^{\dagger}c_{j\downarrow}^{\dagger} = \frac{1}{\sqrt{2}}\left(s_{ij}^{\dagger} - t_{ij}^{z\dagger}\right) \qquad c_{i\downarrow}^{\dagger}c_{j\uparrow}^{\dagger} = -\frac{1}{\sqrt{2}}\left(s_{ij}^{\dagger} + t_{ij}^{z\dagger}\right)$$

Decoupling Scheme

$$\boldsymbol{S}_i \cdot \boldsymbol{S}_j - \frac{1}{4}n_i n_j = -s_{ij}^{\dagger}s_{ij} \qquad S_i^{\alpha}S_j^{\beta} + S_i^{\beta}S_j^{\alpha} = \frac{1}{2}\left(t_{ij}^{\alpha\dagger}t_{ij}^{\beta} + t_{ij}^{\beta\dagger}t_{ij}^{\alpha}\right)$$

$$S_i^x S_j^x = \frac{1}{4}\left(-s_{ij}^{\dagger}s_{ij} - t_{ij}^{x\dagger}t_{ij}^{x} + t_{ij}^{y\dagger}t_{ij}^{y} + t_{ij}^{z\dagger}t_{ij}^{z}\right)$$

$$S_i^y S_j^y = \frac{1}{4}\left(-s_{ij}^{\dagger}s_{ij} + t_{ij}^{x\dagger}t_{ij}^{x} - t_{ij}^{y\dagger}t_{ij}^{y} + t_{ij}^{z\dagger}t_{ij}^{z}\right)$$

$$S_i^z S_j^z = \frac{1}{4}\left(-s_{ij}^{\dagger}s_{ij} + t_{ij}^{x\dagger}t_{ij}^{x} + t_{ij}^{y\dagger}t_{ij}^{y} - t_{ij}^{z\dagger}t_{ij}^{z}\right)$$

- Xiao-Gang Wen, Phys. Rev. B **65,** 165113 (2002)
- S. Okamoto, Phys. Rev. Lett. **110,** 066403 (2013)
- Kai Li, Shun-Li Yu, Jian-Xin Li, New J. Phys. **17,** 043032 (2015)

Mean-Field Approximation

$$\hat{A}\hat{B} = (\hat{A} - \langle\hat{A}\rangle + \langle\hat{A}\rangle) + (\hat{B} - \langle\hat{B}\rangle + \langle\hat{B}\rangle)$$

$$\hat{A}\hat{B} = \hat{A}\langle\hat{B}\rangle + \hat{B}\langle\hat{A}\rangle - \langle\hat{A}\rangle\langle\hat{B}\rangle + (\hat{A} - \langle\hat{A}\rangle)(\hat{B} - \langle\hat{B}\rangle)$$

$$\begin{aligned} \mathrm{H}_{\mathrm{JK\Gamma}} = & \; J\sum_{\langle ij\rangle} -s_{ij}^{\dagger}s_{ij} + \frac{\Gamma}{2}\sum_{\langle ij\rangle}\left(t_{ij}^{\alpha_{ij}\dagger}t_{ij}^{\beta_{ij}} + t_{ij}^{\beta_{ij}\dagger}t_{ij}^{\alpha_{ij}}\right) \\ & + \frac{K}{4}\sum_{\langle ij\rangle}\left(-s_{ij}^{\dagger}s_{ij} + t_{ij}^{\alpha_{ij}\dagger}t_{ij}^{\alpha_{ij}} + t_{ij}^{\beta_{ij}\dagger}t_{ij}^{\beta_{ij}} - t_{ij}^{\gamma_{ij}\dagger}t_{ij}^{\gamma_{ij}}\right) \end{aligned}$$

Replacing the singlet and triplet pairing operators by their expectation values. For complete generality, there are in total 12 different order parameters. Three of these are singlet order parameters, one for each nearest-neighbor bond. The remaining nine are triplet order parameters which make up the usual $\boldsymbol{d}$ vector.

$$\boldsymbol{d} = \begin{bmatrix} d_1^x & d_2^x & d_3^x \\ d_1^y & d_2^y & d_3^y \\ d_1^z & d_2^z & d_3^z \end{bmatrix}$$

The resulting mean-field Hamiltonian is:

$$H_{JK\Gamma}^{mean} = \sum_{\langle ij\rangle}\left(\Delta_{ij}s_{ij}^{\dagger} + \sum_{\alpha} d_{ij}^{\alpha}t_{ij}^{\alpha\dagger} + h.c\right)$$

where we have dropped constant terms that only change the overall energy of the system.

Self-consistency equations:

$$\Delta = \frac{1}{\sqrt{2}}\left(-J-\frac{K}{4}\right)\left(\langle s_{i\delta_1}\rangle, \langle s_{i\delta_2}\rangle, \langle s_{i\delta_3}\rangle\right)$$

$$\boldsymbol{d}^x = \frac{1}{\sqrt{2}}\left(-\frac{K}{4}\langle t^x_{i\delta_1}\rangle, \frac{K}{4}\langle t^x_{i\delta_2}\rangle + \frac{\Gamma}{2}\langle t^z_{i\delta_2}\rangle, \frac{K}{4}\langle t^x_{i\delta_3}\rangle + \frac{\Gamma}{2}\langle t^y_{i\delta_3}\rangle\right)$$

$$\boldsymbol{d}^y = \frac{1}{\sqrt{2}}\left(\frac{K}{4}\langle t^y_{i\delta_1}\rangle + \frac{\Gamma}{2}\langle t^z_{i\delta_1}\rangle, -\frac{K}{4}\langle t^y_{i\delta_2}\rangle, \frac{K}{4}\langle t^y_{i\delta_3}\rangle + \frac{\Gamma}{2}\langle t^x_{i\delta_3}\rangle\right)$$

$$\boldsymbol{d}^z = \frac{1}{\sqrt{2}}\left(\frac{K}{4}\langle t^z_{i\delta_1}\rangle + \frac{\Gamma}{2}\langle t^y_{i\delta_1}\rangle, \frac{K}{4}\langle t^z_{i\delta_2}\rangle + \frac{\Gamma}{2}\langle t^x_{i\delta_2}\rangle, -\frac{K}{4}\langle t^z_{i\delta_3}\rangle\right)$$

- The Heisenberg term J only gives rise to singlet pairing
- The Kitaev K and off-diagonal Γ exchange term generate triplet pairing
- The Γ term couples two different triplet components on the same bond
- This may leads to a competition between triplet states driven by the K and Γ terms and singlet states from the J interaction

The kinetic part

At half-filling, the $JK\Gamma$ interaction is the effective interaction in a (spin-orbit) Mott insulator. It is thus reasonable to expect finite doping to induce superconductivity, similar to the situation considered in other Mutt insulators.

$$H_k = -\tilde{t}\sum_{\langle ij\rangle\sigma}\left(c_{i,\sigma,a}^{\dagger}c_{j,\sigma,b} + h.c.\right) + \tilde{\mu}\sum_{i\sigma a} c_{i,\sigma,a}^{\dagger}c_{i,\sigma,a}$$

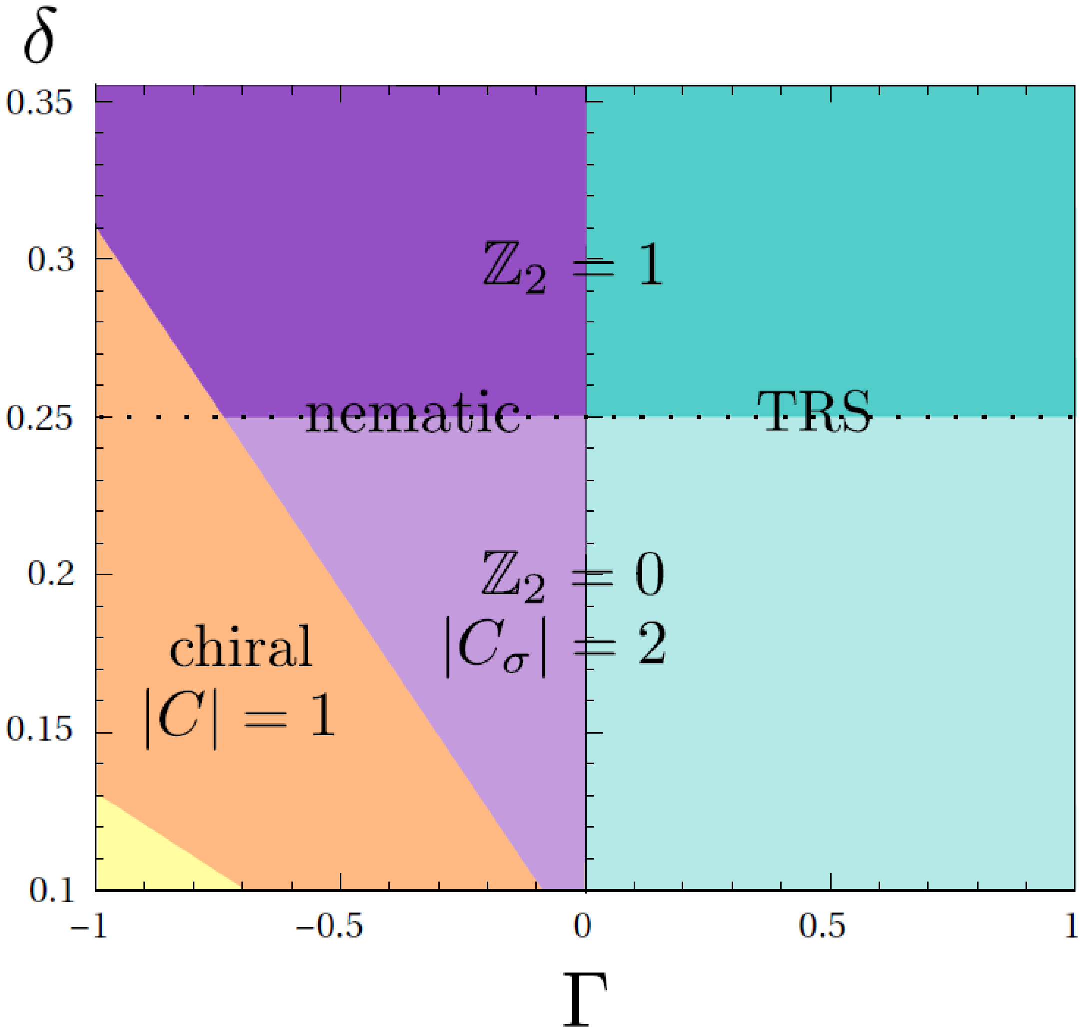
To exclude the double occupancy, we include the Gutzwiller approximation in $\tilde{t}$ through a slave-boson mean-field approach, which leads to rescaling of the effective hopping amplitude. Thus, $\tilde{t} = t\delta$, where t is the bare hopping parameter and δ corresponds to the hole-doping level, such that the number of electrons per site is given by $1-\delta$.
This approximation also requires an adjustment of the chemical potential $\tilde{\mu}$ for each δ.

The final quadratic Hamiltonian

$$H_{quad} = H_k + H_{JK\Gamma}^{mean} \qquad H_{JK\Gamma}^{mean} = \sum_{\langle ij\rangle}\left(\Delta_{ij}s_{ij}^{\dagger} + \sum_{\alpha} d_{ij}^{\alpha}t_{ij}^{\alpha\dagger} + h.c\right)$$

Phase diagram

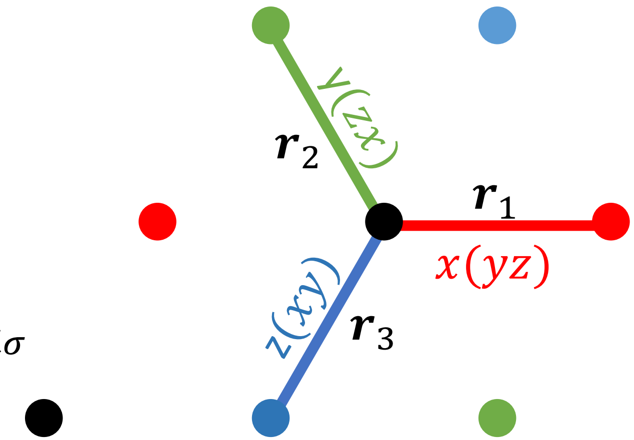
Johann Schmidt et al., Phys. Rev. B **97,** 014504 (2018)



Phase diagram of the triplet order parameters for *K=-t* and *J=0*

- For $\Gamma > 0$, the time-reversal symmetric solution $\boldsymbol{d}_{TRS}$ is stable at all doping level. Beneath $\delta = 0.25$, it hosts a symmetry-protected topological phase, while above the stronger $\mathbb{Z}_2$ invariant becomes nontrivial.
- For $\Gamma < 0$, at large doping, the superconducting order $\boldsymbol{d}_{nematic}$ breaks the C_3 symmetry but it topologically equivalent to $\boldsymbol{d}_{TRS}$; at intermediate doping, the $\boldsymbol{d}_{chiral}$ breaks time-reversal symmetry and classified by a nonzero Chern number.

$J-K-\Gamma$ model on triangular lattice



$$H = H_k + H_{JK\Gamma}$$

$$H_k = -\tilde{t}\sum_{\langle ij\rangle\sigma}\left(c_{i\sigma}^{\dagger}c_{i\sigma} + h.c.\right) + \tilde{\mu}\sum_{i\sigma} c_{i\sigma}^{\dagger}c_{i\sigma}$$

$$H_{JK\Gamma} = J\sum_{\langle ij\rangle}\left(\boldsymbol{S}_i\cdot\boldsymbol{S}_j - \frac{1}{4}n_i n_j\right) + K\sum_{\langle ij\rangle} S_i^{\gamma(ij)}S_j^{\gamma(ij)} + \Gamma\sum_{\langle ij\rangle}\left(S_i^{\alpha(ij)}S_j^{\beta(ij)} + S_i^{\beta(ij)}S_j^{\alpha(ij)}\right)$$

Fourier Transformation

$$\sum_{\langle ij\rangle} s_{ij}^{\dagger} = \frac{1}{\sqrt{2}}\sum_{\langle ij\rangle}\left[c_{i\uparrow}^{\dagger}, c_{i\downarrow}^{\dagger}\right] i\sigma_y\sigma_0 \begin{bmatrix} c_{j\uparrow}^{\dagger} \\ c_{j\downarrow}^{\dagger} \end{bmatrix}$$

$$c_{i\sigma} = \frac{1}{\sqrt{N}}\sum_{\boldsymbol{k}\in BZ} c_{\boldsymbol{k}\sigma}e^{i\boldsymbol{k}\cdot\boldsymbol{r}_i} \qquad = \frac{1}{\sqrt{2}}\sum_{\boldsymbol{k},\boldsymbol{k}'\in BZ}\left[c_{\boldsymbol{k}\uparrow}^{\dagger}, c_{\boldsymbol{k}\downarrow}^{\dagger}\right] i\sigma_y\sigma_0 \begin{bmatrix} c_{\boldsymbol{k}'\uparrow}^{\dagger} \\ c_{\boldsymbol{k}'\downarrow}^{\dagger} \end{bmatrix} \frac{1}{N}\sum_{\langle ij\rangle} e^{-i\boldsymbol{k}\cdot\boldsymbol{r}_i - \boldsymbol{k}'\cdot\boldsymbol{r}_j}$$

$$c_{\boldsymbol{k}\sigma} = \frac{1}{\sqrt{N}}\sum_{i} c_{i\sigma}e^{-i\boldsymbol{k}\cdot\boldsymbol{r}_i} \qquad = \frac{1}{\sqrt{2}}\sum_{\boldsymbol{k}\in BZ}\left[c_{\boldsymbol{k}\uparrow}^{\dagger}, c_{\boldsymbol{k}\downarrow}^{\dagger}\right] i\sigma_y\sigma_0 \begin{bmatrix} c_{-\boldsymbol{k}\uparrow}^{\dagger} \\ c_{-\boldsymbol{k}\downarrow}^{\dagger} \end{bmatrix} e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_j - \boldsymbol{r}_i)}$$

Mean-Field Hamiltonian in $\boldsymbol{k}$ space:

$$H_{JK\Gamma}^{mean} = \frac{1}{\sqrt{2}} \sum_{\boldsymbol{k}\in BZ} \left[c_{\boldsymbol{k}\uparrow}^{\dagger}, c_{\boldsymbol{k}\downarrow}^{\dagger}\right] M \begin{bmatrix} c_{-\boldsymbol{k}\uparrow}^{\dagger} \\ c_{-\boldsymbol{k}\downarrow}^{\dagger} \end{bmatrix} + h.c.$$

$$\begin{aligned} M = &\quad i\sigma_y\sigma_0\left(\Delta_1 e^{i\boldsymbol{k}\cdot\boldsymbol{r}_1} + \Delta_2 e^{i\boldsymbol{k}\cdot\boldsymbol{r}_2} + \Delta_3 e^{i\boldsymbol{k}\cdot\boldsymbol{r}_3}\right) \\ &+ i\sigma_y\sigma_x\left(d_1^x e^{i\boldsymbol{k}\cdot\boldsymbol{r}_1} + d_2^x e^{i\boldsymbol{k}\cdot\boldsymbol{r}_2} + d_3^x e^{i\boldsymbol{k}\cdot\boldsymbol{r}_3}\right) \\ &+ i\sigma_y\sigma_y\left(d_1^y e^{i\boldsymbol{k}\cdot\boldsymbol{r}_1} + d_2^y e^{i\boldsymbol{k}\cdot\boldsymbol{r}_2} + d_3^y e^{i\boldsymbol{k}\cdot\boldsymbol{r}_3}\right) \\ &+ i\sigma_y\sigma_z\left(d_1^z e^{i\boldsymbol{k}\cdot\boldsymbol{r}_1} + d_2^z e^{i\boldsymbol{k}\cdot\boldsymbol{r}_2} + d_3^z e^{i\boldsymbol{k}\cdot\boldsymbol{r}_3}\right) \end{aligned}$$

$$\begin{aligned} \Delta &= \frac{1}{\sqrt{2}}\left(-J - \frac{K}{4}\right)\left(\langle s_{i\delta_1}\rangle, \langle s_{i\delta_2}\rangle, \langle s_{i\delta_3}\rangle\right) \\ \boldsymbol{d}^x &= \frac{1}{\sqrt{2}}\left(-\frac{K}{4}\langle t_{i\delta_1}^x\rangle, \frac{K}{4}\langle t_{i\delta_2}^x\rangle + \frac{\Gamma}{2}\langle t_{i\delta_2}^z\rangle, \frac{K}{4}\langle t_{i\delta_3}^x\rangle + \frac{\Gamma}{2}\langle t_{i\delta_3}^y\rangle\right) \\ \boldsymbol{d}^y &= \frac{1}{\sqrt{2}}\left(\frac{K}{4}\langle t_{i\delta_1}^y\rangle + \frac{\Gamma}{2}\langle t_{i\delta_1}^z\rangle, -\frac{K}{4}\langle t_{i\delta_2}^y\rangle, \frac{K}{4}\langle t_{i\delta_3}^y\rangle + \frac{\Gamma}{2}\langle t_{i\delta_3}^x\rangle\right) \\ \boldsymbol{d}^z &= \frac{1}{\sqrt{2}}\left(\frac{K}{4}\langle t_{i\delta_1}^z\rangle + \frac{\Gamma}{2}\langle t_{i\delta_1}^y\rangle, \frac{K}{4}\langle t_{i\delta_2}^z\rangle + \frac{\Gamma}{2}\langle t_{i\delta_2}^x\rangle, -\frac{K}{4}\langle t_{i\delta_3}^z\rangle\right) \end{aligned}$$

Hopping terms in $\boldsymbol{k}$ space:

$$H_k = -\tilde{t}\sum_{\langle ij\rangle\sigma}\left(c_{i\sigma}^{\dagger}c_{j\sigma} + h.c.\right) - \tilde{\mu}\sum_{i\sigma} c_{i\sigma}^{\dagger}c_{i\sigma} = -\sum_{\boldsymbol{k}\in BZ,\sigma}\left[2\tilde{t}f(\boldsymbol{k}) + \tilde{\mu}\right]c_{\boldsymbol{k}\sigma}^{\dagger}c_{\boldsymbol{k}\sigma} \qquad (1)$$

$$f(\boldsymbol{k}) = cos(\boldsymbol{k}\cdot\boldsymbol{r}_1) + cos(\boldsymbol{k}\cdot\boldsymbol{r}_2) + cos(\boldsymbol{k}\cdot\boldsymbol{r}_3) \qquad f(\boldsymbol{k}) = f(-\boldsymbol{k})$$

$$\begin{aligned} H_k &= -\sum_{\boldsymbol{k}\in BZ,\sigma}\left[2\tilde{t}f(-\boldsymbol{k}) + \tilde{\mu}\right]c_{-\boldsymbol{k}\sigma}^{\dagger}c_{-\boldsymbol{k}\sigma} = -\sum_{\boldsymbol{k}\in BZ,\sigma}\left[2\tilde{t}f(-\boldsymbol{k}) + \tilde{\mu}\right]\left(1 - c_{-\boldsymbol{k}\sigma}c_{-\boldsymbol{k}\sigma}^{\dagger}\right) \\ &= \sum_{\boldsymbol{k}\in BZ,\sigma}\left[2\tilde{t}f(\boldsymbol{k}) + \tilde{\mu}\right]c_{-\boldsymbol{k}\sigma}c_{-\boldsymbol{k}\sigma}^{\dagger} - \sum_{\boldsymbol{k}\in BZ,\sigma}\left[2\tilde{t}f(k) + \tilde{\mu}\right] \qquad (2) \end{aligned}$$

$$H = H_k + H^{mean}_{JK\Gamma} = \sum_{\boldsymbol{k}\in BZ} \left[c^\dagger_{\boldsymbol{k}\uparrow}, c^\dagger_{\boldsymbol{k}\downarrow}, c^\dagger_{-\boldsymbol{k}\uparrow}, c_{-\boldsymbol{k}\downarrow}\right] H_M \begin{bmatrix} c_{\boldsymbol{k}\uparrow} \\ c_{\boldsymbol{k}\downarrow} \\ c^\dagger_{-\boldsymbol{k}\uparrow} \\ c^\dagger_{-\boldsymbol{k}\downarrow} \end{bmatrix}$$

$$H_M = \begin{bmatrix} \begin{matrix} -\tilde{t}f(\boldsymbol{k}) - \tilde{\mu}/2 & 0 \\ 0 & -\tilde{t}f(\boldsymbol{k}) - \tilde{\mu}/2 \end{matrix} & M \\ M^\dagger & \begin{matrix} \tilde{t}f(\boldsymbol{k}) + \tilde{\mu}/2 & 0 \\ 0 & \tilde{t}f(\boldsymbol{k}) + \tilde{\mu}/2 \end{matrix} \end{bmatrix}$$

$$U^\dagger H_M U = \begin{bmatrix} -\epsilon_{0\boldsymbol{k}} & 0 & 0 & 0 \\ 0 & -\epsilon_{1\boldsymbol{k}} & 0 & 0 \\ 0 & 0 & \epsilon_{1\boldsymbol{k}} & 0 \\ 0 & 0 & 0 & \epsilon_{0\boldsymbol{k}} \end{bmatrix} \qquad U^\dagger U = UU^\dagger = I \qquad \epsilon_{0\boldsymbol{k}} \geq \epsilon_{1\boldsymbol{k}} \geq 0$$

$$\left[A^\dagger_{\boldsymbol{k}}, B^\dagger_{\boldsymbol{k}}, C^\dagger_{\boldsymbol{k}}, D^\dagger_{\boldsymbol{k}}\right] = \left[c^\dagger_{\boldsymbol{k}\uparrow}, c^\dagger_{\boldsymbol{k}\downarrow}, c^\dagger_{-\boldsymbol{k}\uparrow}, c_{-\boldsymbol{k}\downarrow}\right] U$$

$$H = \sum_{\boldsymbol{k}\in BZ} \left[-\left(\epsilon_{0\boldsymbol{k}} A^\dagger_{\boldsymbol{k}} A_{\boldsymbol{k}} + \epsilon_{1\boldsymbol{k}} B^\dagger_{\boldsymbol{k}} B_{\boldsymbol{k}}\right) + \left(\epsilon_{1\boldsymbol{k}} C^\dagger_{\boldsymbol{k}} C_{\boldsymbol{k}} + \epsilon_{0\boldsymbol{k}} D^\dagger_{\boldsymbol{k}} D_{\boldsymbol{k}}\right)\right]$$

The ground state: $|\,\Omega\rangle$

The *A*, *B* quasiparticle states are fully occupied and *C*, *D* quasiparticle states are empty.

$$\langle \Omega \,|\, A^\dagger_{\boldsymbol{k}} A_{\boldsymbol{k}'} \,|\, \Omega \rangle = \delta_{\boldsymbol{k}\boldsymbol{k}'} \qquad \langle \Omega \,|\, B^\dagger_{\boldsymbol{k}} B_{\boldsymbol{k}'} \,|\, \Omega \rangle = \delta_{\boldsymbol{k}\boldsymbol{k}'}$$

$$\langle \Omega \,|\, C^\dagger_{\boldsymbol{k}} C_{\boldsymbol{k}'} \,|\, \Omega \rangle = 0 \qquad \langle \Omega \,|\, D^\dagger_{\boldsymbol{k}} D_{\boldsymbol{k}'} \,|\, \Omega \rangle = 0$$

The ground state averages

$$\langle \hat{n}_i \rangle = \left\langle \Omega \,\middle|\, [c_{i\uparrow}^\dagger, c_{i\downarrow}^\dagger] \begin{bmatrix} c_{i\uparrow} \\ c_{i\downarrow} \end{bmatrix} \,\middle|\, \Omega \right\rangle = \frac{1}{N} \sum_{\boldsymbol{k},\boldsymbol{k}' \in BZ} e^{-i(\boldsymbol{k}\cdot\boldsymbol{r}_i + \boldsymbol{k}'\cdot\boldsymbol{r}_j)} \left\langle \Omega \,\middle|\, [c_{\boldsymbol{k}\uparrow}^\dagger, c_{\boldsymbol{k}\downarrow}^\dagger] \begin{bmatrix} c_{\boldsymbol{k}'\uparrow} \\ c_{\boldsymbol{k}'\downarrow} \end{bmatrix} \,\middle|\, \Omega \right\rangle$$

$$= \frac{1}{N} \sum_{\boldsymbol{k},\boldsymbol{k}' \in BZ} e^{-i(\boldsymbol{k}\cdot\boldsymbol{r}_i + \boldsymbol{k}'\cdot\boldsymbol{r}_j)} \langle \Omega \mid [A_{\boldsymbol{k}'}^\dagger, B_{\boldsymbol{k}'}^\dagger, C_{\boldsymbol{k}'}^\dagger, D_{\boldsymbol{k}}^\dagger] U_0^\dagger U_0 [A_{\boldsymbol{k}}, B_{\boldsymbol{k}}, C_{\boldsymbol{k}}, D_{\boldsymbol{k}}]^T \mid \Omega \rangle$$

$$= \frac{1}{N} \sum_{\boldsymbol{k},\boldsymbol{k}' \in BZ} (M_{00} + M_{11}) \qquad \mathrm{M} = U_0^\dagger U_0 \quad \text{and } U_0 \text{ is the first two rows of } U$$

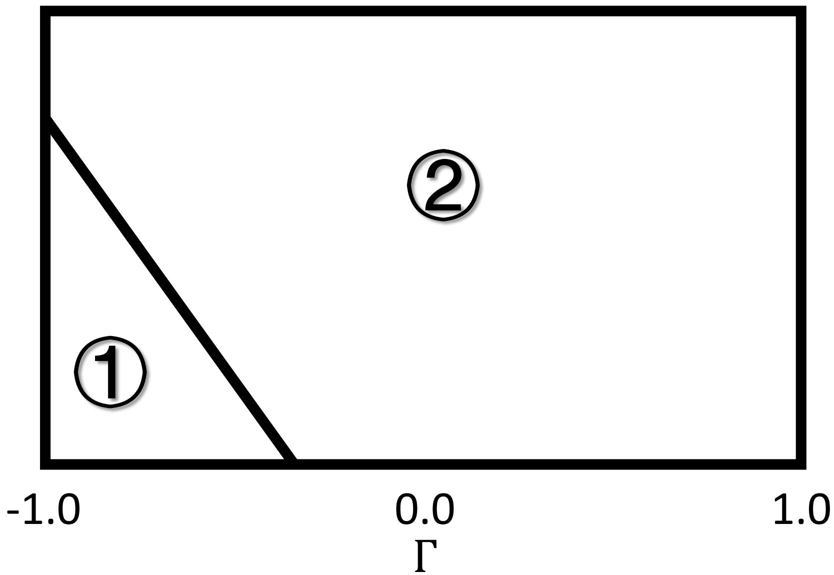
$$\langle \Omega \mid [c_{i\uparrow}^\dagger, c_{i\downarrow}^\dagger] T \begin{bmatrix} c_{j\uparrow} \\ c_{j\downarrow} \end{bmatrix} \mid \Omega \rangle = \frac{1}{N} \sum_{\boldsymbol{k},\boldsymbol{k}' \in BZ} e^{-i(\boldsymbol{k}\cdot\boldsymbol{r}_i - \boldsymbol{k}'\cdot\boldsymbol{r}_j)} \left\langle \Omega \,\middle|\, [c_{\boldsymbol{k}\uparrow}^\dagger, c_{\boldsymbol{k}\downarrow}^\dagger] P \begin{bmatrix} c_{\boldsymbol{k}'\uparrow} \\ c_{\boldsymbol{k}'\downarrow} \end{bmatrix} \,\middle|\, \Omega \right\rangle$$

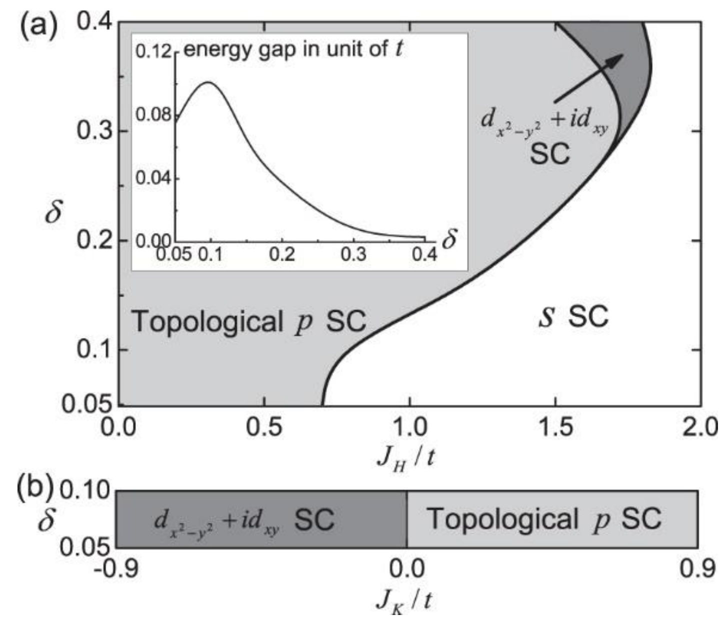
$$= \frac{1}{N} \sum_{\boldsymbol{k},\boldsymbol{k}' \in BZ} e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_j - \boldsymbol{r}_i)} (M_{00} + M_{11}) \quad \mathrm{M} = U_0^\dagger P U_0$$

$$\langle \Omega \mid [c_{i\uparrow}^\dagger, c_{i\downarrow}^\dagger] P \begin{bmatrix} c_{j\uparrow}^\dagger \\ c_{j\downarrow}^\dagger \end{bmatrix} \mid \Omega \rangle = \frac{1}{N} \sum_{\boldsymbol{k},\boldsymbol{k}' \in BZ} e^{-i(\boldsymbol{k}\cdot\boldsymbol{r}_i + \boldsymbol{k}'\cdot\boldsymbol{r}_j)} \left\langle \Omega \,\middle|\, [c_{\boldsymbol{k}\uparrow}^\dagger, c_{\boldsymbol{k}\downarrow}^\dagger] P \begin{bmatrix} c_{-\boldsymbol{k}'\uparrow}^\dagger \\ c_{-\boldsymbol{k}'\downarrow}^\dagger \end{bmatrix} \,\middle|\, \Omega \right\rangle$$

$$= \frac{1}{N} \sum_{\boldsymbol{k},\boldsymbol{k}' \in BZ} e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_j - \boldsymbol{r}_i)} (M_{00} + M_{11}) \quad \mathrm{M} = U_0^\dagger P U_1$$

Mean-Field Results





① $\boldsymbol{d}_1 = \eta \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix} \quad \boldsymbol{d}_2 = \eta \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \quad \boldsymbol{d}_3 = \eta \begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}$

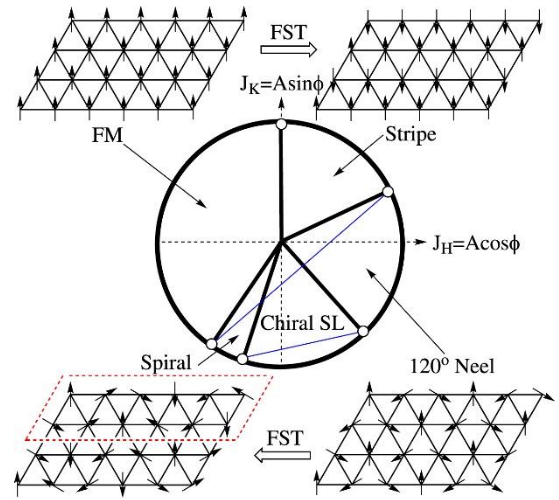
② $\boldsymbol{d} = \eta_1 \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & -1 \\ 0 & 0 & 0 \end{bmatrix} + \eta_2 \begin{bmatrix} 0 & -1 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} + \eta_3 \begin{bmatrix} 0 & 0 & 0 \\ -1 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}$

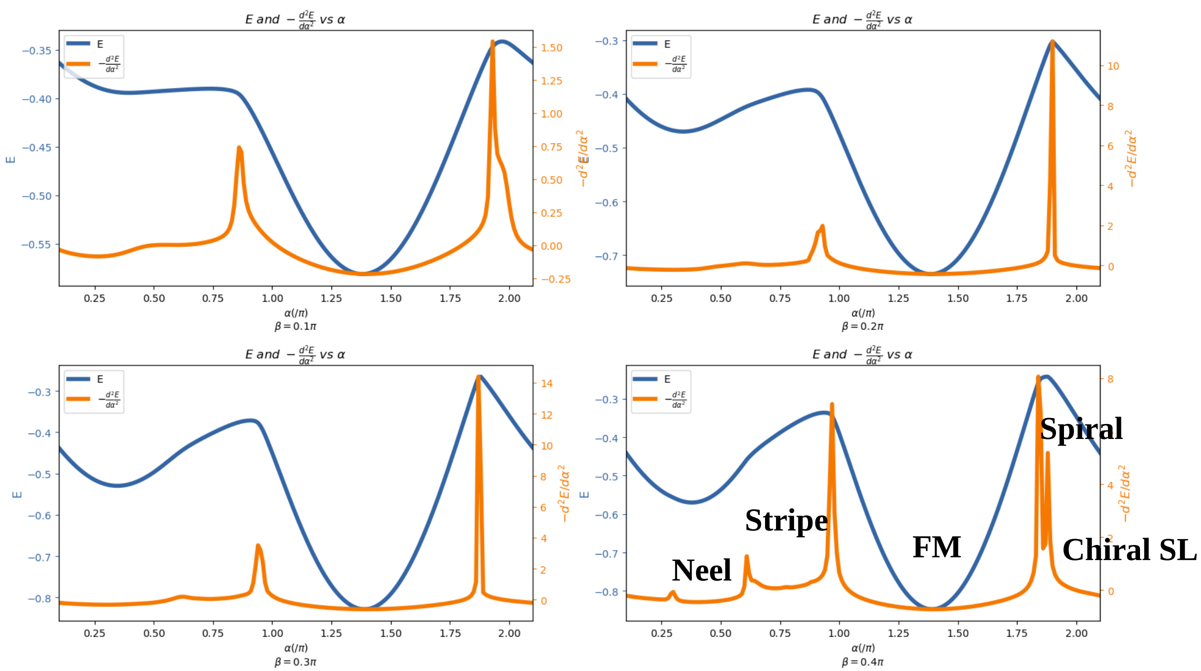
Exact diagonalization of the spin model

Kai Li, Shun-Li Yu, Jian-Xin Li,
New J. Phys. **17,** 043032 (2015)

$$J = A\sin(\beta)\sin(\alpha)$$
$$K = A\sin(\beta)\cos(\alpha)$$
$$\Gamma = A\cos(\beta)$$

Global phase diagram for $\Gamma = 0$





Thank you!