# The Landscape of the Hubbard model

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Talk online: sachdev.physics.harvard.edu

# The Hubbard Model

$$H = -\sum_{i<j} t_{ij} c^\dagger_{i\alpha} c_{j\alpha} + U \sum_i \left( n_{i\uparrow} - \frac{1}{2} \right) \left( n_{i\downarrow} - \frac{1}{2} \right) - \mu \sum_i c^\dagger_{i\alpha} c_{i\alpha}$$

$t_{ij} \rightarrow$ "hopping". $U \rightarrow$ local repulsion, $\mu \rightarrow$ chemical potential

Spin index $\alpha = \uparrow, \downarrow$

$$n_{i\alpha} = c^\dagger_{i\alpha} c_{i\alpha}$$

$$c^\dagger_{i\alpha} c_{j\beta} + c_{j\beta} c^\dagger_{i\alpha} = \delta_{ij} \delta_{\alpha\beta}$$
$$c_{i\alpha} c_{j\beta} + c_{j\beta} c_{i\alpha} = 0$$

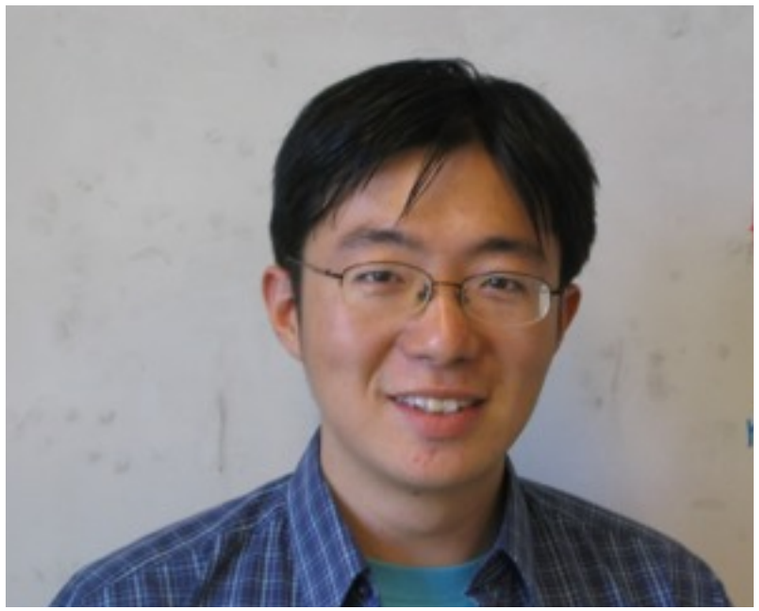
Will study the honeycomb and square lattices.

# Outline

1. Honeycomb lattice:
   semi-metal and antiferromagnetism
   *Dirac fermions and the Gross-Neveu model*

2. Spin liquids
   *Unified formulation as a SO(4) gauge theory*

3. Instabilities of spin liquids
   *Geometric phases, valence bond solids, and other competing orders*



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Physical Review Letters **105**, 057201 (2010)
and to appear

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In the limit of large $U$, and at a density of one particle per site, this maps onto the Heisenberg antiferromagnet

$$H_{AF} = \sum_{i<j} J_{ij} S^a_i S^a_j$$

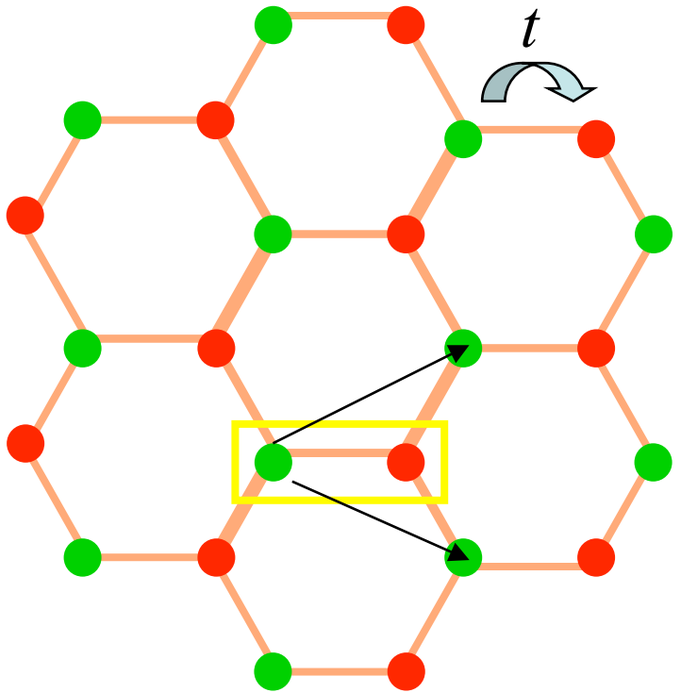
where $a = x, y, z$,

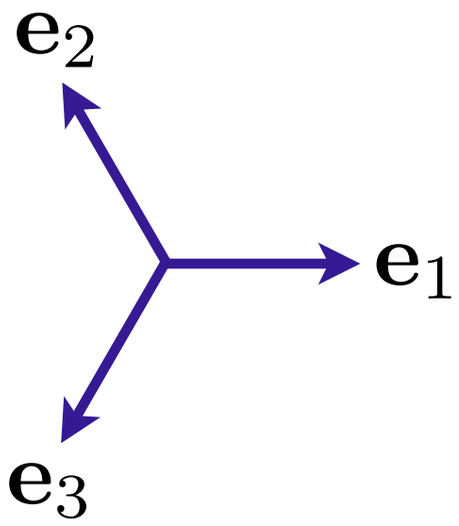
$$S^a_i = \frac{1}{2} c^{a\dagger}_{i\alpha} \sigma^a_{\alpha\beta} c_{i\beta},$$

with $\sigma^a$ the Pauli matrices and

$$J_{ij} = \frac{4t^2_{ij}}{U}$$

# Graphene



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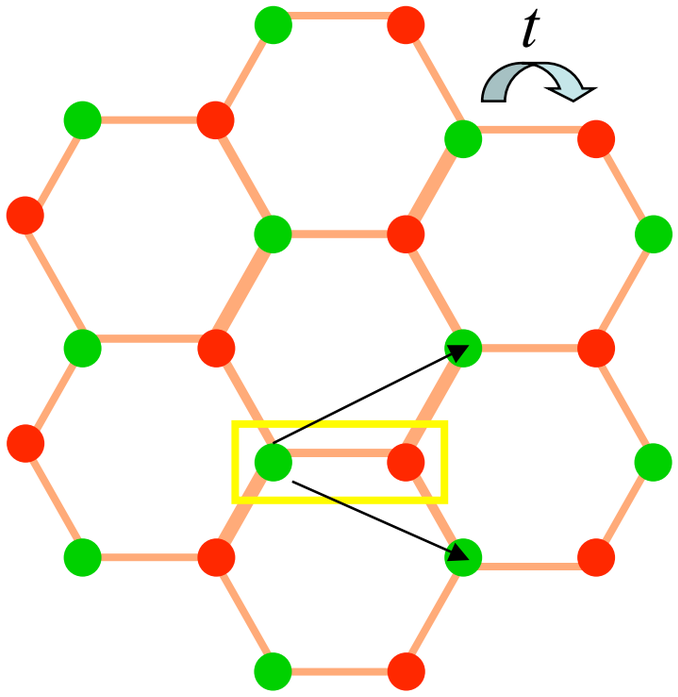
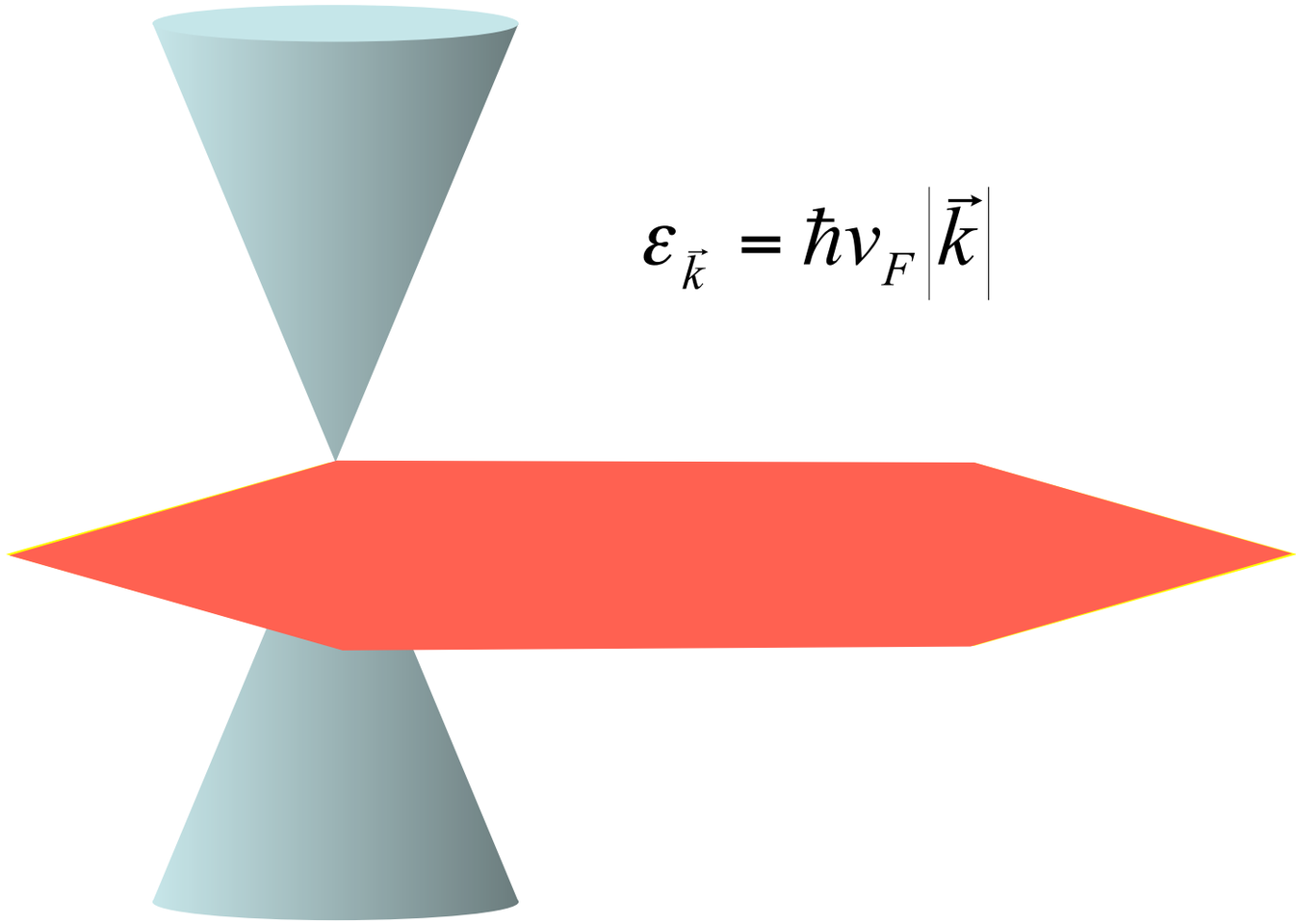
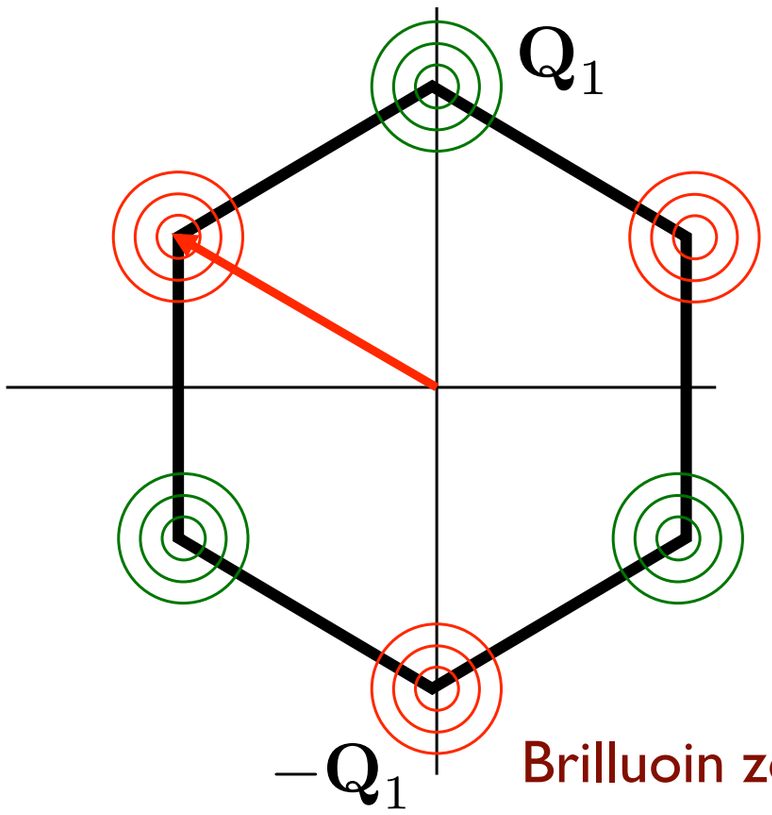


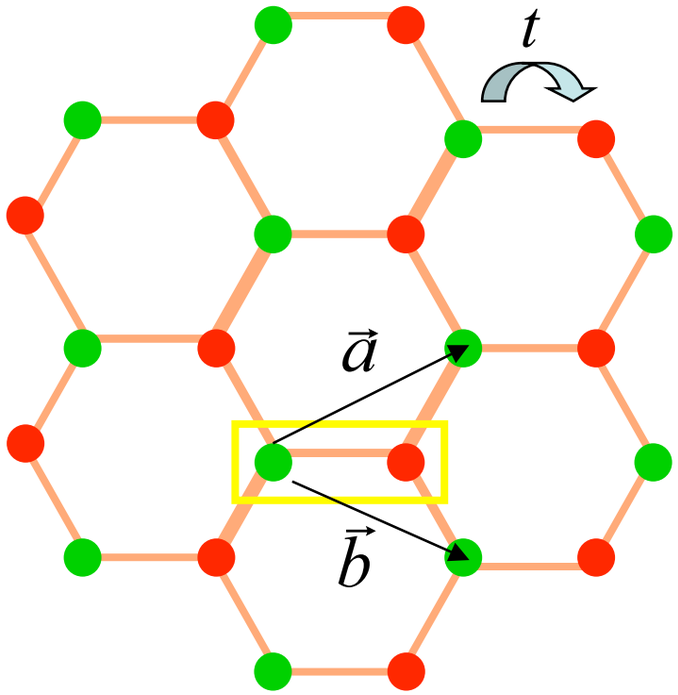
$$\varepsilon_{\vec{k}} = \hbar v_F \left| \vec{k} \right|$$



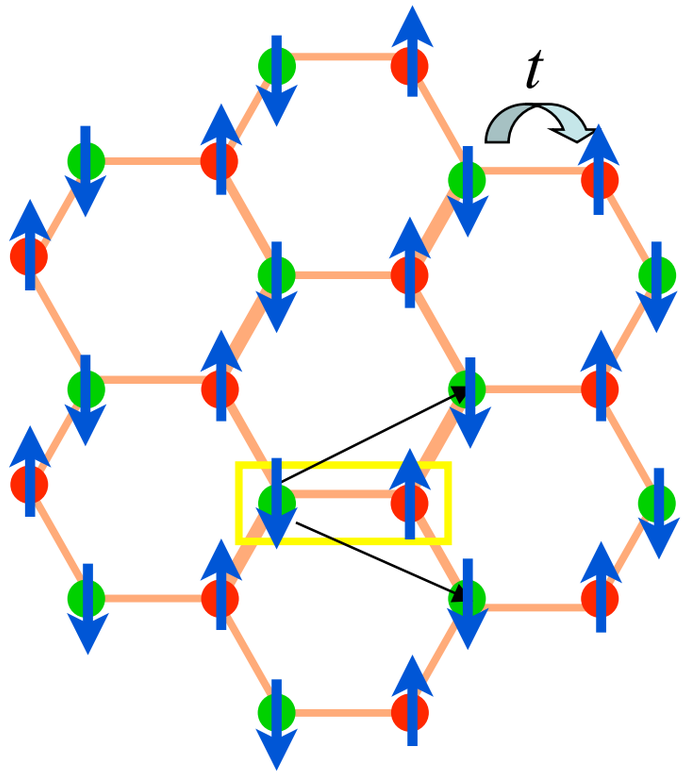

Brilluoin zone

Semi-metal with
massless Dirac fermions

# Graphene

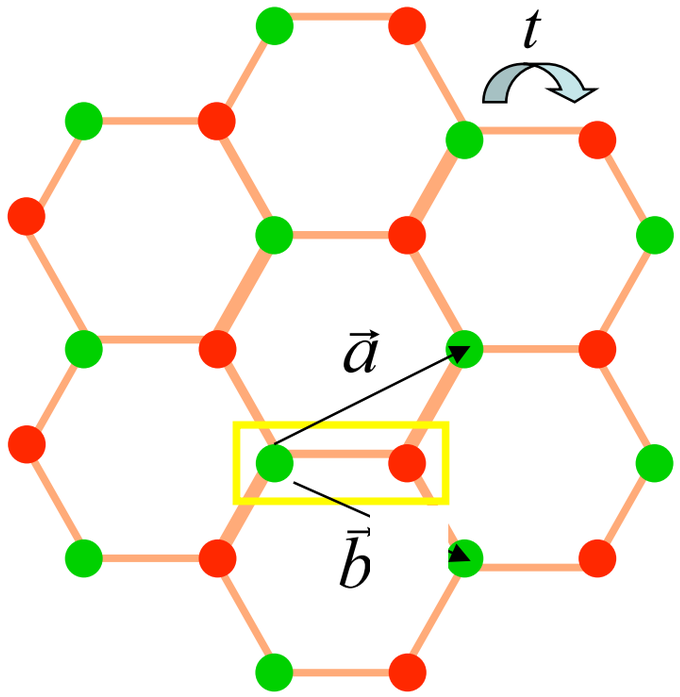


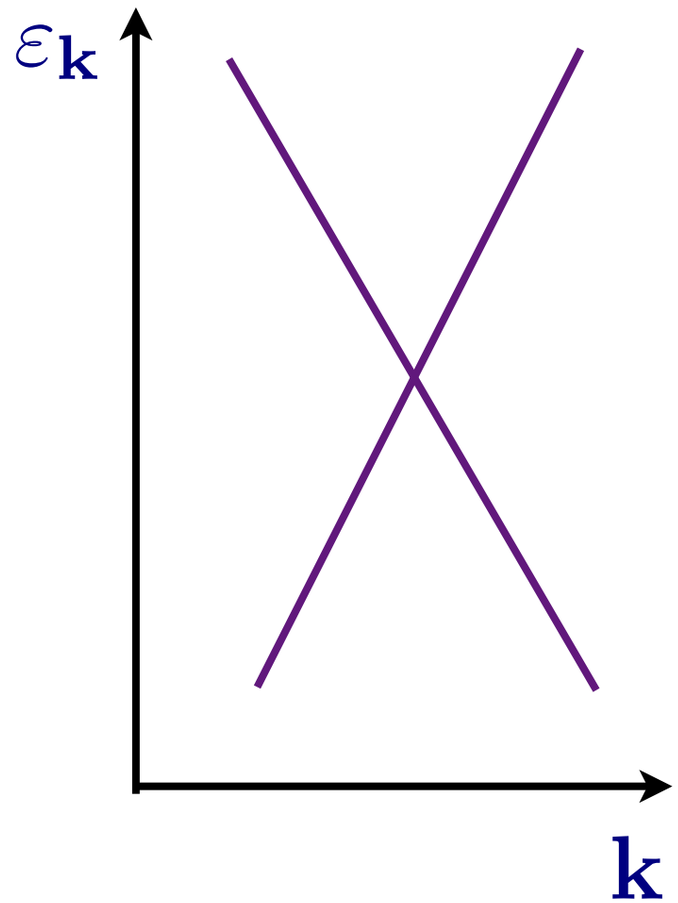

Dirac
semi-metal




Insulating
antiferromagnet
with Neel order

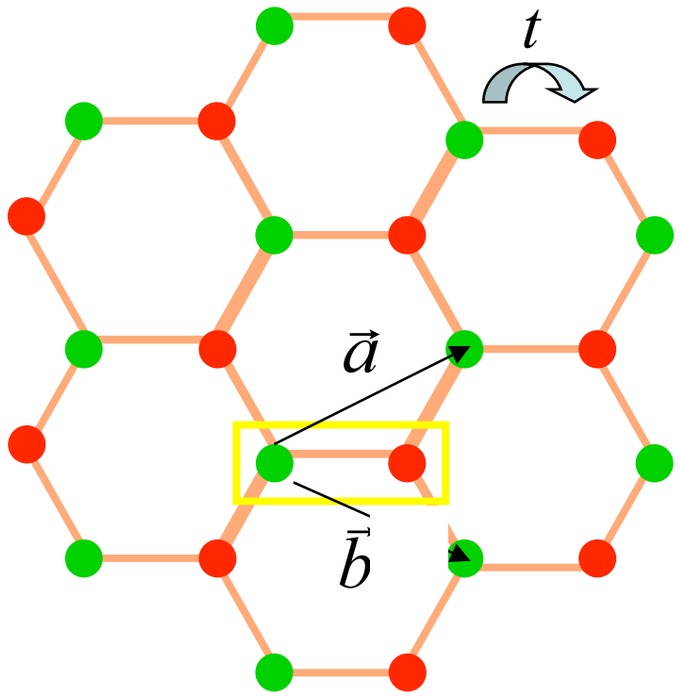
$U/t$

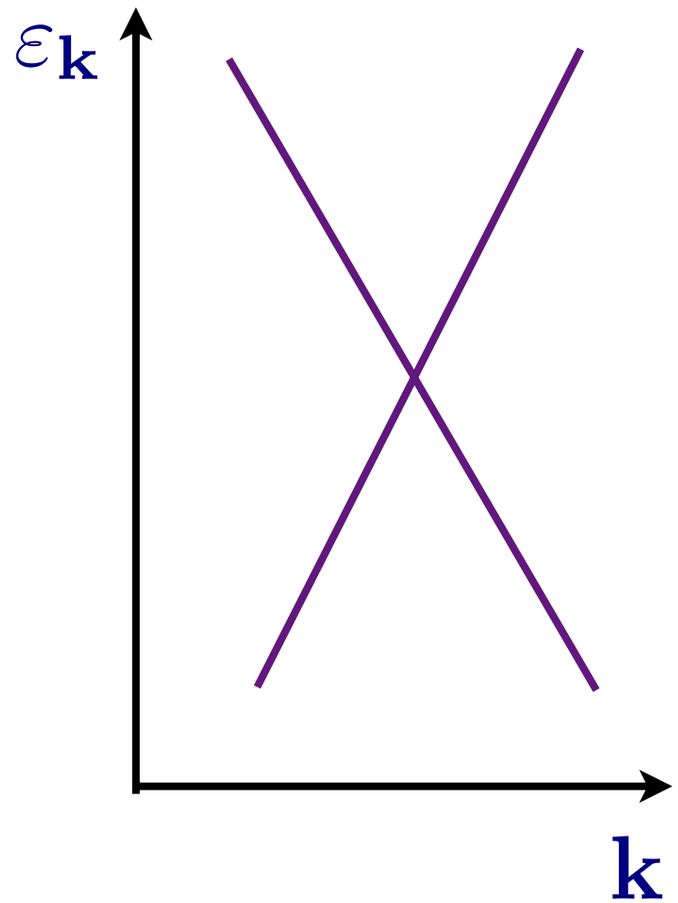



$$H_0 = -\sum_{i<j} t_{ij} c^{\dagger}_{i\alpha} c_{i\alpha}$$

- Begin with free electrons.

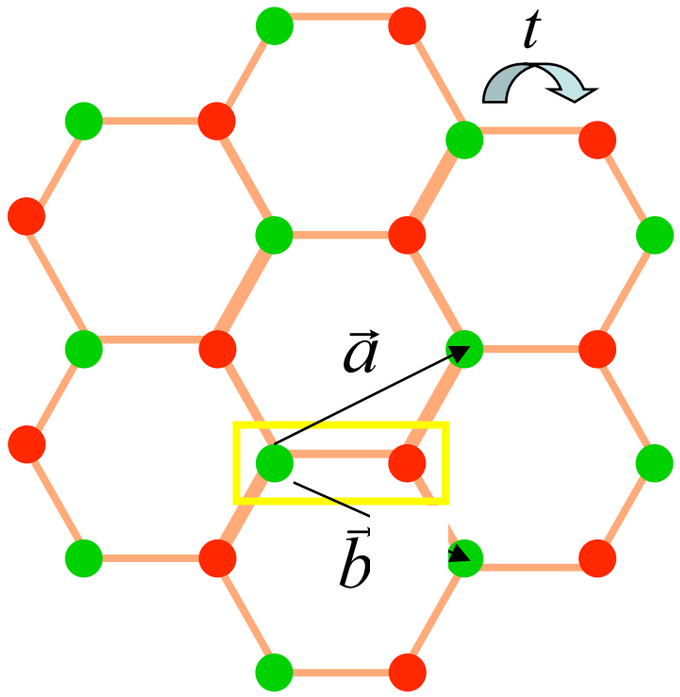


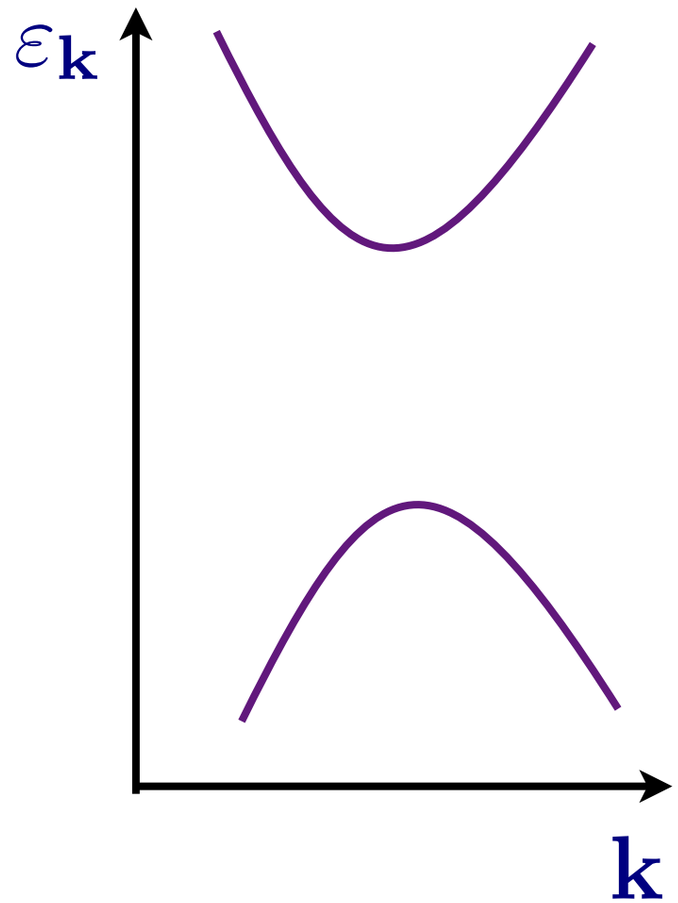




$$H_0 = -\sum_{i<j} t_{ij} c^\dagger_{i\alpha} c_{i\alpha}$$

- Begin with free electrons.
- Add local antiferromagnetism with order parameter $\vec{\varphi}$

$$H_{sdw} = -\sum_i \vec{\varphi}(\mathbf{r}_i)(-1)^i c^\dagger_{i\alpha} \vec{\sigma}_{\alpha\beta} c_{i\beta}$$

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- The phase with $\langle\vec{\varphi}\rangle \neq 0$ is an insulator with a gap between conduction and valence bands.

## **Honeycomb lattice at half filling**.

We define the unit length vectors

$$\mathbf{e}_1 = (1, 0) \quad , \quad \mathbf{e}_2 = (-1/2, \sqrt{3}/2) \quad , \quad \mathbf{e}_3 = (-1/2, -\sqrt{3}/2). \tag{1}$$

Note that $\mathbf{e}_i \cdot \mathbf{e}_j = -1/2$ for $i \neq j$, and $\mathbf{e}_1 + \mathbf{e}_2 + \mathbf{e}_3 = 0$.
We take the origin of co-ordinates of the honeycomb lattice at the center of an *empty hexagon*. The A sublattice sites closest to the origin are at $\mathbf{e}_1$, $\mathbf{e}_2$, and $\mathbf{e}_3$, while the B sublattice sites closest to the origin are at $-\mathbf{e}_1$, $-\mathbf{e}_2$, and $-\mathbf{e}_3$.
The reciprocal lattice is generated by the wavevectors

$$\mathbf{G}_1 = \frac{4\pi}{3}\mathbf{e}_1 \quad , \quad \mathbf{G}_2 = \frac{4\pi}{3}\mathbf{e}_2 \quad , \quad \mathbf{G}_3 = \frac{4\pi}{3}\mathbf{e}_3 \tag{2}$$

The first Brillouin zone is a hexagon whose vertices are given by

$$\mathbf{Q}_1 = \frac{1}{3}(\mathbf{G}_2 - \mathbf{G}_3) \quad , \quad \mathbf{Q}_2 = \frac{1}{3}(\mathbf{G}_3 - \mathbf{G}_1) \quad , \quad \mathbf{Q}_3 = \frac{1}{3}(\mathbf{G}_1 - \mathbf{G}_2), \tag{3}$$

and $-\mathbf{Q}_1$, $-\mathbf{Q}_2$, and $-\mathbf{Q}_3$.

We define the Fourier transform of the fermions by

$$c_A(\mathbf{k}) = \sum_{\mathbf{r}} c_A(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} \tag{4}$$

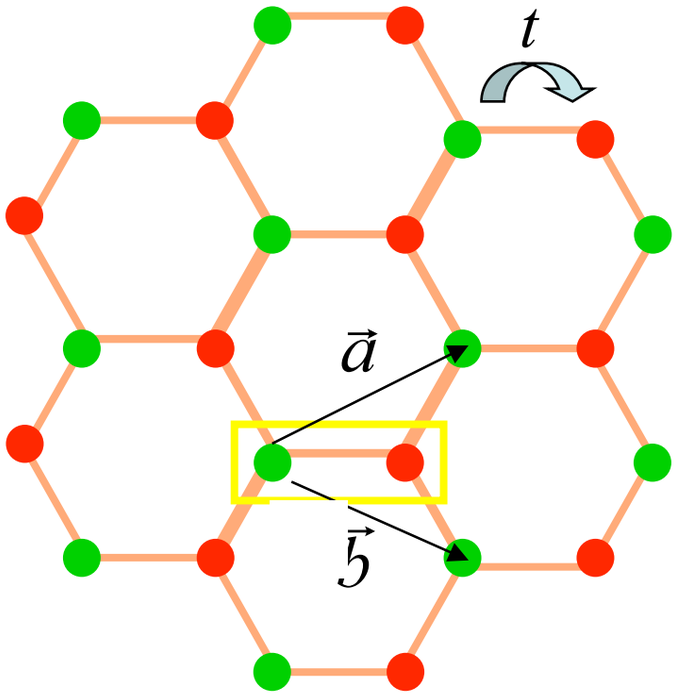
and similarly for $c_B$.
The hopping Hamiltonian is

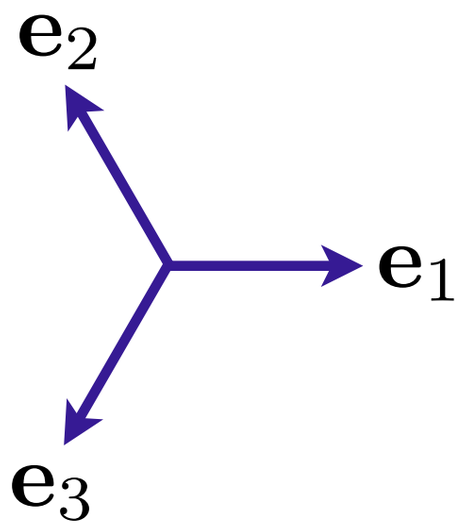
$$H_0 = -t \sum_{\langle ij \rangle} \left( c^\dagger_{Ai\alpha} c_{Bj\alpha} + c^\dagger_{Bj\alpha} c_{Ai\alpha} \right) \tag{5}$$

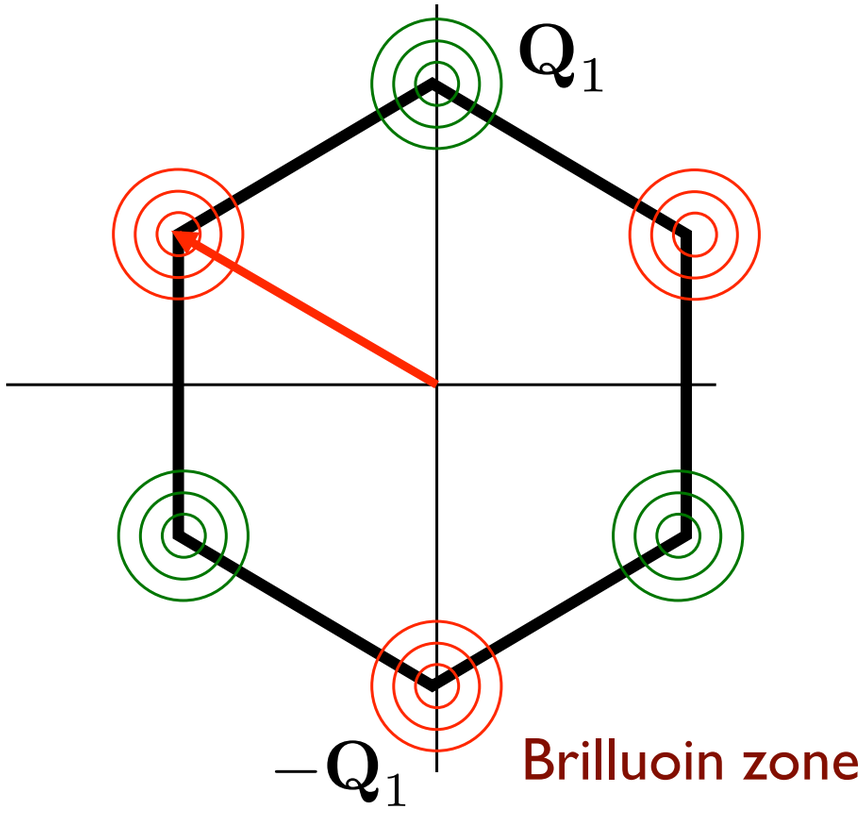
where $\alpha$ is a spin index. If we introduce Pauli matrices $\tau^a$ in sublattice space ($a = x, y, z$), this Hamiltonian can be written as

$$\begin{aligned} H_0 \;=\; & \int \frac{d^2k}{4\pi^2} c^\dagger(\mathbf{k}) \Big[ -t \Big( \cos(\mathbf{k}\cdot\mathbf{e}_1) + \cos(\mathbf{k}\cdot\mathbf{e}_2) + \cos(\mathbf{k}\cdot\mathbf{e}_3) \Big) \tau^x \\ & + t \Big( \sin(\mathbf{k}\cdot\mathbf{e}_1) + \sin(\mathbf{k}\cdot\mathbf{e}_2) + \sin(\mathbf{k}\cdot\mathbf{e}_3) \Big) \tau^y \Big] c(\mathbf{k}) \end{aligned} \tag{6}$$

The low energy excitations of this Hamiltonian are near $\mathbf{k} \approx \pm\mathbf{Q}_1$.


t
$\vec{a}$
$\vec{b}$


$\mathbf{e}_2$
$\mathbf{e}_1$
$\mathbf{e}_3$


$\mathbf{Q}_1$
$-\mathbf{Q}_1$
Brilluoin zone

In terms of the fields near $\mathbf{Q}_1$ and $-\mathbf{Q}_1$, we define

$$\begin{aligned}
\Psi_{A1\alpha}(\mathbf{k}) &= c_{A\alpha}(\mathbf{Q}+\mathbf{k}) \\
\Psi_{A2\alpha}(\mathbf{k}) &= c_{A\alpha}(-\mathbf{Q}+\mathbf{k}) \\
\Psi_{B1\alpha}(\mathbf{k}) &= c_{B\alpha}(\mathbf{Q}+\mathbf{k}) \\
\Psi_{B2\alpha}(\mathbf{k}) &= c_{B\alpha}(-\mathbf{Q}+\mathbf{k})
\end{aligned} \tag{7}$$

We consider $\Psi$ to be a 8 component vector, and introduce Pauli matrices $\rho^a$ which act in the $1,2$ valley space. Then the Hamiltonian is

$$H_0 = \int \frac{d^2k}{4\pi^2} \Psi^\dagger(\mathbf{k}) \Big( v\tau^y k_x + v\tau^x \rho^z k_y \Big) \Psi(\mathbf{k}), \tag{8}$$

where $v = 3t/2$; below we set $v = 1$. Now define $\overline{\Psi} = \Psi^\dagger \rho^z \tau^z$. Then we can write the imaginary time Lagrangian as

$$\mathcal{L}_0 = -i\overline{\Psi}\left(\omega\gamma_0 + k_x\gamma_1 + k_y\gamma_2\right)\Psi \tag{9}$$

where

$$\gamma_0 = -\rho^z\tau^z \quad \gamma_1 = \rho^z\tau^x \quad \gamma_2 = -\tau^y \tag{10}$$

# Antiferromagnetism

We use the operator equation (valid on each site $i$):

$$U\left(n_\uparrow - \frac{1}{2}\right)\left(n_\downarrow - \frac{1}{2}\right) = -\frac{2U}{3}S^{a2} + \frac{U}{4} \tag{11}$$

Then we decouple the interaction via

$$\exp\left(\frac{2U}{3}\sum_i \int d\tau S_i^{a2}\right) = \int \mathcal{D}J_i^a(\tau)\exp\left(-\sum_i \int d\tau \left[\frac{3U}{8}J_i^{a2} - J_i^a S_i^a\right]\right.$$

(12)

We now integrate out the fermions, and look for the saddle point of the resulting effective action for $J_i^a$. At the saddle-point we find that the lowest energy is achieved when the vector has opposite orientations on the A and B sublattices. Anticipating this, we look for a continuum limit in terms of a field $\varphi^a$ where

$$J_A^a = \varphi^a \quad , \quad J_B^a = -\varphi^a \tag{13}$$

The coupling between the field $\varphi^a$ and the $\Psi$ fermions is given by

$$\sum_i J_i^a c_{i\alpha}^\dagger \sigma_{\alpha\beta}^a c_{i\beta} = \varphi^a \left( c_{A\alpha}^\dagger \sigma_{\alpha\beta}^a c_{A\beta} - c_{B\alpha}^\dagger \sigma_{\alpha\beta}^a c_{B\beta} \right)$$

$$= \varphi^a \Psi^\dagger \tau^z \sigma^a \Psi = -\varphi^a \overline{\Psi} \rho^z \sigma^a \Psi \tag{14}$$

From this we motivate the low energy theory

$$\mathcal{L} = \overline{\Psi} \gamma_\mu \partial_\mu \Psi + \frac{1}{2} \left[ (\partial_\mu \varphi^a)^2 + s \varphi^{a2} \right] + \frac{u}{24} \left( \varphi^{a2} \right)^2 - \lambda \varphi^a \overline{\Psi} \rho^z \sigma^a \Psi \tag{15}$$

Note that the matrix $\rho^z \sigma^a$ commutes with all the $\gamma_\mu$; hence $\rho^z \sigma^a$ is a matrix in "flavor" space. This is the Gross-Neveu model, and it describes the quantum phase transition from the Dirac semi-metal to an insulating Néel state. In mean-field theory, the Dirac semi-metal is obtained for $s > 0$ with $\langle \varphi^a \rangle = 0$. The Néel state obtains for $s < 0$, and we have $\varphi^a = N_0 \delta_{az}$ (say), and so the dispersion of the electrons is

$$\omega_k = \pm \sqrt{k^2 + \lambda^2 N_0^2} \tag{16}$$

near the points $\pm \mathbf{Q}_1$. These form the conduction and valence bands of the insulator.

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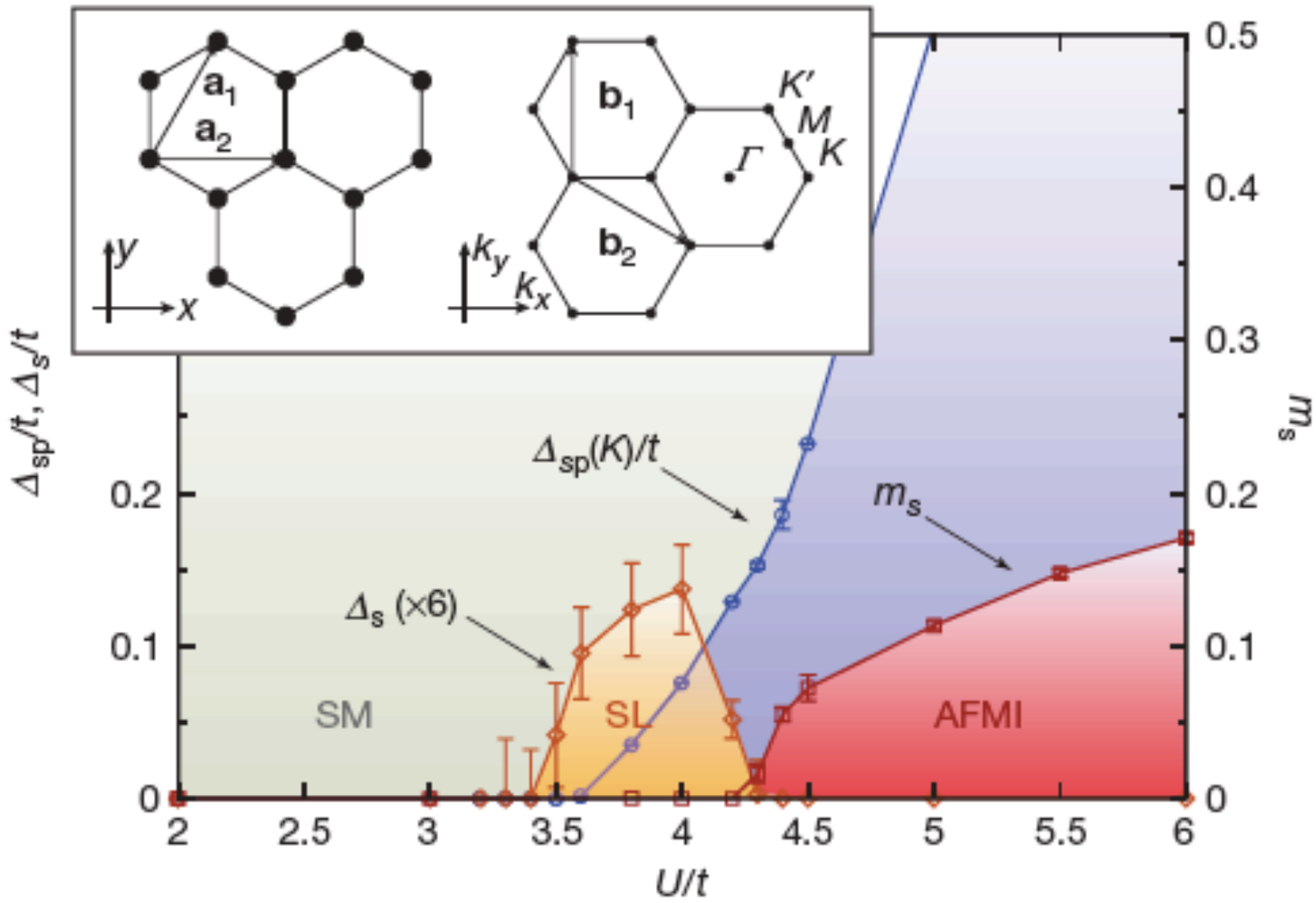


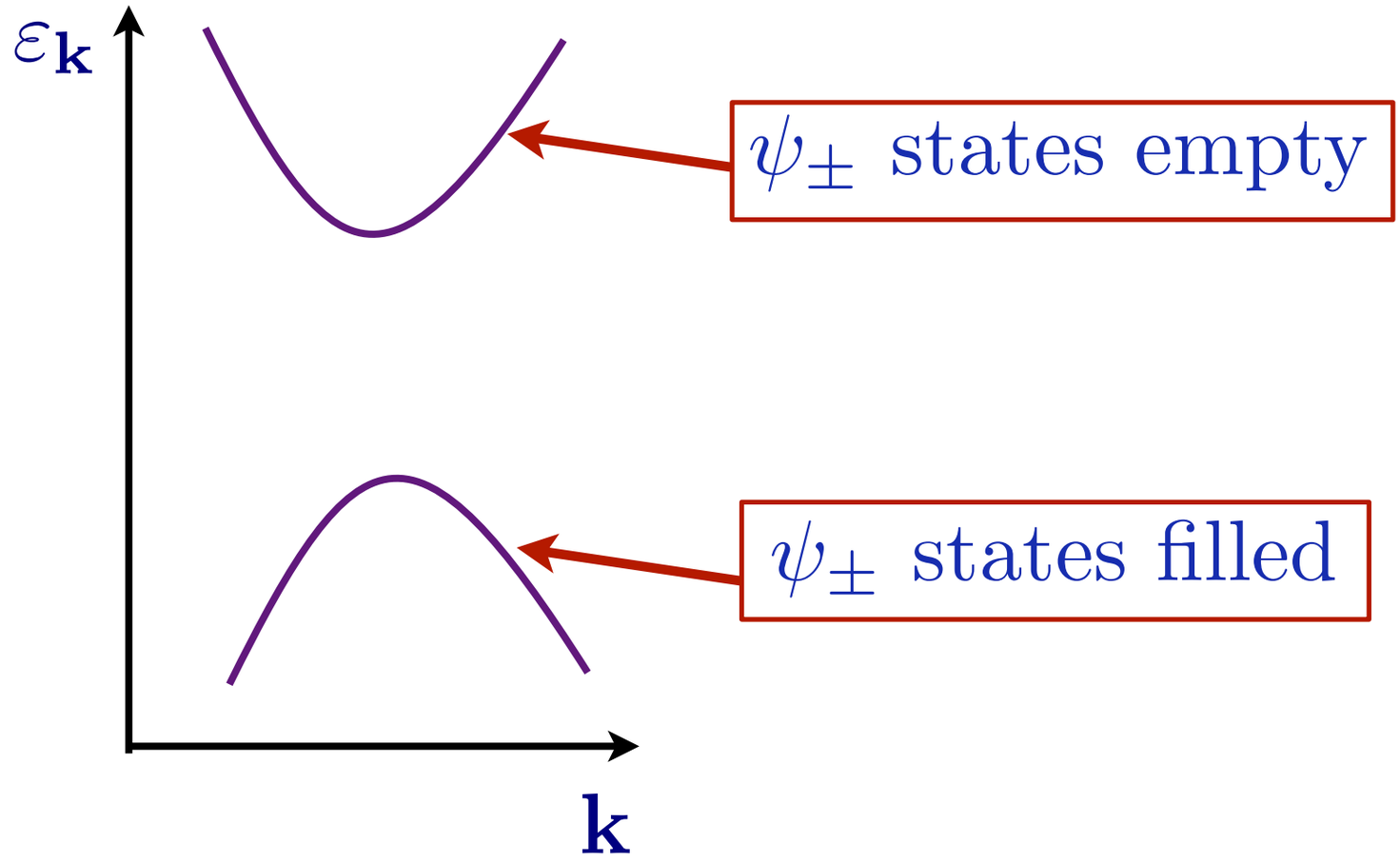

**Figure 1 | Phase diagram for the Hubbard model on the honeycomb lattice at half-filling.** The semimetal (SM) and the antiferromagnetic Mott insulator (AFMI) are separated by a gapped spin-liquid (SL) phase in an intermediate-coupling regime. $\Delta_{sp}(K)$ denotes the single-particle gap and $\Delta_s$ denotes the spin gap; $m_s$ denotes the staggered magnetization, whose saturation value is 1/2. Error bars, s.e.m. Inset, the honeycomb lattice with primitive vectors $\mathbf{a}_1$ and $\mathbf{a}_2$, and the reciprocal lattice with primitive vectors $\mathbf{b}_1$ and $\mathbf{b}_2$. Open and filled sites respectively indicate two different sublattices. The Dirac points $K$ and $K'$ and the $M$ and $\Gamma$ points are marked.

Z. Y. Meng *et al.*, Nature **464**, 847 (2010).

$$\mathcal{R}_z(x,\tau)\,|\text{Néel}\rangle$$

Perform SU(2) rotation $\mathcal{R}_z$ on filled band of electrons:

$$\begin{pmatrix} c_\uparrow \\ c_\downarrow \end{pmatrix} = \begin{pmatrix} z_\uparrow & -z_\downarrow^* \\ z_\downarrow & z_\uparrow^* \end{pmatrix} \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix}$$



# Quantum "disordering" magnetic order

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$\mathrm{SU}(2)_{\mathrm{spin}}$

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$\mathrm{U}(1)_{\mathrm{charge}}$

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$U \times U^{-1}$

$\mathrm{SU}(2)_{\mathrm{s;gauge}}$

S. Sachdev, M. A. Metlitski, Y. Qi, and S. Sachdev *Phys. Rev. B* **80**, 155129 (2009)

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The Hubbard model can be written *exactly* as a lattice gauge theory with a

$$\mathrm{SU}(2)_{s;g} \times \mathrm{SU}(2)_{\mathrm{spin}} \times \mathrm{U}(1)_{\mathrm{charge}}$$

invariance.

The $\mathrm{SU}(2)_{s;g}$ is a gauge invariance,
while $\mathrm{SU}(2)_{\mathrm{spin}} \times \mathrm{U}(1)_{\mathrm{charge}}$ is a global symmetry

Global symmetry operations:

- Spin rotations, $\mathrm{SU}(2)_{\mathrm{spin}}$
- Combine electromagnetic charge (electron number) $\mathrm{U}(1)_{\mathrm{charge}}$ with particle-hole transformations to obtain $\mathrm{SU}(2)_{\mathrm{pseudospin}}$.

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Projected fermion wavefunctions (Fisher, Wen, Lee, Kim, Senthil)

$$\begin{pmatrix} c_\uparrow \\ c_\downarrow^\dagger \end{pmatrix} = \begin{pmatrix} b_1^* & b_2^* \\ -b_2 & b_1 \end{pmatrix} \begin{pmatrix} f_1 \\ f_2^\dagger \end{pmatrix}$$

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neutral fermionic spinons

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charged slave boson/rotor

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$U \times U^{-1}$
$\mathrm{SU}(2)_{\mathrm{p;gauge}}$

# Unified spin liquid theory

Decompose electron operator into real fermions, $\chi$:

$$c_\uparrow = \chi_1 + i\chi_2 \quad ; \quad c_\downarrow = \chi_3 + i\chi_4$$

Introduce a 4-component Majorana fermion $\zeta_i$, $i = 1 \ldots 4$ and a SO(4) matrix $\mathcal{R}$, and decompose:

$$\chi = \quad \mathcal{R} \quad \zeta$$

# Unified spin liquid theory

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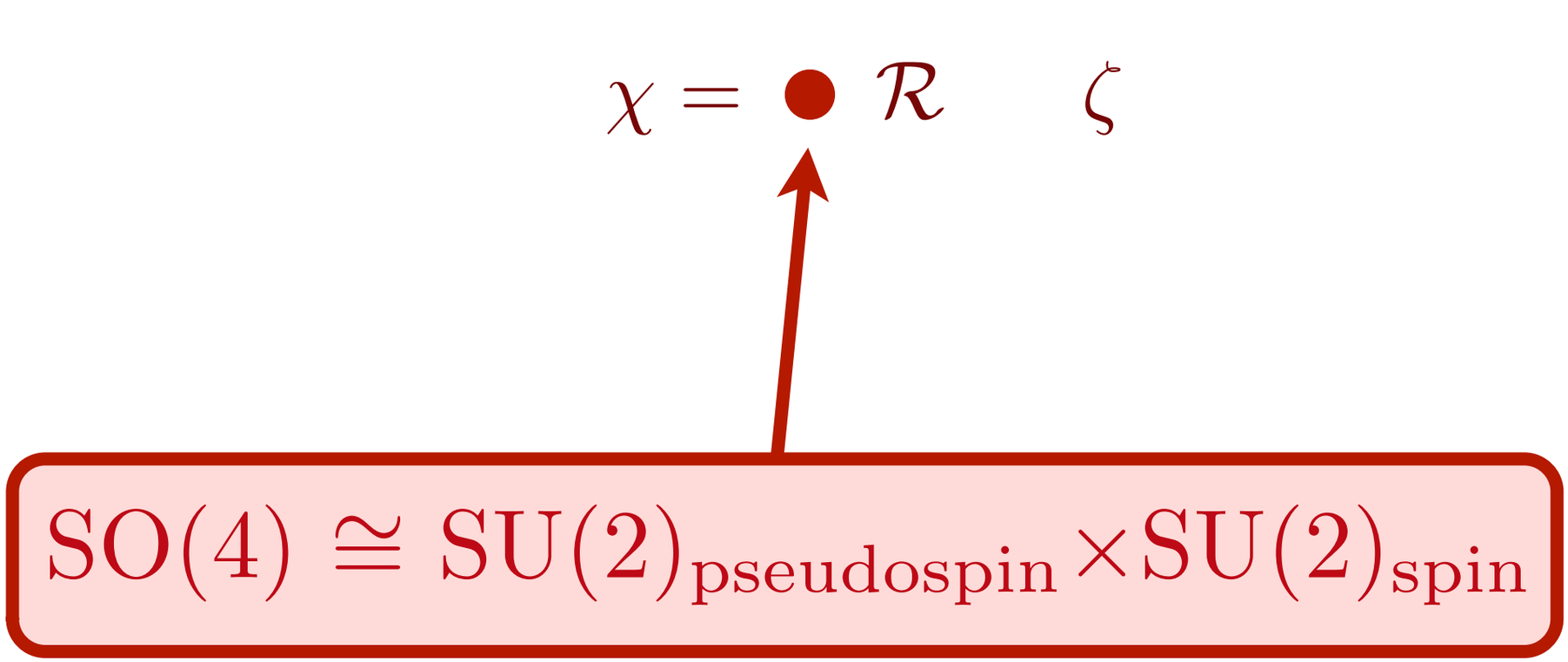
$$c_\uparrow = \chi_1 + i\chi_2 \quad ; \quad c_\downarrow = \chi_3 + i\chi_4$$

Introduce a 4-component Majorana fermion $\zeta_i$, $i = 1 \ldots 4$ and a SO(4) matrix $\mathcal{R}$, and decompose:



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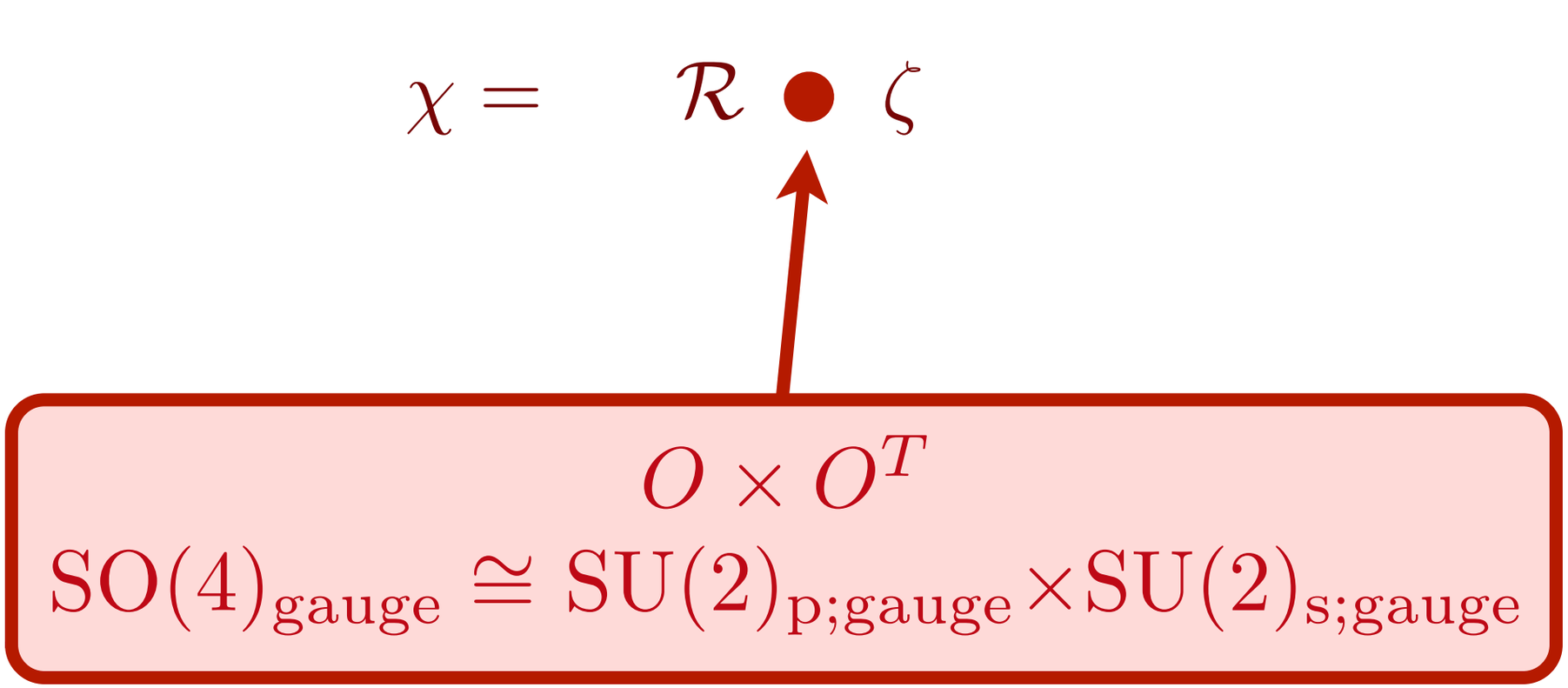

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$$\chi = \quad \mathcal{R} \quad \zeta$$

By breaking $SO(4)_{gauge}$ with different Higgs fields, we can reproduce essentially all earlier theories of spin liquids.

We also find many new spin liquid phases, some with Majorana fermion excitations which carry neither spin nor charge

# Quantum "disordering" magnetic order

$$\begin{pmatrix} c_\uparrow \\ c_\downarrow \end{pmatrix} = \begin{pmatrix} z_\uparrow & -z_\downarrow^* \\ z_\downarrow & z_\uparrow^* \end{pmatrix} \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix}$$

The Hubbard model can be written *exactly* as a lattice gauge theory with a

$$\mathrm{SU}(2)_{s;g} \times \mathrm{SU}(2)_{\mathrm{spin}} \times \mathrm{U}(1)_{\mathrm{charge}}$$

invariance.

The $\mathrm{SU}(2)_{s;g}$ is a gauge invariance,
while $\mathrm{SU}(2)_{\mathrm{spin}} \times \mathrm{U}(1)_{\mathrm{charge}}$ is a global symmetry

Matter context of $\mathrm{SU}(2)_{s;g} \times \mathrm{SU}(2)_{\mathrm{spin}} \times \mathrm{U}(1)_{\mathrm{charge}}$ theory

- Fundamental fermions $\psi$ transforming as $(\mathbf{2}, \mathbf{1}, 1)$,
- Fundamental scalar $z$ transforming as $(\bar{\mathbf{2}}, \mathbf{2}, 0)$, connecting local to global Néel order,
- Adjoint scalar $\vec{N}(\mathbf{r}_i) = \psi_i^\dagger \vec{\sigma} \psi_i$ transforming as $(\mathbf{3}, \mathbf{1}, 0)$, measuring local Néel order.

# Phase diagram

"Frustration"

$U/t$

# Phase diagram

"Frustration"

$\langle z \rangle \neq 0 \quad , \quad \langle N \rangle = 0$

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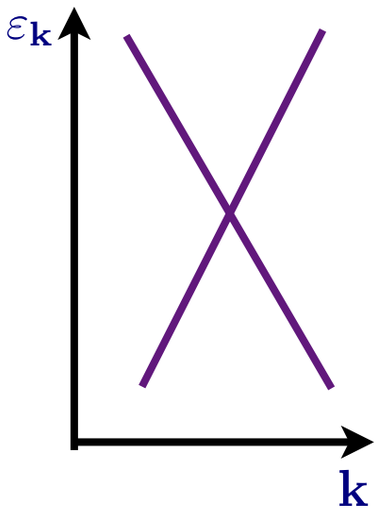


Semi-metal

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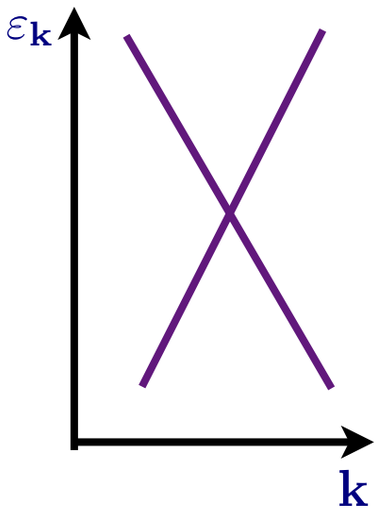


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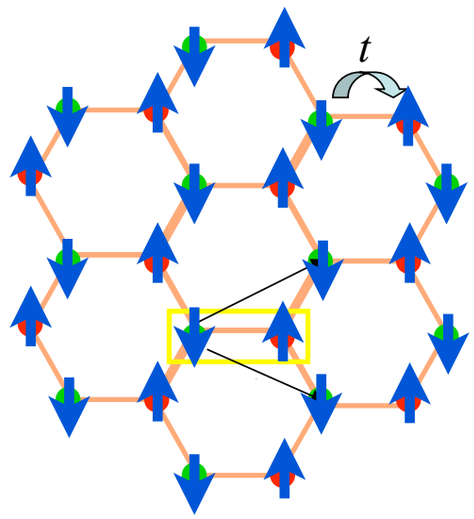


Insulator with Neel order

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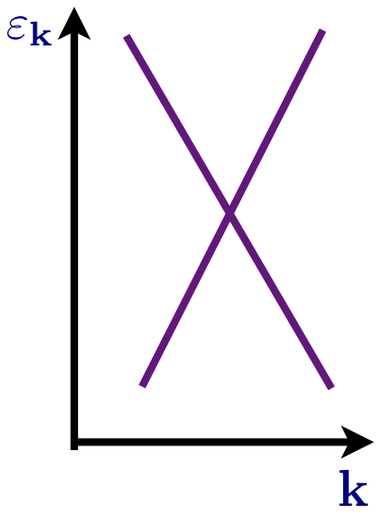


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SU(2) QCD with $N_f = 4$ massless Dirac quarks

$$\mathcal{L} = \frac{1}{g^2} F_{\mu\nu}^2 + \overline{\psi} \gamma_\mu (\partial_\mu - i A_\mu) \psi$$

Could describe a CFT3 like SYM, but could also be unstable to confinement.

or

eel

$J/t$

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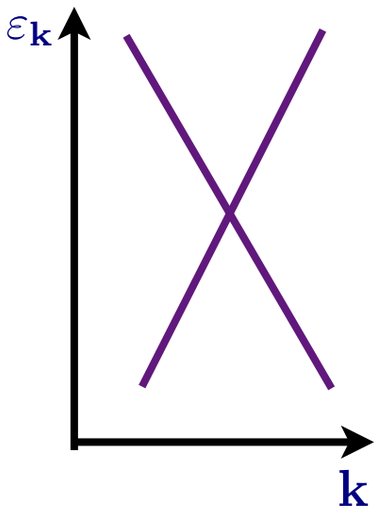


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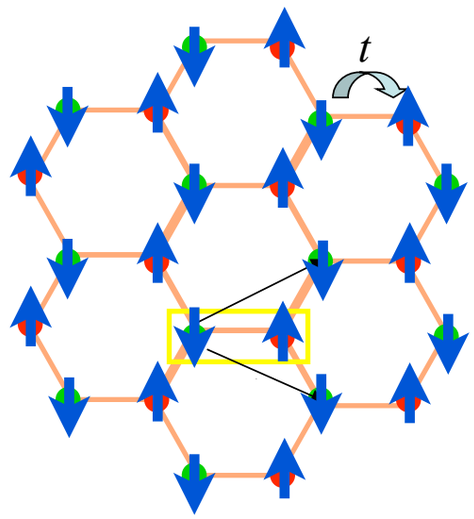


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Spin liquid:
CFT of SU(2) QCD with $N_f$=4 massless Dirac quarks

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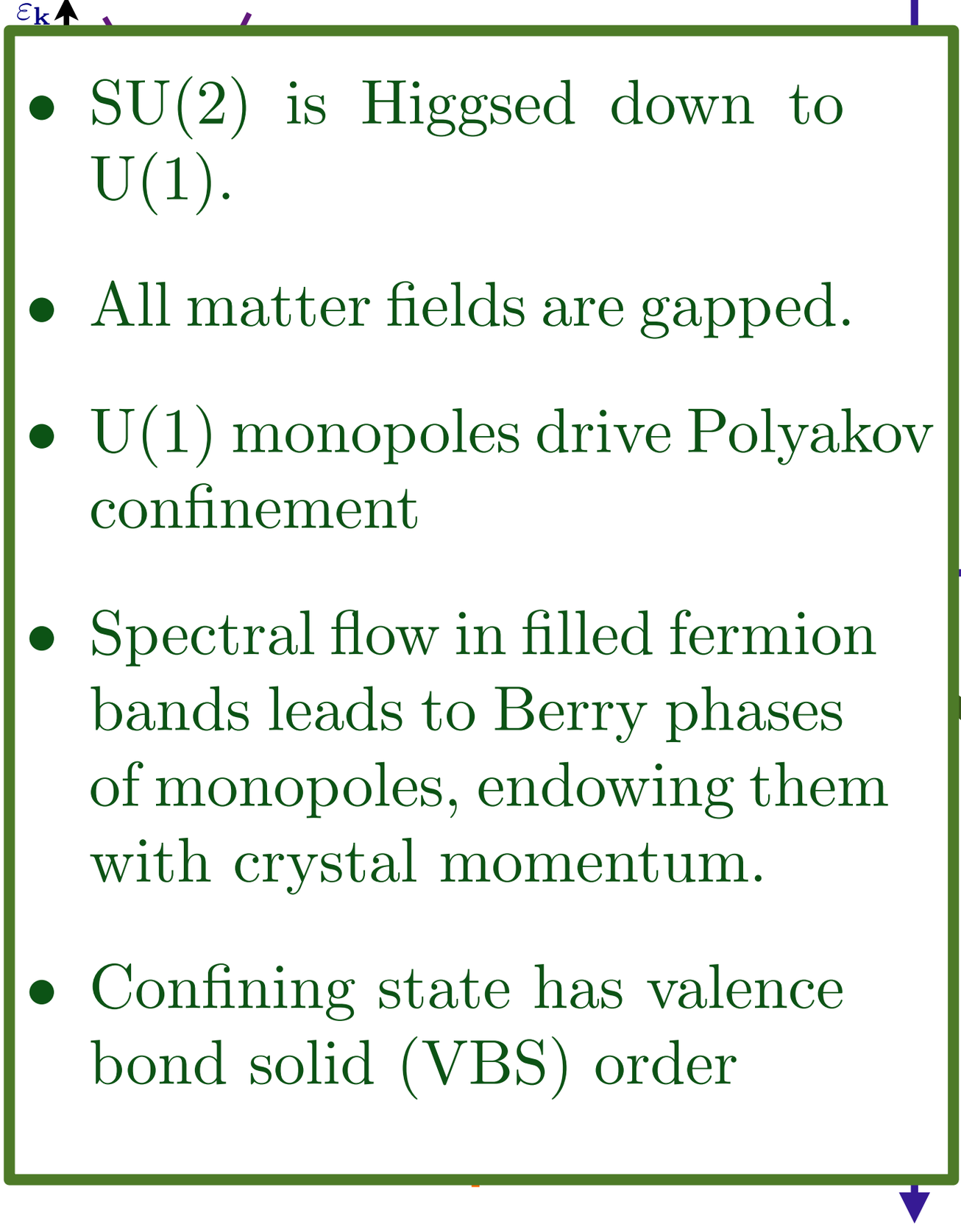
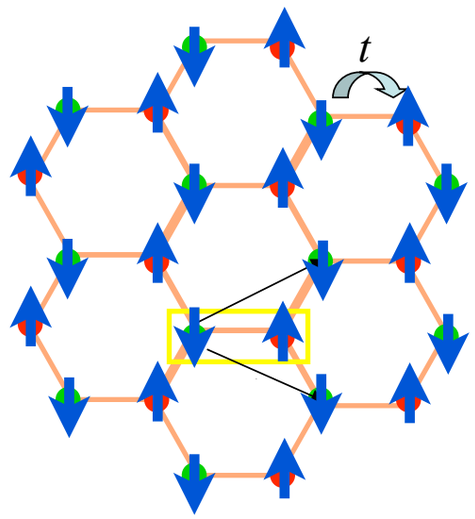



- SU(2) is Higgsed down to U(1).
- All matter fields are gapped.
- U(1) monopoles drive Polyakov confinement
- Spectral flow in filled fermion bands leads to Berry phases of monopoles, endowing them with crystal momentum.
- Confining state has valence bond solid (VBS) order

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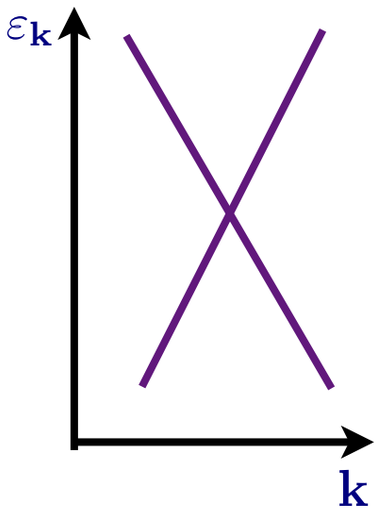


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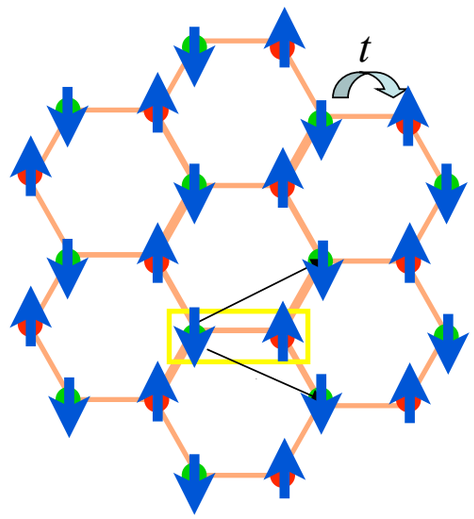


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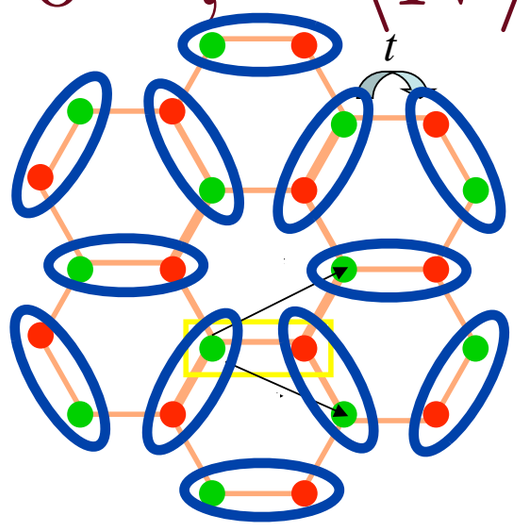


Confining insulator with VBS (kekule) order

# Outline

1. Honeycomb lattice:
   semi-metal and antiferromagnetism
   *Dirac fermions and the Gross-Neveu model*

2. Spin liquids
   *Unified formulation as a SO(4) gauge theory*

3. Instabilities of spin liquids
   *Geometric phases, valence bond solids, and other competing orders*

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# Fluctuating Néel states

Begin with the electronic Hamiltonian on the square lattice

$$H_0 = -\sum_{i,j} t(\mathbf{r}_i - \mathbf{r}_j) c^\dagger_\alpha(\mathbf{r}_i) c_\alpha(\mathbf{r}_j) \tag{1}$$

Now we allow for a spatially varying Néel order $n^a(\mathbf{r})$ $(a = x, y, z)$. Then the Hamiltonian is

$$H_0 = -\sum_{i,j} t(\mathbf{r}_i - \mathbf{r}_j) c^\dagger_\alpha(\mathbf{r}_i) c_\alpha(\mathbf{r}_j) + N_0 \sum_i \eta_i n^a(\mathbf{r}_i) c^\dagger_\alpha(\mathbf{r}_i) \sigma^a_{\alpha\beta} c_\beta(\mathbf{r}_i) \tag{2}$$

where $\eta_i = \pm 1$ on the two sublattices. We transform to a rotating reference frame in the varying Néel background so that the Néel order points in the constant direction (0,0,1) in the new reference frame:

$$\begin{pmatrix} c_\uparrow \\ c_\downarrow \end{pmatrix} = \begin{pmatrix} z_\uparrow & -z^*_\downarrow \\ z_\downarrow & z^*_\uparrow \end{pmatrix} \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix} \tag{3}$$

where $\psi_p$, $p = \pm$, are the "electrons" in the rotating reference frame. A fixed orientation of the Néel order is realized in the

rotating reference frame by choosing the $z_\alpha$ so that

$$n^a = z^*_\alpha \sigma^a_{\alpha\beta} z_\beta \tag{4}$$

However, we will *not* assume any slow variations in the fermions $c_\alpha$ and $\psi_p$, allowing them to carry arbitrary momenta and band structures.
Inserting Eq. (3) into Eq. (2), we obtain the theory for the $\psi_\pm$ fermions, which we write in the form

$$H = -\sum_{i,j} t(\mathbf{r}_i - \mathbf{r}_j)\psi^\dagger_p(\mathbf{r}_i)e^{ipA_{ij}}\psi_p(\mathbf{r}_j) + N_0 \sum_i \eta_i\, p\, \psi^\dagger_p(\mathbf{r}_i)\psi_p(\mathbf{r}_i) + \ldots \tag{5}$$

The flux in the continuum gauge field **A** can be related to gradients in the antiferromagnetic order parameter by

$$\partial_x A_y - \partial_y A_x = \frac{1}{2}\epsilon_{abc} n^a \partial_x n^b \partial_y n^c. \tag{6}$$

Thus inducing a $2\pi$ flux in **A** corresponds to changing the skyrmion number of the field $n^a(\mathbf{r})$ by unity *i.e.* to introducing a hedgehog defect in the Néel order.

## Linear response

Now we compute the linear response of Eq. (5) to the gauge field $A_{ij}$, for a slowly varying spacetime dependence. After a Fourier transform of Eq. (5), we can write for zero $A_{ij}$

$$H_0 \;=\; \sum_{\mathbf{k}} \Big( \varepsilon_{\mathbf{k}} \psi^\dagger(\mathbf{k}) \psi(\mathbf{k}) + N_0 \psi^\dagger(\mathbf{k}+\mathbf{Q}) \sigma^z \psi(\mathbf{k}) \Big) \qquad (7)$$

where $\mathbf{Q} = (\pi, \pi)$ and

$$\varepsilon_{\mathbf{k}} = -\sum_{\mathbf{s}} t(\mathbf{s}) \cos(\mathbf{k}\cdot\mathbf{s}), \qquad (8)$$

with $t(-\mathbf{s}) = t(\mathbf{s})$. The summation over momenta extends over the entire square lattice Brillouin zone. Also, we will drop the $\pm$ indices of the $\psi_\pm$, and all Pauli matrices are assumed to act on the $\pm$ space. The single fermion Green's function of $H_0$ is

$$\begin{aligned} \langle \psi(\mathbf{k})\,;\, \psi^\dagger(\mathbf{p}) \rangle &= \delta_{\mathbf{k},\mathbf{p}} \left( \frac{u_{\mathbf{k}}^2}{-i\omega + E_{1\mathbf{k}}} + \frac{v_{\mathbf{k}}^2}{-i\omega + E_{2\mathbf{k}}} \right) \\ &+ \delta_{\mathbf{k}+\mathbf{Q},\mathbf{p}} \sigma^z u_{\mathbf{k}} v_{\mathbf{k}} \left( \frac{1}{-i\omega + E_{1\mathbf{k}}} - \frac{1}{-i\omega + E_{2\mathbf{k}}} \right). \qquad (9) \end{aligned}$$

The eigenenergies in Eq. (9) are

$$E_{1,2\mathbf{k}} = \frac{\varepsilon_{\mathbf{k}} + \varepsilon_{\mathbf{k}+\mathbf{Q}}}{2} \pm \sqrt{\left(\frac{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}+\mathbf{Q}}}{2}\right)^2 + N_0^2}, \tag{10}$$

and the parameters are

$$u_{\mathbf{k}} = \cos(\theta_{\mathbf{k}}/2) \quad , \quad v_{\mathbf{k}} = \sin(\theta_{\mathbf{k}}/2) \tag{11}$$

with

$$\tan\theta_{\mathbf{k}} = \frac{N_0}{(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}+\mathbf{Q}})/2} \quad , \quad 0 < \theta_{\mathbf{k}} < \pi \tag{12}$$

Note that these relations imply

$$u_{\mathbf{k}+\mathbf{Q}} = v_{\mathbf{k}} \quad , \quad v_{\mathbf{k}+\mathbf{Q}} = u_{\mathbf{k}} \quad , \quad E_{1,\mathbf{k}+\mathbf{Q}} = E_{1\mathbf{k}} \quad , \quad E_{2,\mathbf{k}+\mathbf{Q}} = E_{2\mathbf{k}}. \tag{13}$$

Now we expand Eq. (5) to first order in $A_{ij}$

$$\begin{aligned} H_1 &= -i\sum_{i<j} t(\mathbf{r}_i - \mathbf{r}_j) A_{ij} \left(\psi_i^\dagger \sigma^z \psi_j - \psi_j^\dagger \sigma^z \psi_i\right) \qquad (14) \\ &= \sum_{\mathbf{k},\mathbf{q}} \left[\mathbf{A}(\mathbf{q}) \cdot \frac{\partial \varepsilon_{\mathbf{k}}}{\partial \mathbf{k}}\right] \psi^\dagger(\mathbf{k}+\mathbf{q}/2)\sigma^z\psi(\mathbf{k}-\mathbf{q}/2) + \mathcal{O}(\mathbf{q}^2) \end{aligned}$$

Now we will use the Kubo formula to determine the response to this applied gauge field. We will work to linear response order $\mathbf{A}$, and to linear order in $\mathbf{q}$.
We have to carefully define an observable: it should be gauge invariant and spin-rotation invariant. For this reason we look at the response in the following

$$M_{ij} \equiv \psi_i^\dagger e^{i\sigma^z A_{ij}} \psi_j \tag{15}$$

We want to compute the change in $\langle M_{ij} \rangle$ to linear order in $\mathbf{A}(\mathbf{q})$, and in the limit of small $\mathbf{q}$. We find

$$\delta\langle M_{ij} \rangle = 2 \sum_{\mathbf{k},\mathbf{q}} e^{-i\mathbf{k}\cdot(\mathbf{r}_i - \mathbf{r}_j)} e^{i\mathbf{q}\cdot(\mathbf{r}_j + \mathbf{r}_i)/2} e^{i\mathbf{Q}\cdot\mathbf{r}_j} \mathbf{A}(\mathbf{q}) \cdot \mathbf{I}(\mathbf{k},\mathbf{q}) \tag{16}$$

where

$$\mathbf{I}(\mathbf{k},\mathbf{q}) = \frac{N_0}{(E_{1\mathbf{k}} - E_{2\mathbf{k}})^3} \left[ \frac{\partial \varepsilon_{\mathbf{k}}}{\partial \mathbf{k}} \left( \mathbf{q} \cdot \frac{\partial \varepsilon_{\mathbf{k}+\mathbf{Q}}}{\partial \mathbf{k}} \right) - \frac{\partial \varepsilon_{\mathbf{k}+\mathbf{Q}}}{\partial \mathbf{k}} \left( \mathbf{q} \cdot \frac{\partial \varepsilon_{\mathbf{k}}}{\partial \mathbf{k}} \right) \right] \tag{17}$$

Combining (16) and (17), we have the main result

$$\left\langle c^{\dagger}(\mathbf{k})c(\mathbf{k}+\mathbf{Q})\right\rangle = -i\mathcal{F}(\mathbf{k})\left(\partial_x A_y - \partial_y A_x\right) \tag{18}$$

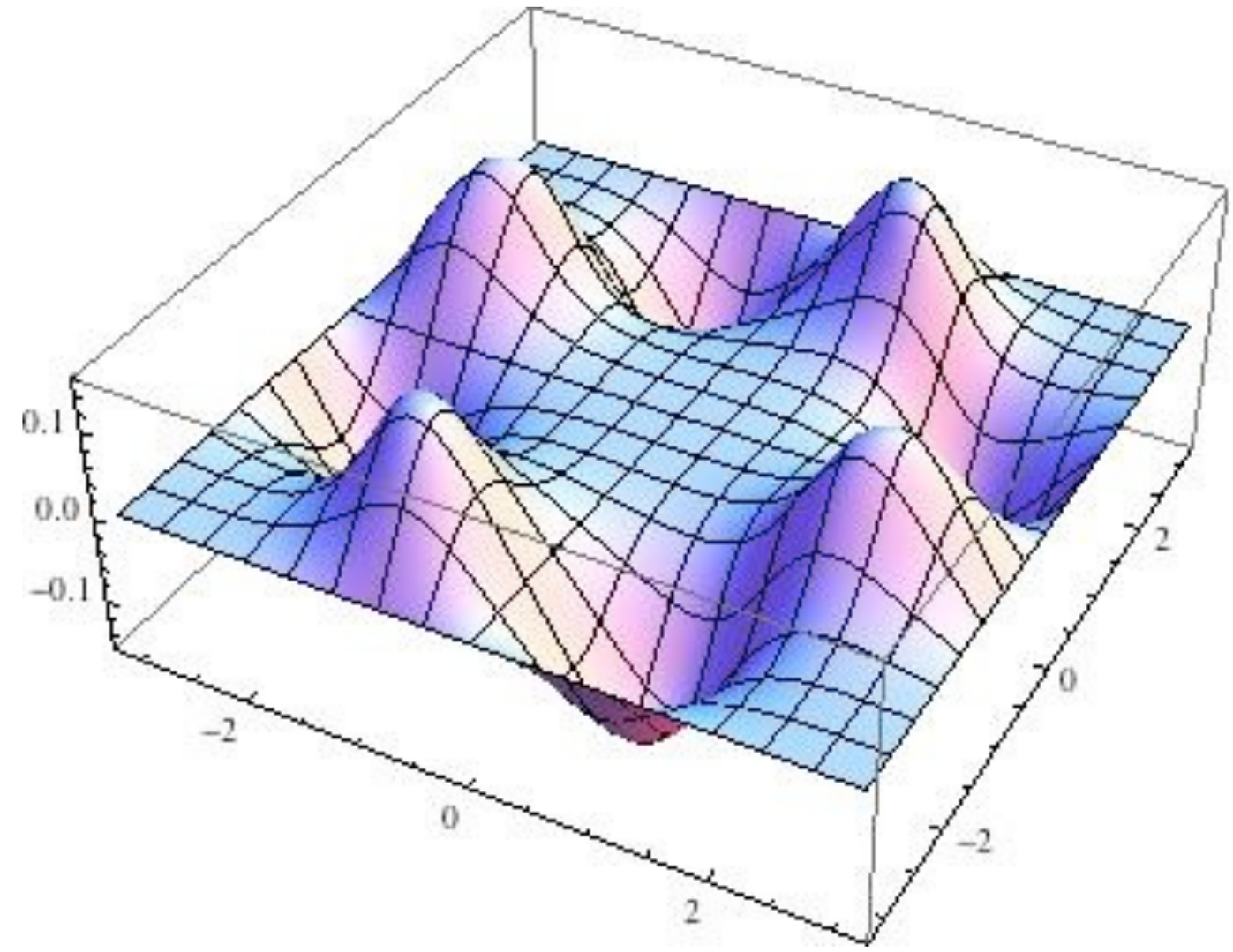
where

$$\mathcal{F}(\mathbf{k}) = \frac{N_0}{(E_{1\mathbf{k}} - E_{2\mathbf{k}})^3}\left(\frac{\partial\varepsilon_{\mathbf{k}+\mathbf{Q}}}{\partial\mathbf{k}} \times \frac{\partial\varepsilon_{\mathbf{k}}}{\partial\mathbf{k}}\right). \tag{19}$$

We have written Eq. (18) in terms of the original electron operators $c(\mathbf{k})$: we are working to linear order in $\mathbf{A}$, and so this order all variables can be mapped onto the original gauge-invariant operators.

Note that $\left\langle c^{\dagger}(\mathbf{k})c(\mathbf{k}+\mathbf{Q})\right\rangle = 0$ before the gauge flux was applied, because we are in the quantum-disordered phase where translational symmetry is preserved. Also, even in mean-field theory of the Hamiltonian in Eq. (7) we have $\left\langle \psi^{\dagger}(\mathbf{k})\psi(\mathbf{k}+\mathbf{Q})\right\rangle = 0$ because of spin inversion. Only $\left\langle \psi^{\dagger}(\mathbf{k})\sigma^{z}\psi(\mathbf{k}+\mathbf{Q})\right\rangle \neq 0$ for Eq. (7) before the gauge flux was applied.

A plot of $\mathcal{F}(\mathbf{k})$ is shown below for $\varepsilon_{\mathbf{k}} = \cos k_x - \cos k_y + 0.4\cos(k_x + k_y) + 0.4\cos(k_x - k_y)$ and $N_0 = 1$.




The integral of $\mathcal{F}(\mathbf{k})$ is zero over the Brillouin zone. However, note that it has the same symmetry as the function $(\cos k_x - \cos k_y)\sin k_x \sin k_y$; so the integral of $\mathcal{F}(\mathbf{k})(\cos k_x - \cos k_y)\sin k_x \sin k_y$ is non-zero.

This suggest we define the charge $\mathcal{Q}_t$ by

$$\mathcal{Q}_t = -i \sum_{\mathbf{k}} c^\dagger(\mathbf{k}) c(\mathbf{k}+\mathbf{Q}) (\cos k_x - \cos k_y) \sin k_x \sin k_y. \quad (20)$$

Note $\mathcal{Q}_t^\dagger = \mathcal{Q}_t$. Before the monopole, $\langle \mathcal{Q}_t \rangle = 0$. After the monopole tunneling event, we have $\langle \mathcal{Q}_t \rangle \neq 0$. We can normalize $\mathcal{Q}_t$ so that $\langle \mathcal{Q}_t \rangle = 1$ for each monopole, and the normalization constant will depend upon (19) and the details on the band structure.

## Competing orders

We now discuss the implications of the main result in Eq. (18) in the 'quantum disordered' phase where Néel order has been lost. Such a phase will have a proliferation of hedgehog/monpole tunnelling events, and so Eq. (18) implies that there will be correspondingly large fluctuations in the charge $\mathcal{Q}_t$. We can therefore expect that fluctuations in variables conjugate to $\mathcal{Q}_t$ will be suppressed, and will therefore have long-range order: this is the competing order induced by the geometric phase in Eq. (18).

Thus any quantum variable conjugate to $\mathcal{Q}_t$ is a bona-fide competing order. There are many possibilities, but for now let us verify that the traditional VBS order does satisfy the requirements. Specifically, the VBS order is $V = V_x + iV_y$ defined by

$$\begin{aligned} V_x &= i\sum_{\mathbf{k}} c^\dagger(\mathbf{k})c(\mathbf{k}+\mathbf{Q}_x)\sin k_x \\ V_y &= i\sum_{\mathbf{k}} c^\dagger(\mathbf{k})c(\mathbf{k}+\mathbf{Q}_y)\sin k_y \end{aligned} \tag{21}$$

where $\mathbf{Q}_x = (\pi, 0)$ and $\mathbf{Q}_y = (0, \pi)$. Now we can commute the commutators

$$[\mathcal{Q}_t, V_x] = -\sum_{\mathbf{k}} c^\dagger(\mathbf{k})c(\mathbf{k}+\mathbf{Q}_y)\sin k_y \frac{(\cos(k_x) - \cos(3k_x))}{2} \simeq iV_y$$

$$[\mathcal{Q}_t, V_y] = \sum_{\mathbf{k}} c^\dagger(\mathbf{k})c(\mathbf{k}+\mathbf{Q}_x)\sin k_x \frac{(\cos(k_y) - \cos(3k_y))}{2} \simeq -iV_x$$

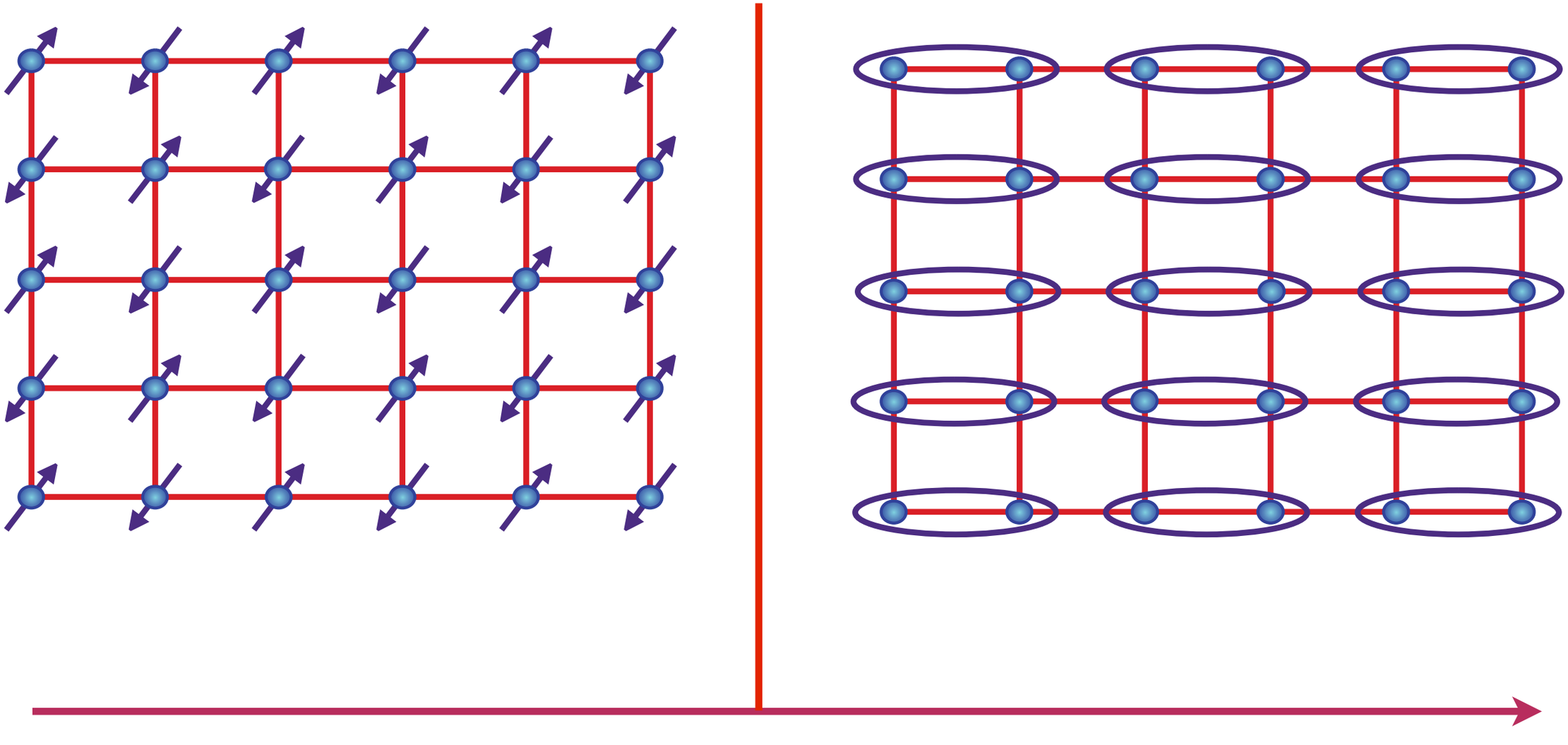
Here the $\simeq$ means that the two operators have the same symmetry under the square lattice space group.

Thus we have the key result

$$[\mathcal{Q}_t, V] \simeq V. \tag{22}$$

This means that $V$ is a raising order for $\mathcal{Q}_t$. But this is precisely the effect of the monopole tunneling event: in other words, $V$ has the same quantum numbers as a monopole operator. Then we conclude that $V$ is a competing order which becomes long-range in the quantum-disordered Néel phase.

# S=1/2 square lattice antiferromagnetic insulator



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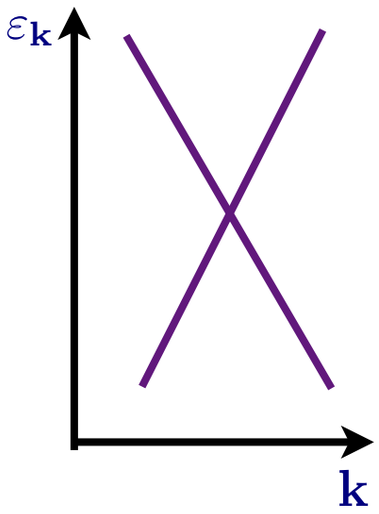


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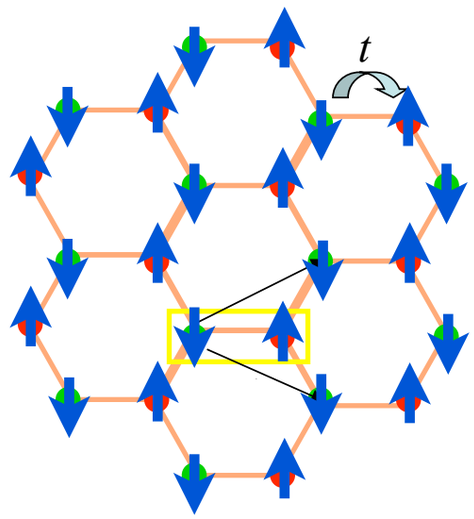


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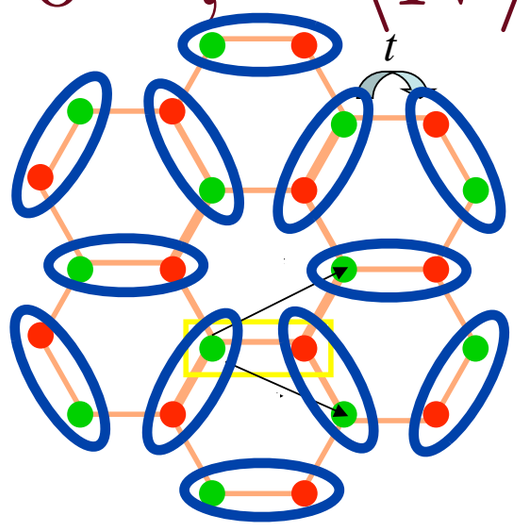


Confining insulator with VBS (kekule) order

Let us now present an alternative version of the above argument. By a suitable Hubbard-Stratonovich transformation of some interaction term, we can think of $\mathcal{Q}_t$ as a dynamic fluctuating field. The quantum-disordered phase has a low energy photon field $A_\mu$, ($\mu$ is a spacetime index). Thus we can write an effective Lagrangian for this photon phase in terms of the dynamic fields $\mathcal{Q}_\mu$ and $A_\mu$:

$$\mathcal{L}_{\text{eff}} = \frac{\mathcal{Q}_\mu^2}{2K} + \frac{1}{2e^2}\left(\epsilon_{\mu\nu\lambda}\partial_\nu A_\lambda\right)^2 + \frac{i}{2\pi K}\mathcal{Q}_\mu\epsilon_{\mu\nu\lambda}\partial_\nu A_\lambda \tag{23}$$

Here the last term represents the linear response computed in Eq. (18), after appropriate renormalization: if we take a derivative of the action with respect to $\mathcal{Q}_t$, we reproduce the response in Eq. (18). The spatial components of $\mathcal{Q}_\mu$ are similarly defined by an appropriate response to the electric components of the photon. The term proportional to $1/e^2$ is the usual Maxwell action for $A_\mu$, obtained after integrating out the $z_\alpha$ and $\psi_{\boldsymbol{p}}$. Now we can perform the standard duality transformation of 2+1 dimensional electrodynamics on $\mathcal{L}_{\text{eff}}$. Here these correspond to decoupling the Maxwell term by a Hubbard-Stratonovich field and then integrating

out the photon; this yields

$$\mathcal{L}_{\text{eff}} = \frac{\mathcal{Q}_\mu^2}{2K} + \frac{e^2}{8\pi^2}\left(\partial_\mu\phi - \frac{\mathcal{Q}_\mu}{K}\right)^2 \tag{24}$$

where $e^{i\phi}$ is the monopole operator. This allows to conclude that the correlations of $\partial_\mu\phi$ are the same as those of $\mathcal{Q}_\mu$, or in other words, we have the operator correspondence $\partial_\mu\phi \simeq \mathcal{Q}_\mu$.
Now let us look for an order parameter $V \sim e^{i\phi}$ so that $\partial_t\phi \simeq \mathcal{Q}_t$. Or more precisely, we need a $V$ so that $-i(V^\dagger\partial_t V - V\partial_t V^\dagger) \simeq \mathcal{Q}_t$. It is easy to check that the definition in Eq. (21) does satisfy the needed requirements.