Spontaneous spin textures in Hubbard systems

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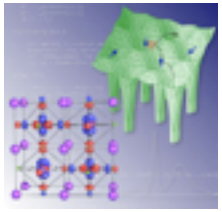

European Research Council

DFG Research Unit FOR1346

Cite as: P. Wadley *et al*., *Science* 10.1126/science.aab1031 (2016).

Electrical switching of an antiferromagnet

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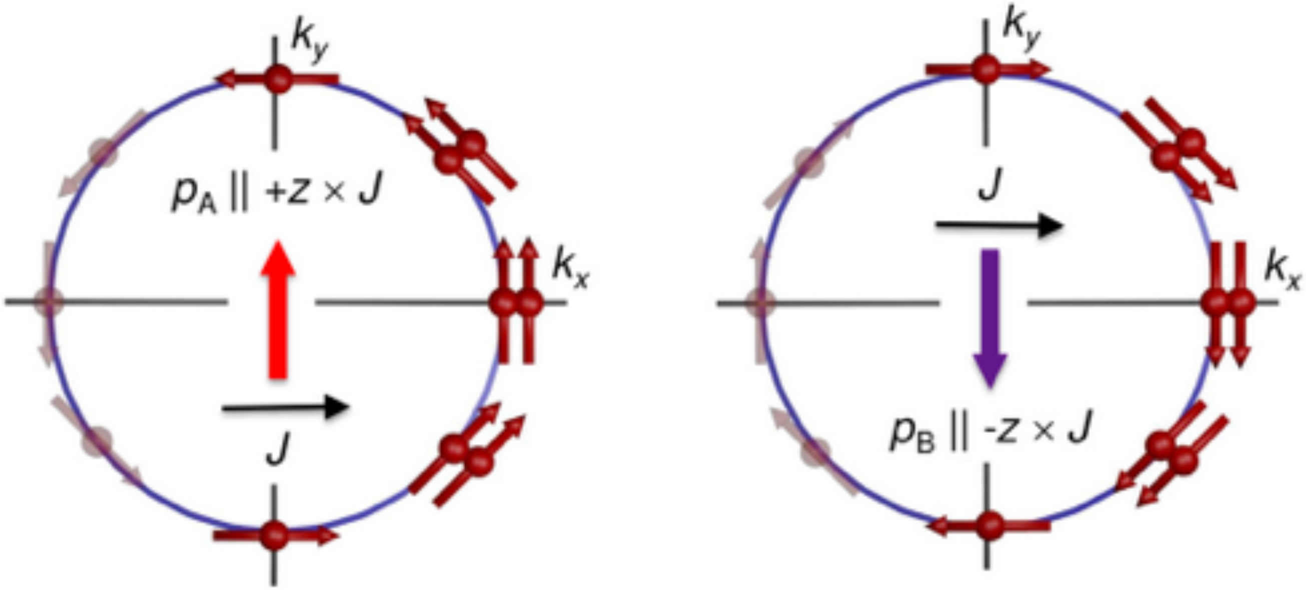

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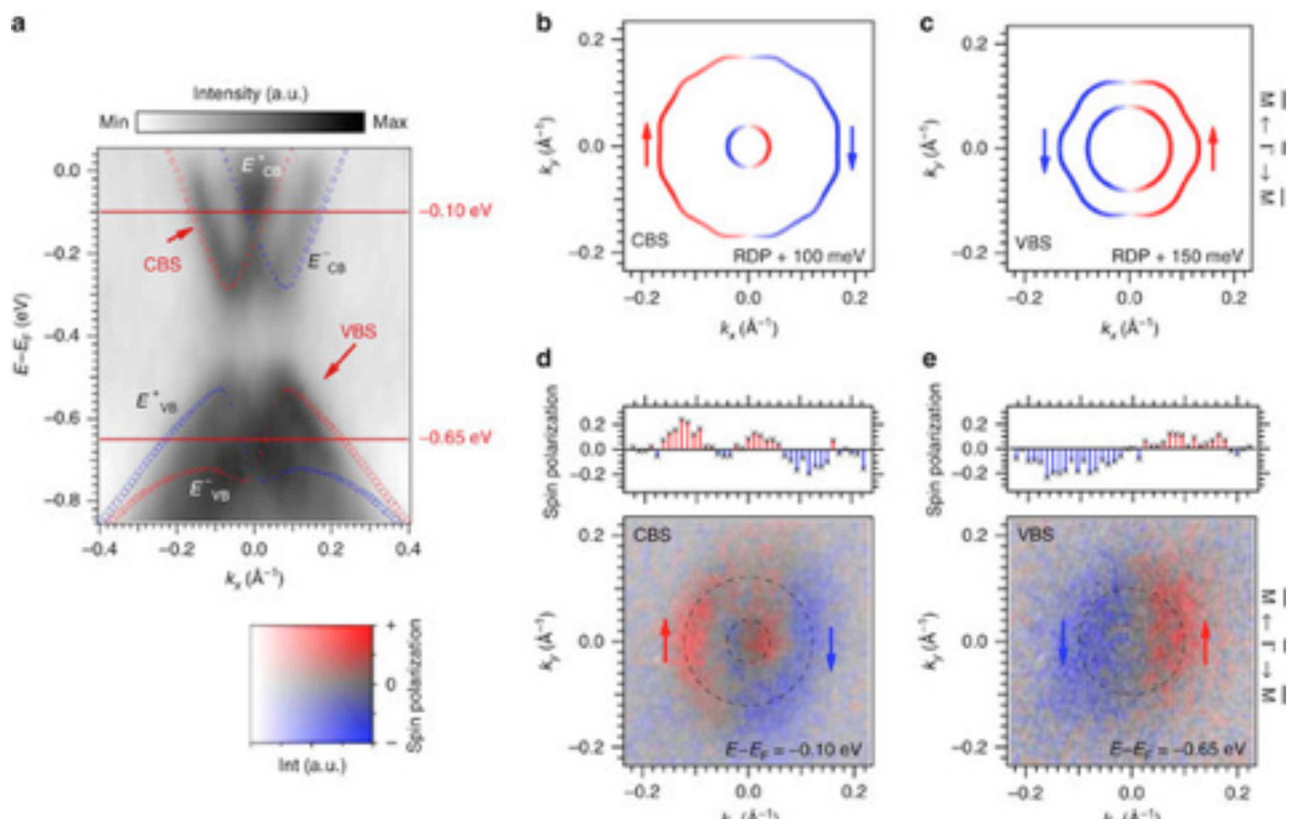
Received 30 Nov 2015 | Accepted 14 Apr 2016 | Published 18 May 2016

DOI: 10.1038/ncomms11621

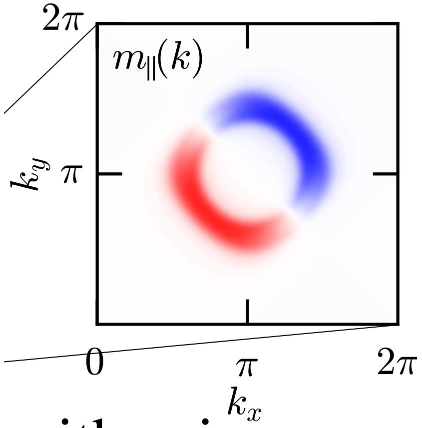
OPEN

Spin-texture inversion in the giant Rashba semiconductor BiTeI

Henriette Maaß[1], Hendrik Bentmann[1], Christoph Seibel[1], Christian Tusche[2], Sergey V. Eremeev[3,4,5], Thiago R.F. Peixoto[1], Oleg E. Tereshchenko[5,6,7], Konstantin A. Kokh[5,7,8], Evgueni V. Chulkov[4,5,9,10], Jürgen Kirschner[2] & Friedrich Reinert[1]



Spin texture



- no spin polarization in direct space $\mathbf{m}(\mathbf{r}) = 0$
- finite polarization in the k-space $\mathbf{m}_{-\mathbf{k}} = -\mathbf{m}_{\mathbf{k}}$

~ can be realized in non-centrosymmetric systems with spin-orbit coupling (Rashba/Dresselhaus SOC).

Here I will present how spin textures can be generated by spontaneous symmetry breaking in multi-band Hubbard models.

The key ingredients are:

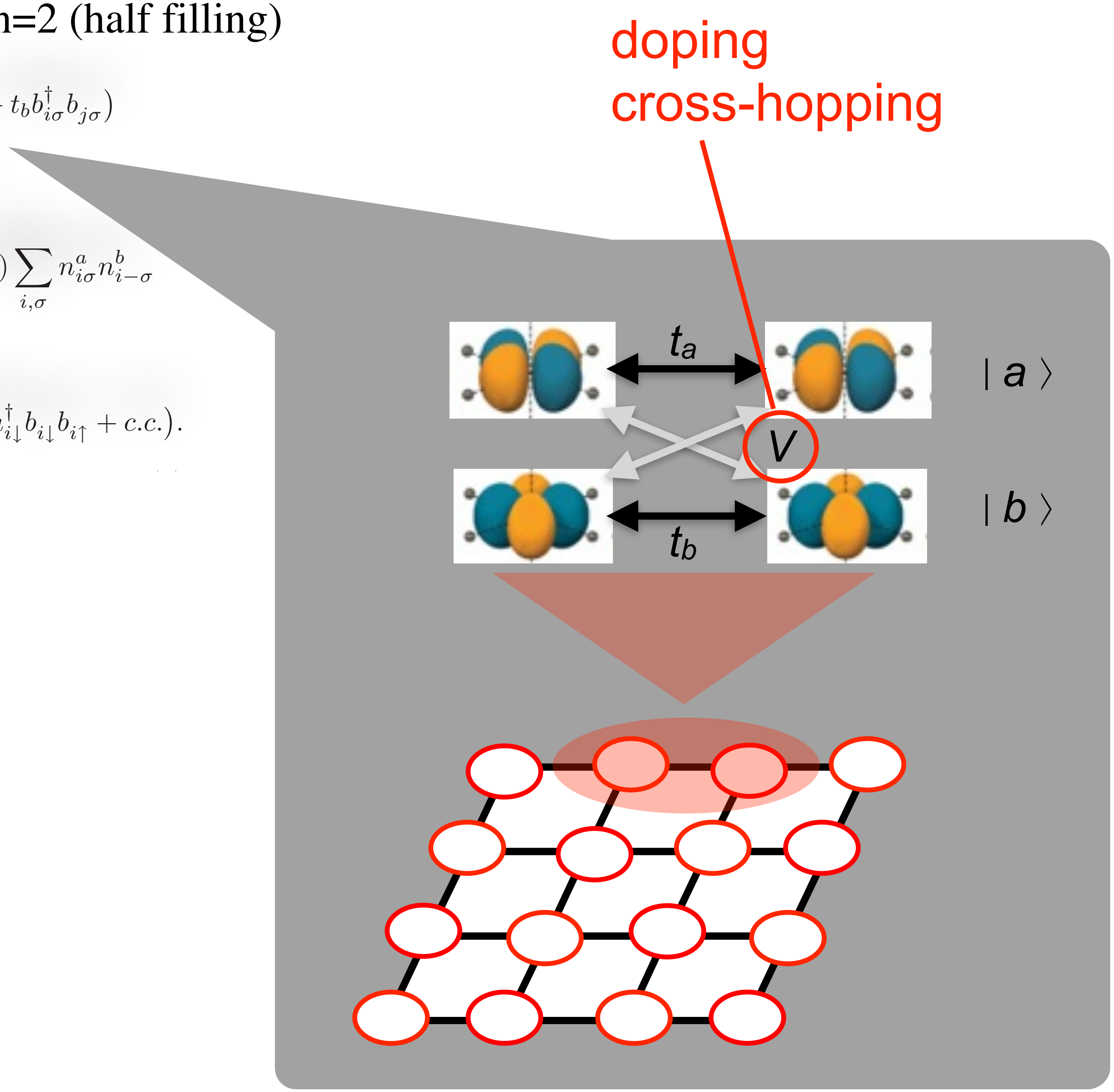
condensation of spinful excitons

generalized double-exchange

The model

Two-band Hubbard model at n=2 (half filling)

$$H_{\rm t} = \frac{\Delta}{2}\sum_{i,\sigma}(n^a_{i\sigma} - n^b_{i\sigma}) + \sum_{i,j,\sigma}(t_a a^\dagger_{i\sigma}a_{j\sigma} + t_b b^\dagger_{i\sigma}b_{j\sigma})$$
$$+ \sum_{\langle ij\rangle,\sigma}(V_1 a^\dagger_{i\sigma}b_{j\sigma} + V_2 b^\dagger_{i\sigma}a_{j\sigma} + c.c.)$$
$$H^{\rm dd}_{\rm int} = U\sum_i(n^a_{i\uparrow}n^a_{i\downarrow} + n^b_{i\uparrow}n^b_{i\downarrow}) + (U-2J)\sum_{i,\sigma}n^a_{i\sigma}n^b_{i-\sigma}$$
$$+ (U-3J)\sum_{i\sigma}n^a_{i\sigma}n^b_{i\sigma}$$
$$H'_{\rm int} = J\sum_{i\sigma}a^\dagger_{i\sigma}b^\dagger_{i-\sigma}a_{i-\sigma}b_{i\sigma} + J'\sum_i(a^\dagger_{i\uparrow}a^\dagger_{i\downarrow}b_{i\downarrow}b_{i\uparrow} + c.c.).$$



John Hubbard

Proximity to spin-state crossover

Two-band Hubbard model at n=2 (half filling)

$$H_{\rm t} = \frac{\Delta}{2}\sum_{i,\sigma}(n^a_{i\sigma} - n^b_{i\sigma}) + \sum_{i,j,\sigma}(t_a a^\dagger_{i\sigma}a_{j\sigma} + t_b b^\dagger_{i\sigma}b_{j\sigma})$$
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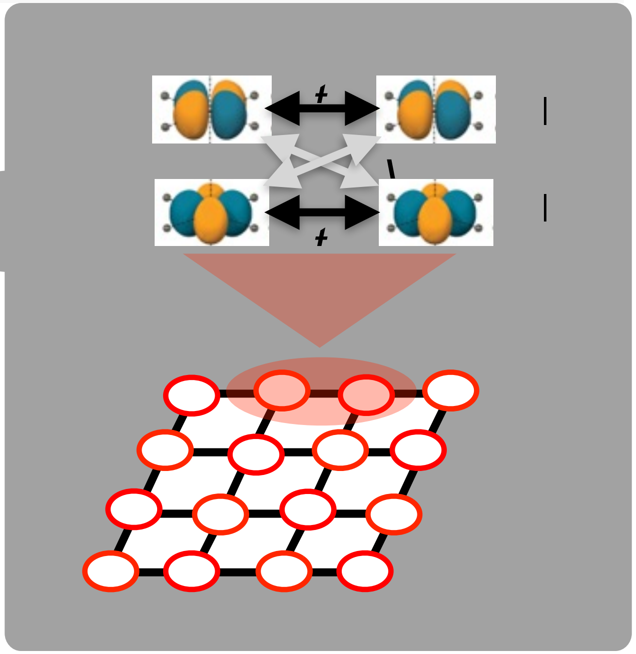
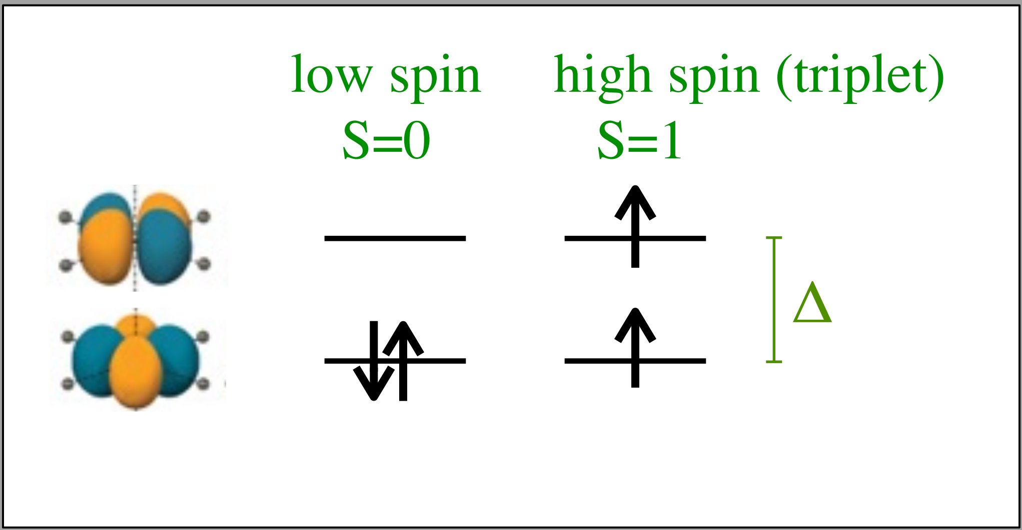
$$H^{\rm dd}_{\rm int} = U\sum(n^a_{i\uparrow}n^a_{i\downarrow} + n^b_{i\uparrow}n^b_{i\downarrow}) + (U-2J) \ldots n^b_{i-\sigma}$$





Competition of Hund's coupling J and crystal-field Δ

We are interested in $E_{LS} \simeq E_{HS}$

Friedrich H. Hund

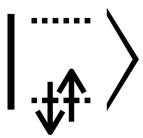
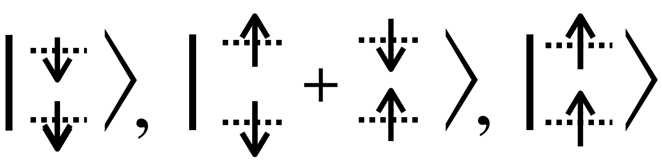
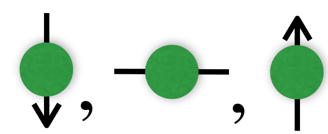
Strong-coupling limit (hard-core bosons)

What is exciton condensate?

Strong coupling theory

Balents 2000
Rademaker et al. 2012-2014
bilayer Heisenberg model

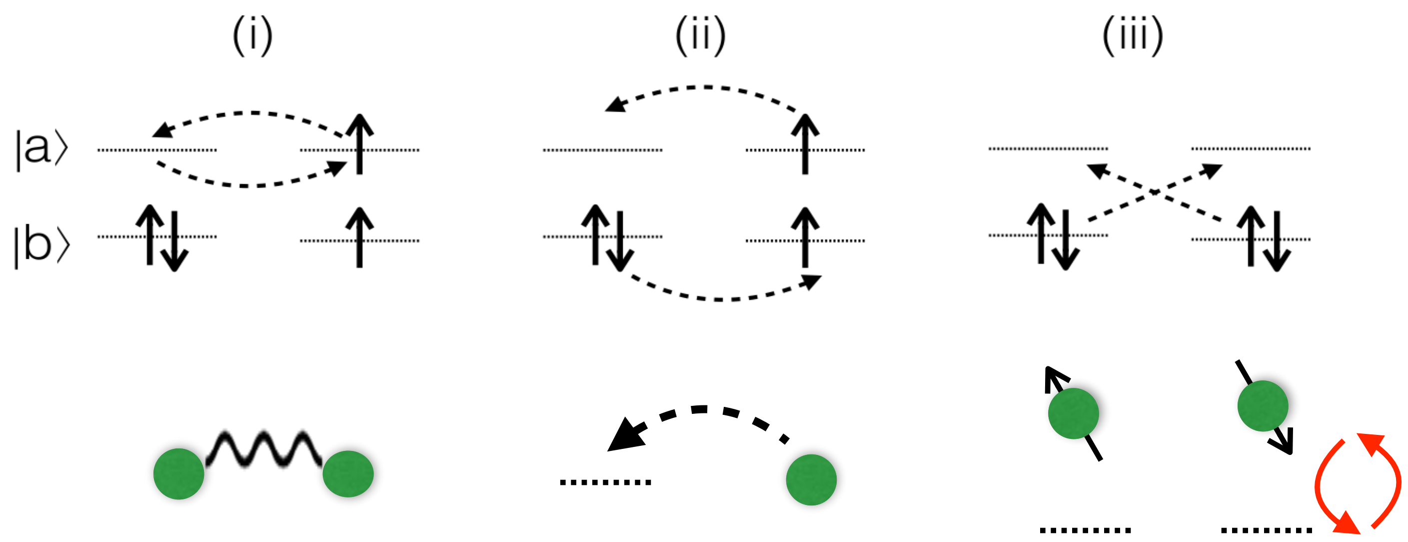
- Define restricted low-energy Hilbert space

Fermions	Bosons (hard-core)
low-spin state 	vacuum
high-spin state 	S=1 boson 
LS -> HS transition $a_\downarrow^\dagger b_\uparrow\,,\,\ldots$	creation of a boson $d_{-1}^\dagger\,,\,\ldots$

Strong coupling theory

- Decouple it from the high-energy states (Schrieffer-Wolff transformation)

Typical 2nd order processes:



Effective Hamiltonian:

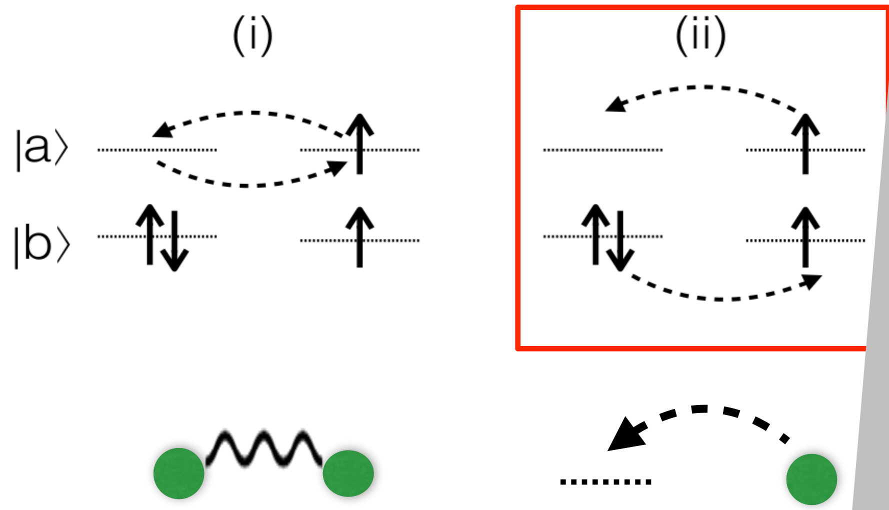
$$H_{\text{eff}} = \varepsilon \sum_i n_i + K_\perp \sum_{\langle ij \rangle} \left(\mathbf{d}_i^\dagger \cdot \mathbf{d}_j + H.c. \right) +$$

$$K_\parallel \sum_{\langle ij \rangle} n_i n_j + K_0 \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + K_1 \sum_{\langle ij \rangle} \left(\mathbf{d}_i^\dagger \cdot \mathbf{d}_j^\dagger + H.c. \right) + \dots$$

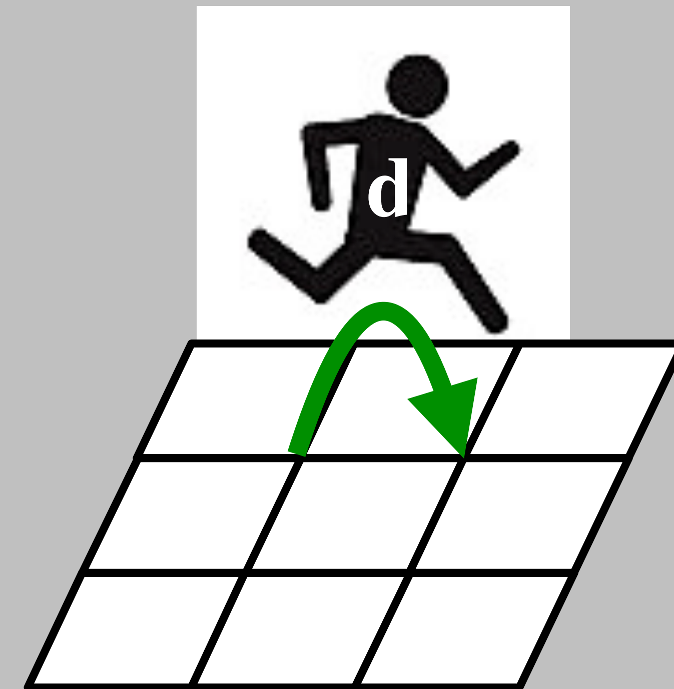
Strong coupling

- Decouple it from the high-energy states (Schrie

Typical 2nd order processes:



d-bosons are mobile !



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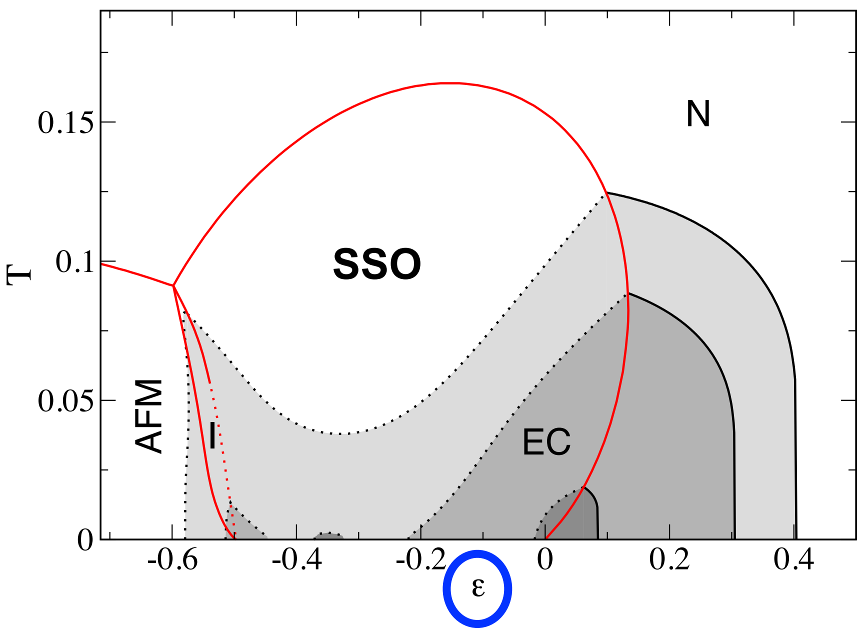
$$K_\parallel \sum_{\langle ij \rangle} n_i n_j + K_0 \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + K_1 \sum_{\langle ij \rangle} \left(\mathbf{d}_i^\dagger \cdot \mathbf{d}_j^\dagger + H.c. \right) + \ldots$$

Mean-field theory

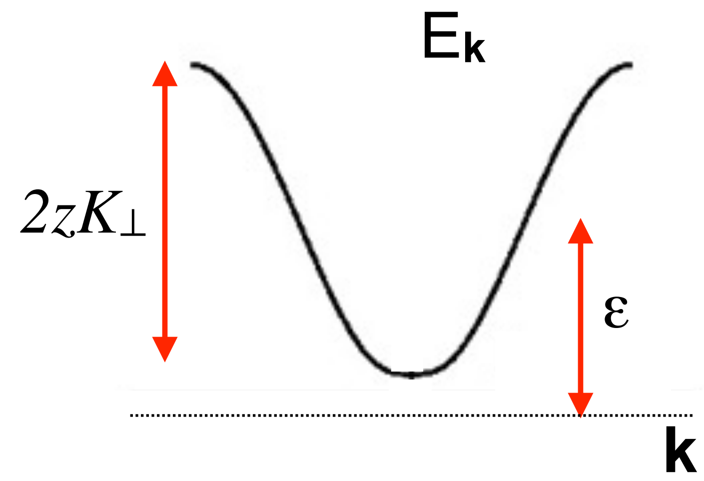
$$H_{\mathrm{eff}} = \varepsilon \sum_i n_i + K_\perp \sum_{\langle ij \rangle} \left(\mathbf{d}_i^\dagger \cdot \mathbf{d}_j + H.c. \right) + K_\parallel \sum_{\langle ij \rangle} n_i n_j + K_0 \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

MF phase diagram:



Augustinský and Kuneš, 2014

excitations in the normal state



d-occupancy: $\langle n \rangle = 0$

Mean-field theory

$$H_{\text{eff}} = \varepsilon \sum_i n_i + K_\perp \sum_{\langle ij \rangle} \left(\mathbf{d}_i^\dagger \cdot \mathbf{d}_j + H.c. \right) + K_\parallel \sum_{\langle ij \rangle} n_i n_j + K_0 \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

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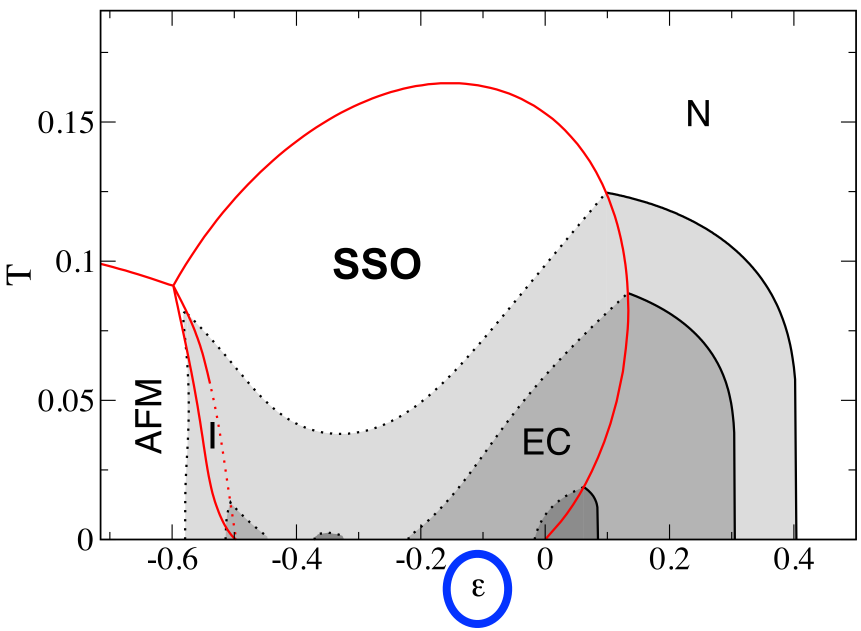
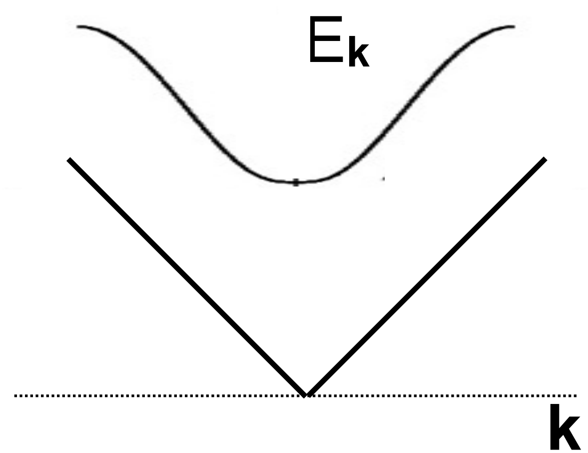


Augustinský and Kuneš, 2014

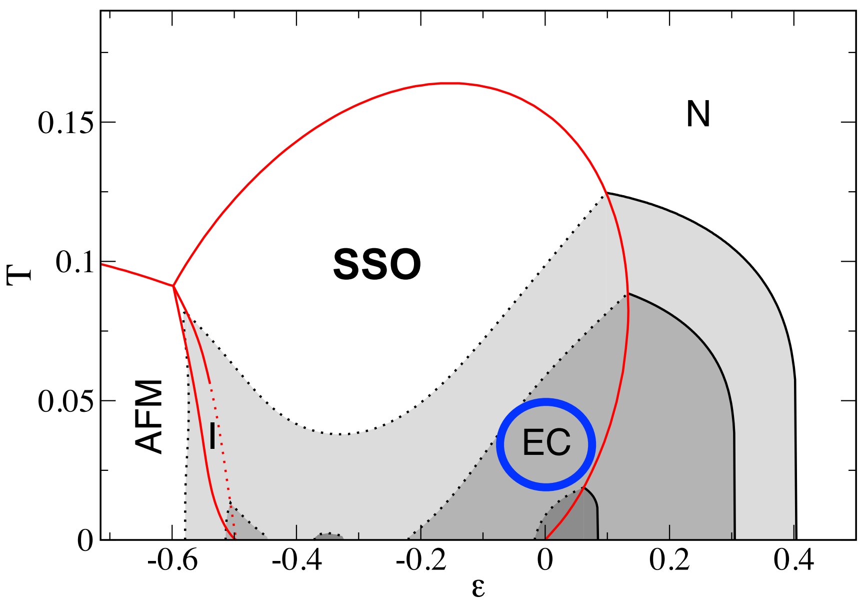
excitations of the condensate



Mean-field theory

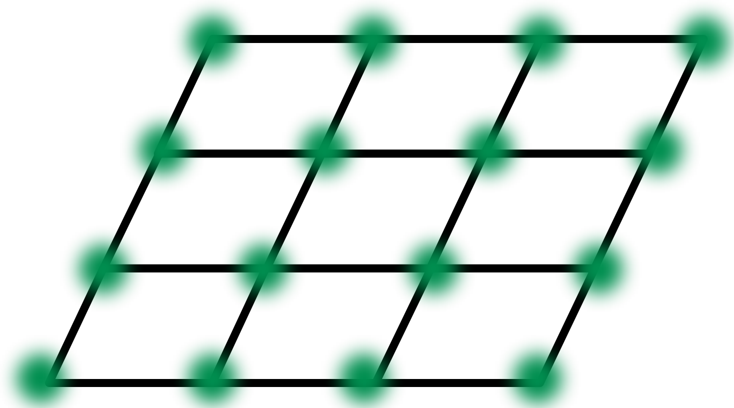
$$H_{\text{eff}} = \varepsilon \sum_i n_i + K_\perp \sum_{\langle ij \rangle} \left(\mathbf{d}_i^\dagger \cdot \mathbf{d}_j + H.c. \right) + K_\parallel \sum_{\langle ij \rangle} n_i n_j + K_0 \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

MF phase diagram:



Augustinský and Kuneš, 2014

Bose-Einstein condensate of d-bosons



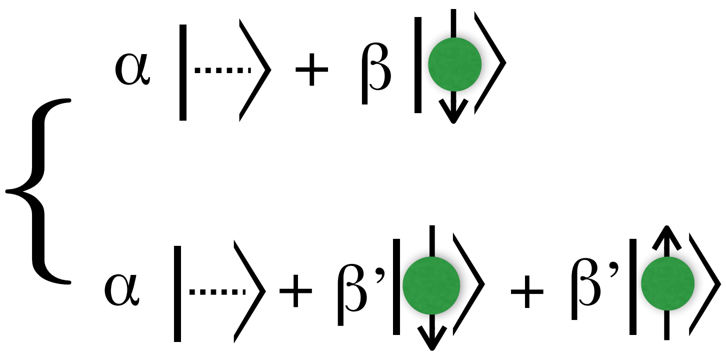
Order parameter: $\langle d_s \rangle$

d-occupancy: $0 < \langle n \rangle < 1$

Exciton condensate

Degenerate excitations -> distinct condensates possible

$|C_i\rangle$



ferromagnetic condensate

polar condensate

$$|C\rangle = \prod_i |C_i\rangle$$

approx. condensate wavefunction

order parameter

$$\vec{\phi} = \sum_{\sigma,\sigma'} \langle a^\dagger_\sigma b_{\sigma'} \rangle \vec{\tau}_{\sigma\sigma'} \sim \alpha^* \beta$$

Back to fermions
(DMFT)

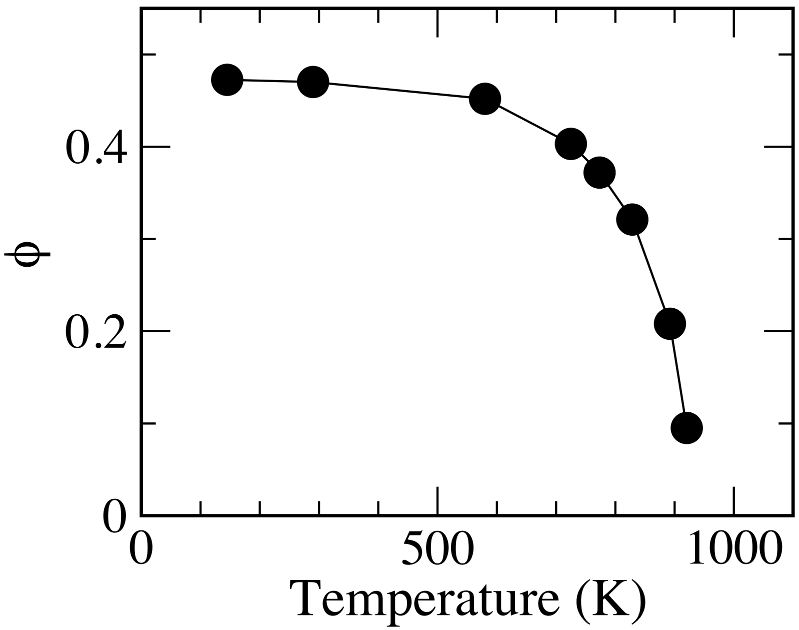
" fermion = boson$^{1/2}$ " adds a lot of extra structure

Undoped system - polar condensate

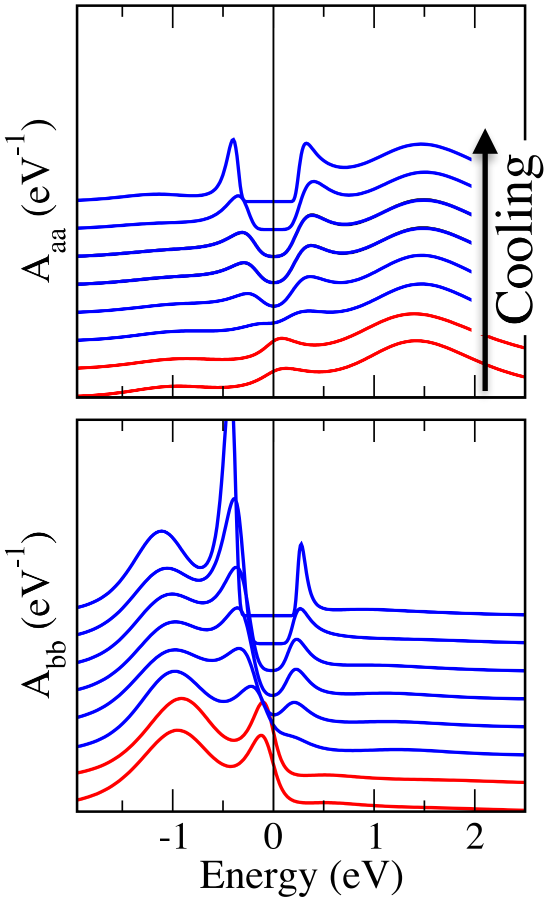
order parameter

$$\vec{\phi} = \sum_{\sigma,\sigma'} \langle a^\dagger_\sigma b_{\sigma'} \rangle \vec{\tau}_{\sigma\sigma'}$$

$$\vec{\phi} = (\phi, 0, 0)$$



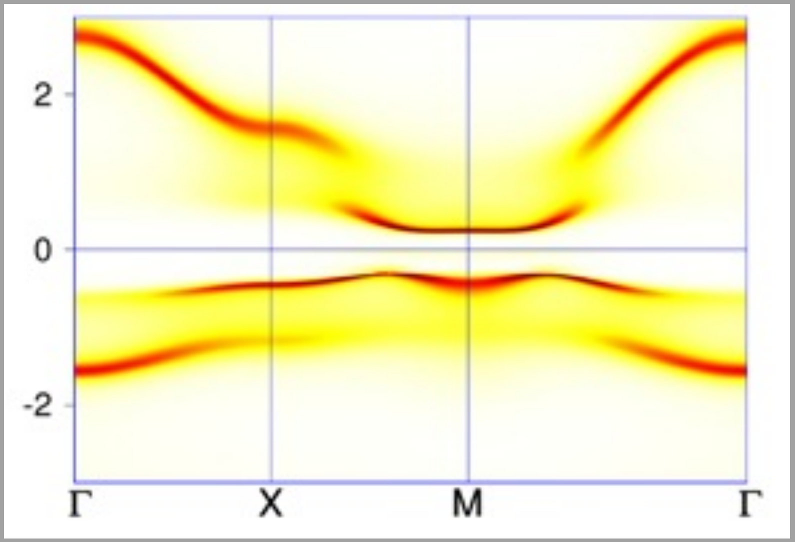
Spectral density (diagonal elements)



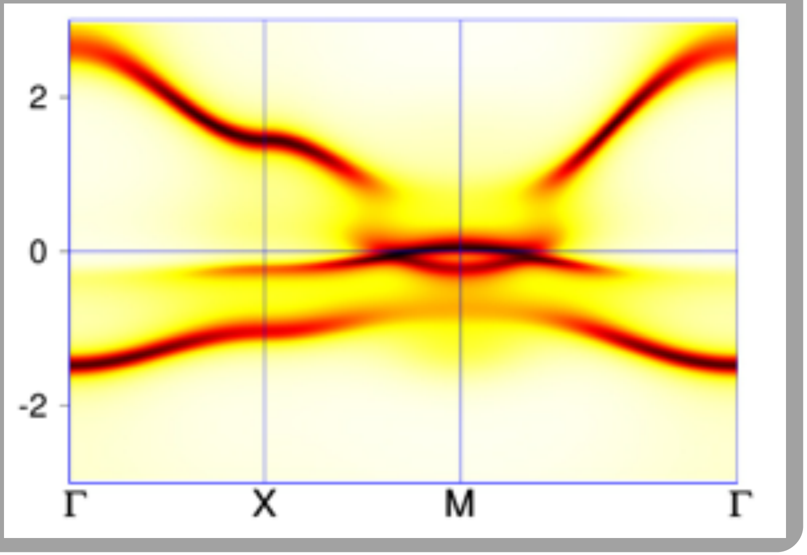
Undoped system - polar condensate

Opening of charge gap

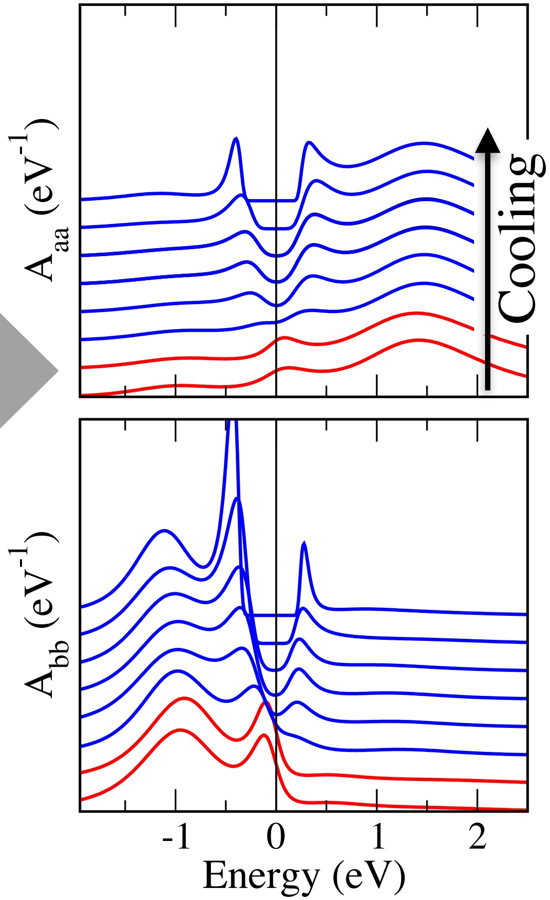
EC phase
(low T)



normal phase
(high T)

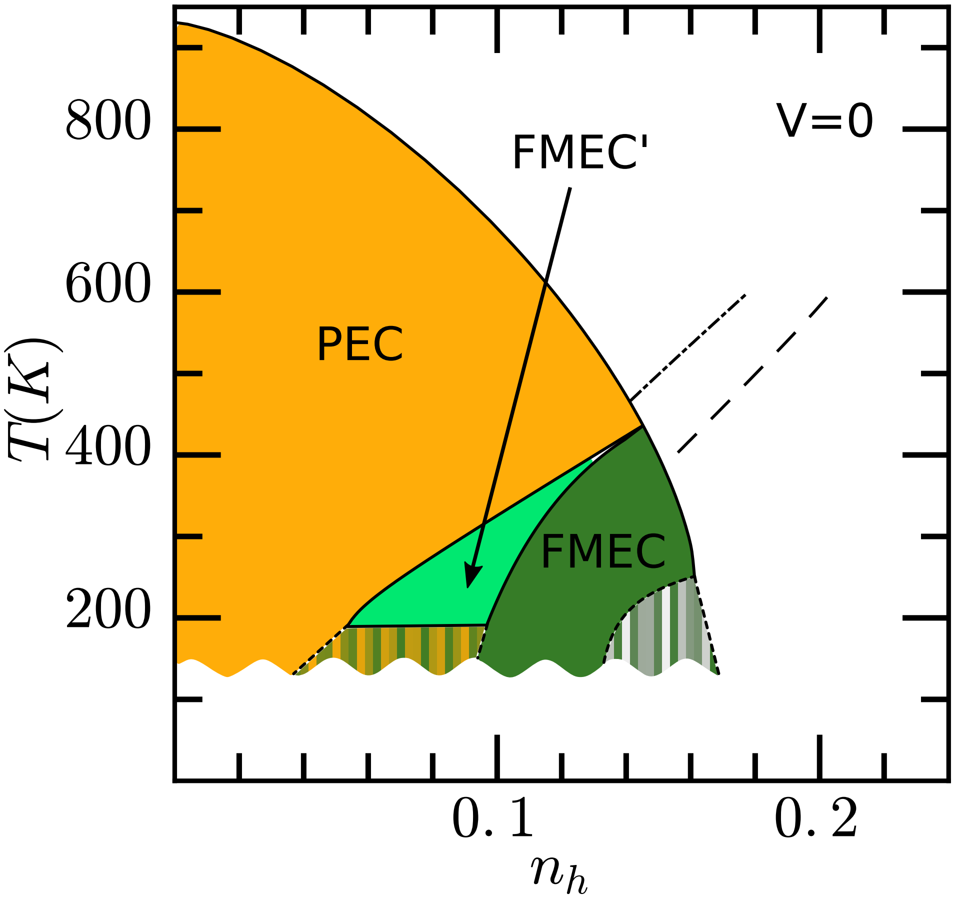


density (diagonal elements)



Doping (V=0)

n-T phase diagram



Competition between
AFM super-exchange (PEC) and
double-exchange (FMEC)

$$\overrightarrow{\phi} = \sum_{\sigma,\sigma'} \langle a^\dagger_\sigma b_{\sigma'} \rangle \overrightarrow{\tau}_{\sigma\sigma'}$$

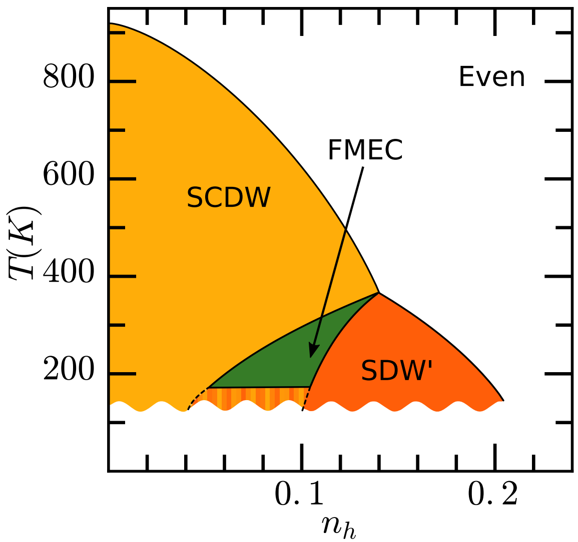
PEC - polar condensate

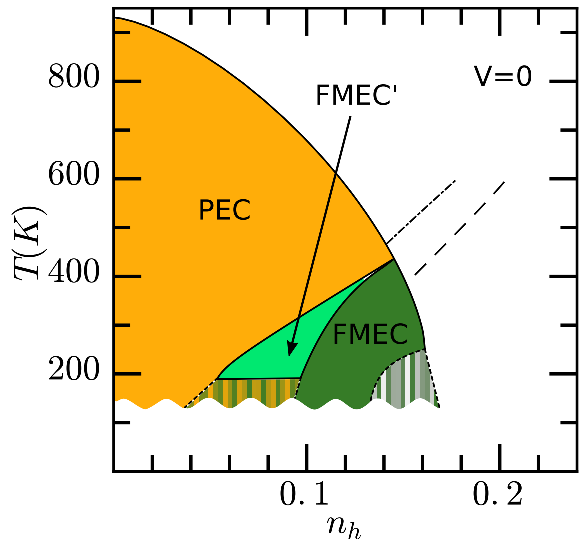
$$\overrightarrow{\phi} = \exp(i\varphi)\overrightarrow{x}$$

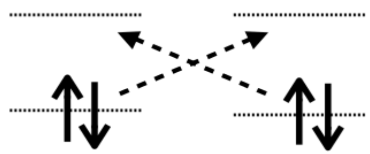
FMEC - ferromagnetic condensate

$$\overrightarrow{M} = i\overrightarrow{\phi}^* \wedge \overrightarrow{\phi}$$

Finite cross-hopping



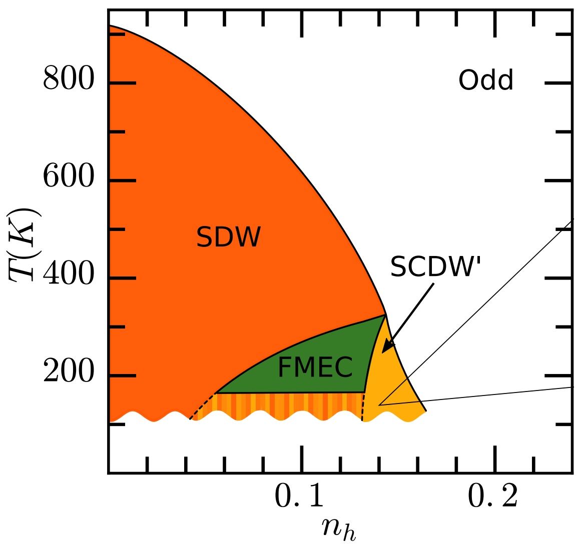




V$_1$=V$_2$ even cross-hopping

V$_1$=-V$_2$ odd cross-hopping

PEC $\begin{cases} \text{SDW} & \vec{\phi} = \vec{x} \\ \text{SCDW} & \vec{\phi} = i\vec{x} \end{cases}$

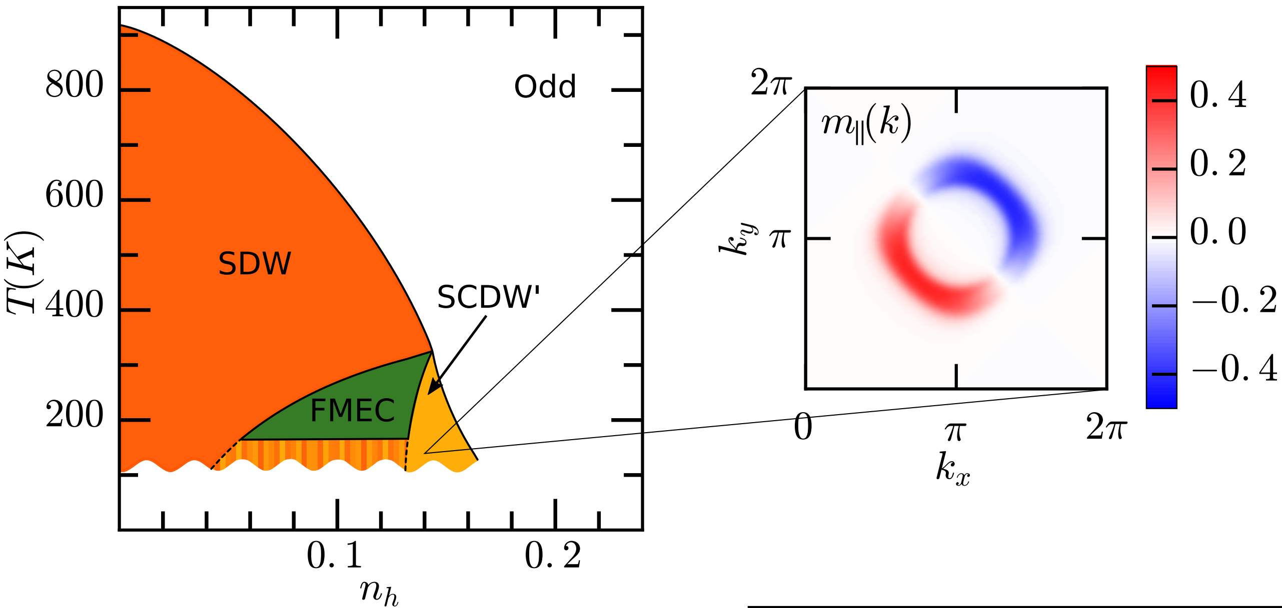


Condensate state	$M_\perp$	$M_\parallel$	$\mathbf{m}(\mathbf{r})$	$\mathbf{m}_\mathbf{k}$	Re $\boldsymbol{\phi}$	Im $\boldsymbol{\phi}$
FMEC	✓	✓, 0	✓	✓	✓	✓
SDW	0	0	✓	0	✓	0
SCDW	0	0	0	0	0	✓
SDW'	0	✓, 0	✓	✓	✓	0
SCDW'	0	0	0	✓	0	✓

$$\mathbf{m}_\mathbf{k} = \sum_{\alpha\beta} \boldsymbol{\sigma}_{\alpha\beta} \langle a^\dagger_{\mathbf{k}\alpha} a_{\mathbf{k}\beta} + b^\dagger_{\mathbf{k}\alpha} b_{\mathbf{k}\beta} \rangle$$

$$\boldsymbol{\phi} = \sum_{\alpha,\beta} \boldsymbol{\sigma}_{\alpha\beta} \langle a^\dagger_{i\alpha} b_{i\beta} \rangle$$

Spin texture



Condensate state	$M_\perp$	$M_\parallel$	$\mathbf{m}(\mathbf{r})$	$\mathbf{m}_\mathbf{k}$	Re ϕ	Im ϕ
FMEC	✓	✓, 0	✓	✓	✓	✓
SDW	0	0	✓	0	✓	0
SCDW	0	0	0	0	0	✓
SDW'	0	✓	✓	✓	✓	0
SCDW'	0	0	0	✓	0	✓

Dynamically generated Dresselhaus-Rashba spin-orbit coupling

centrosymmetric Hamiltonian, no spin-orbit coupling

Propagation of doped carriers in the condensate

$$H_{\rm eff} = \sum_{\langle ij \rangle} \bar{h}_{\alpha\beta} c^\dagger_{i\alpha} c_{j\beta} + {\rm h.c.}$$

$$h^{(ij)}_{\alpha\beta} = \langle \alpha_i C_j | H | C_i \beta_j \rangle$$

$$\alpha, \beta \in \{\uparrow, \downarrow\}$$

$$\bar{h} = t_s \bar{I} - \frac{i t_a}{4 s^2} \left(\boldsymbol{\phi}^* \wedge \boldsymbol{\phi} \right) \cdot \bar{\boldsymbol{\sigma}} + \frac{1}{2} \left(V_1 \boldsymbol{\phi} + V_2 \boldsymbol{\phi}^* \right) \cdot \bar{\boldsymbol{\sigma}}$$

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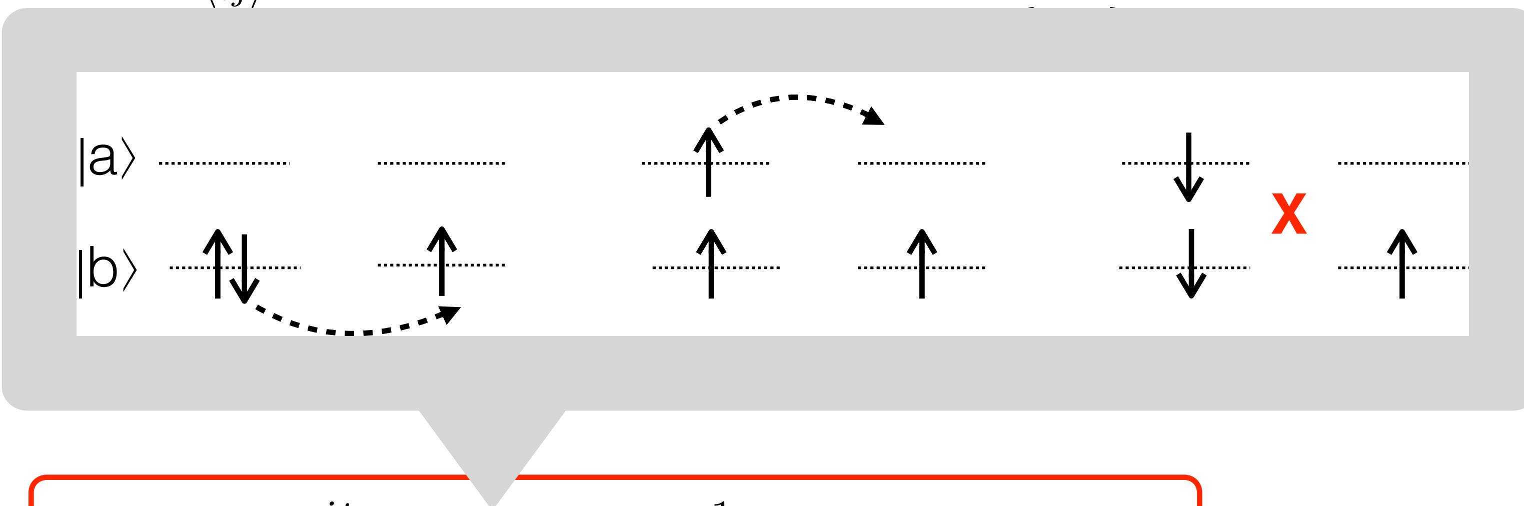

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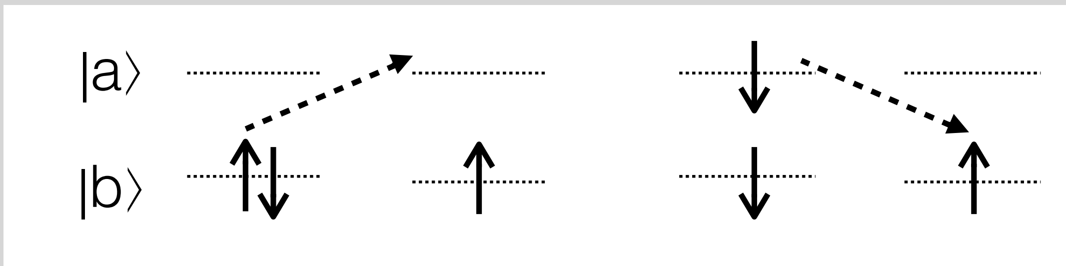

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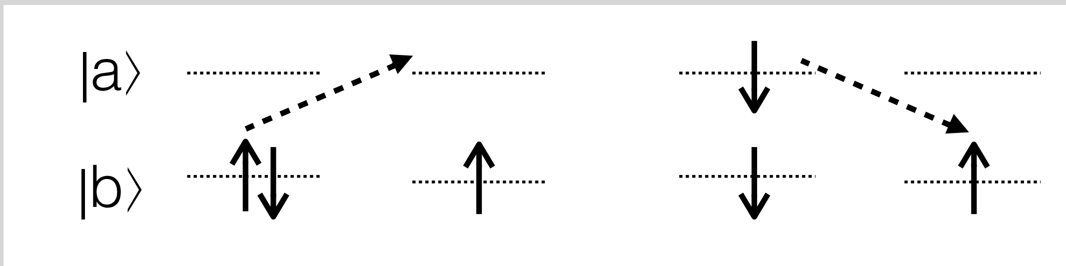

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Field acting on bonds is local in k-space:

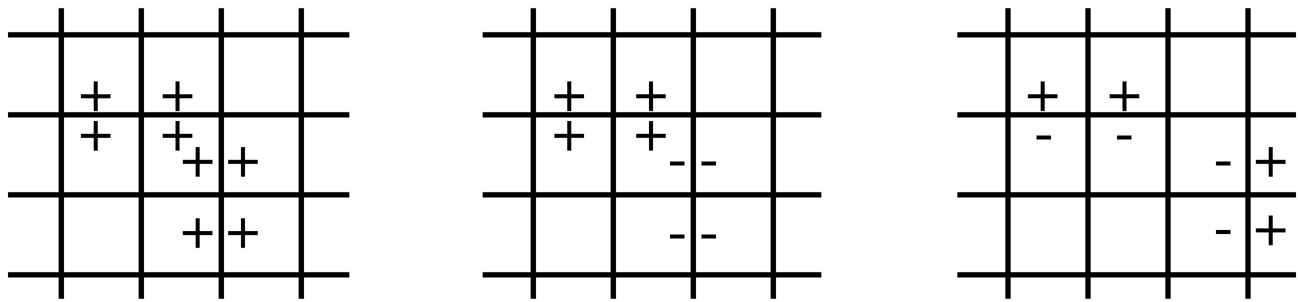
$$\bar{h}_{\mathbf{k}} = 2 t_s \bar{I} C_{\mathbf{k}} + 2 V_1 \boldsymbol{\phi} \cdot \bar{\boldsymbol{\sigma}} \begin{cases} C_{\mathbf{k}} & \text{SDW'} \\ i S_{\mathbf{k}} & \text{CSDW'} \end{cases}$$

with $\quad C_{\mathbf{k}} = \cos k_x + \cos k_y, \quad S_{\mathbf{k}} = \sin k_x + \sin k_y.$

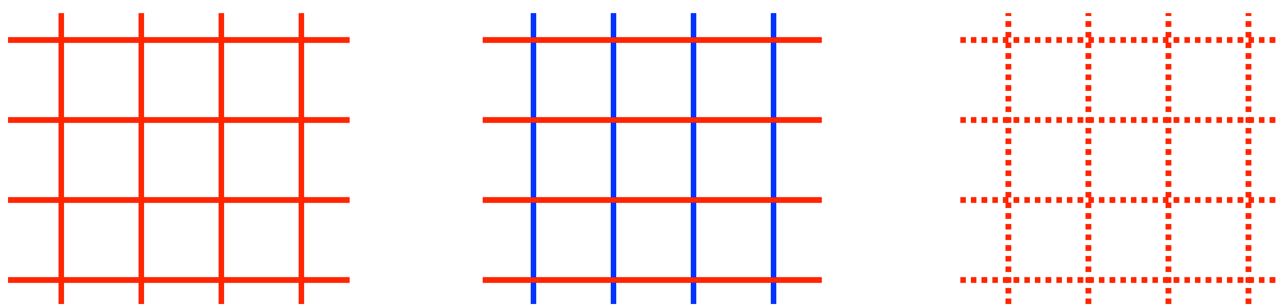
How to realize spin textures

- PEC state (intra atomic level)
- effective exchange on the bonds (inter atomic level)
- global spin-currents or FM polarization (inter cell level)

Cross-hopping:



Bond exchange field:



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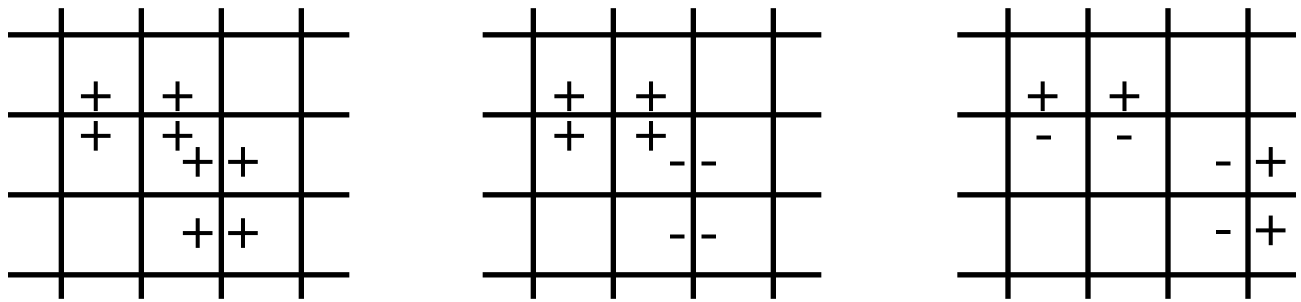

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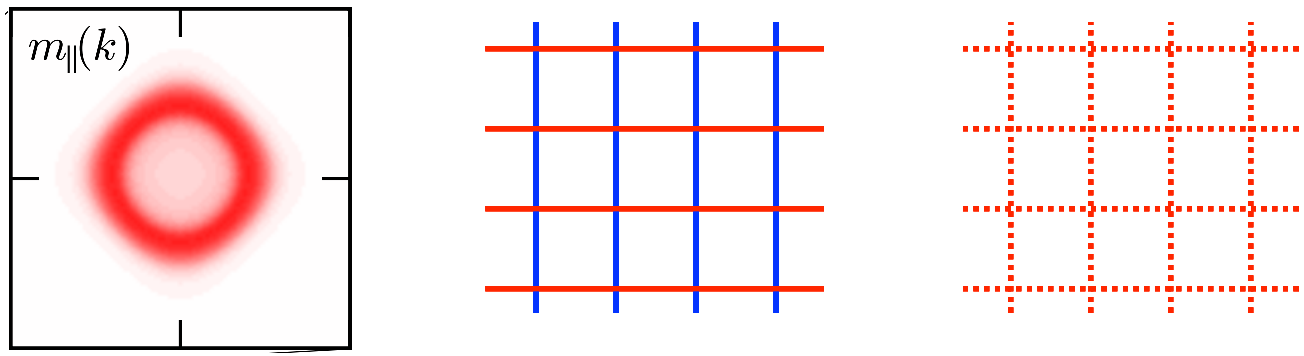
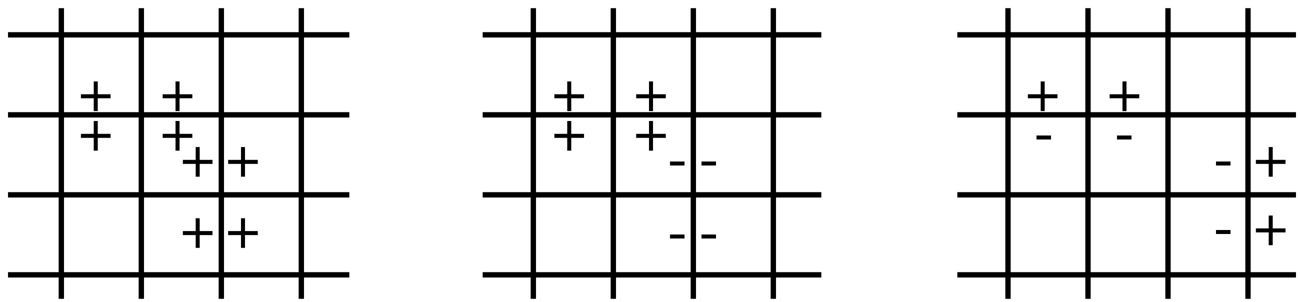


$\cos k_x + \cos k_y$

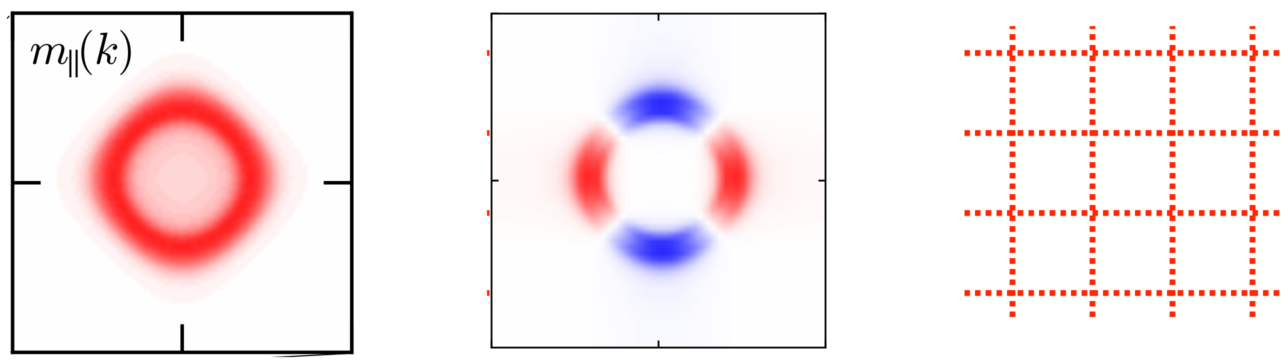
How to realize spin textures

- PEC state (intra atomic level)
- effective exchange on bonds (inter atomic level)
- global spin-currents or FM polarization (inter cell level)

Cross-hopping:



Bond exchange field:



$\cos k_x + \cos k_y$ $\cos k_x - \cos k_y$

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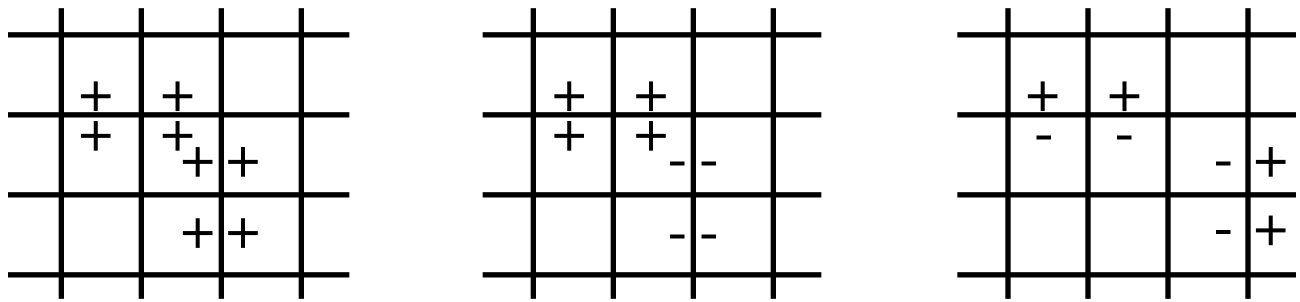

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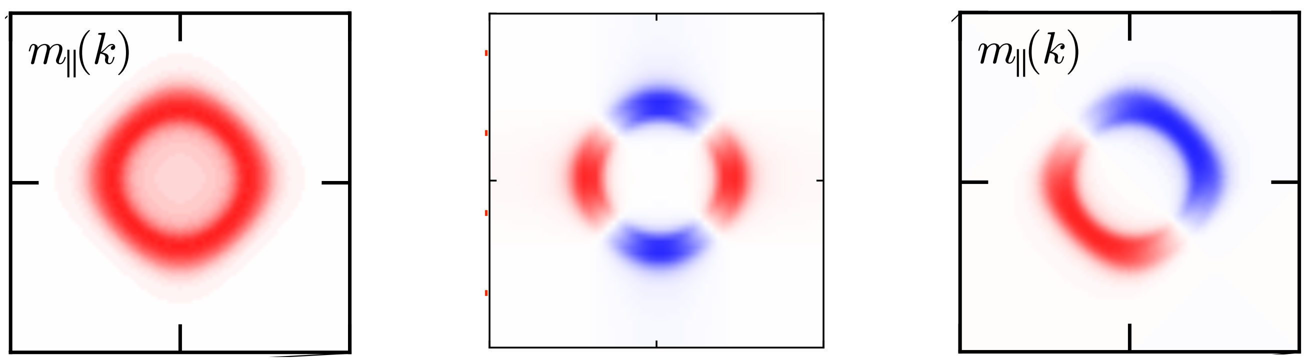


$\cos k_x + \cos k_y$ $\qquad$ $\cos k_x - \cos k_y$ $\qquad$ $\sin k_x + \sin k_y$

Conclusions

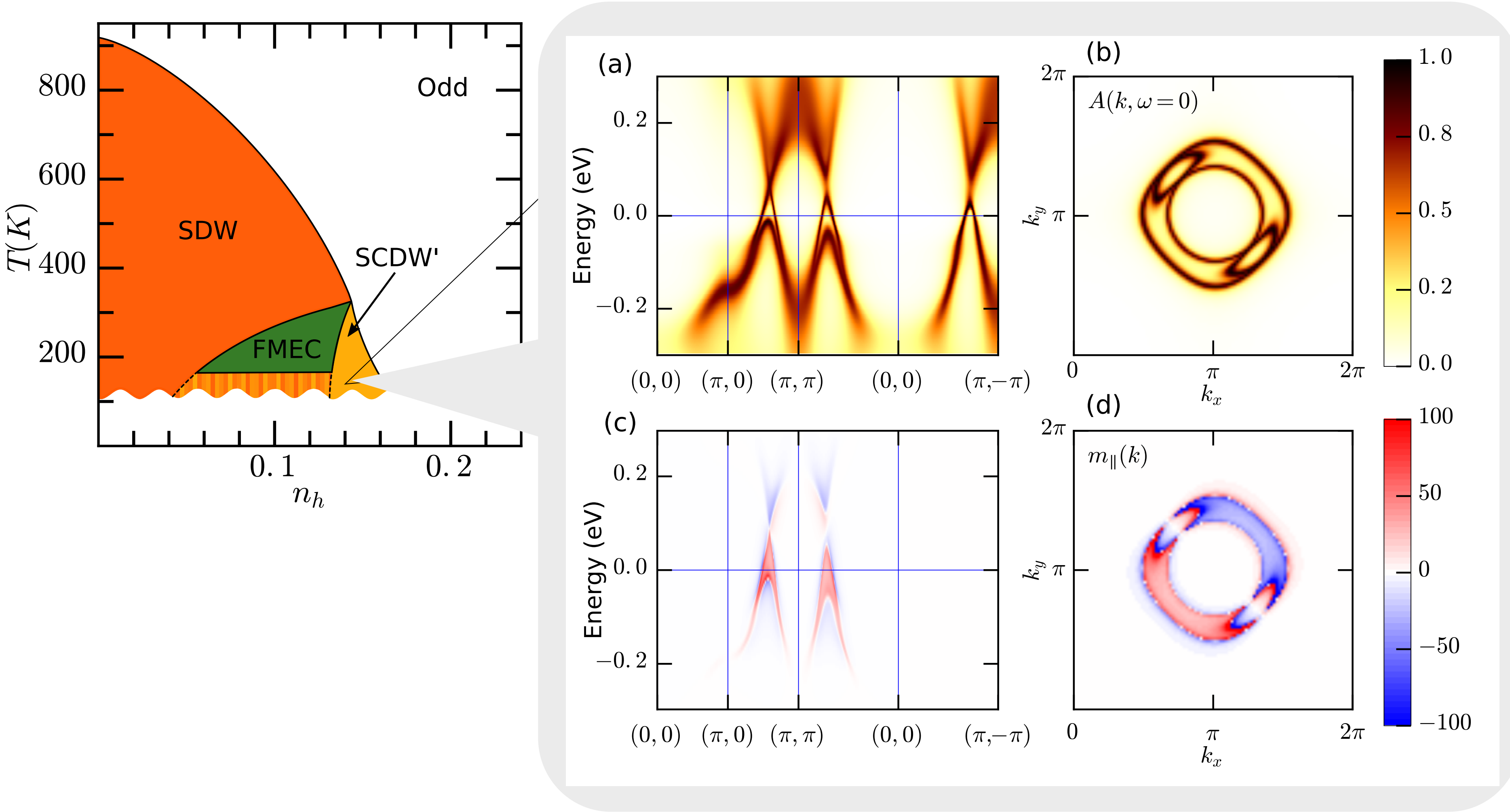
• Solids close to **spin-state transition** are unstable towards **condensation of spinful excitons**.

• Excitonic condensation can give rise to a **number of phases** with rather diverse properties.

• **Doping** activates generalised double-exchange mechanism with interesting consequences (e.g. spontaneous spin texture)

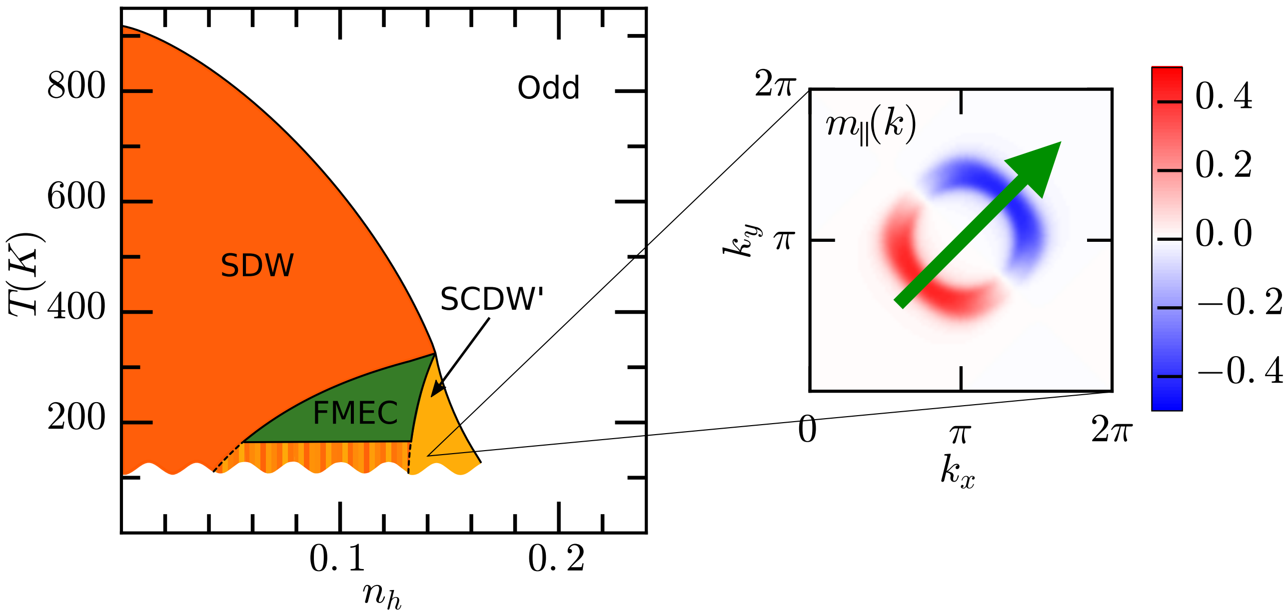
J. Phys.: Condensed. Matter **27**, 333201 (2015) - Topical Review
Phys. Rev. Lett. **116**, 256403 (2016)

Spin texture



Spin-galvanic effect

Magnetic field generates charge current

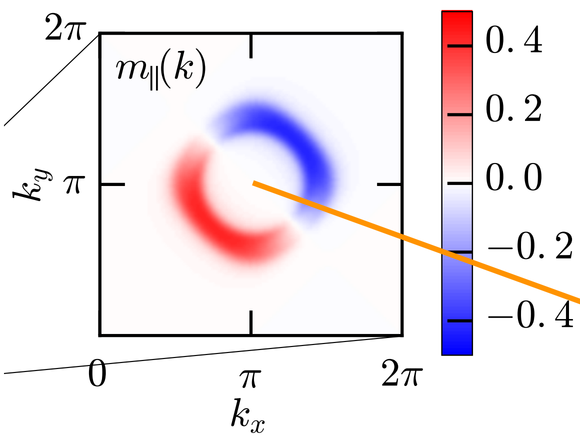


Spin-galvanic effect

Magnetic field generates charge current

poor man's treatment (using $\boldsymbol{\Sigma}_{B=0}$)

spin distribution $m_{\mathbf{k}}$ @ B=0



$\delta n_{\mathbf{k}} = n_{\mathbf{k}}(B) - n_{\mathbf{k}}(0)$

charge distribution $\delta n_{\mathbf{k}}$ @ B=0.001 eV/$\boldsymbol{\mu}_B$