Institute for Basic Science

Center for Theoretical
Physics of Complex Systems

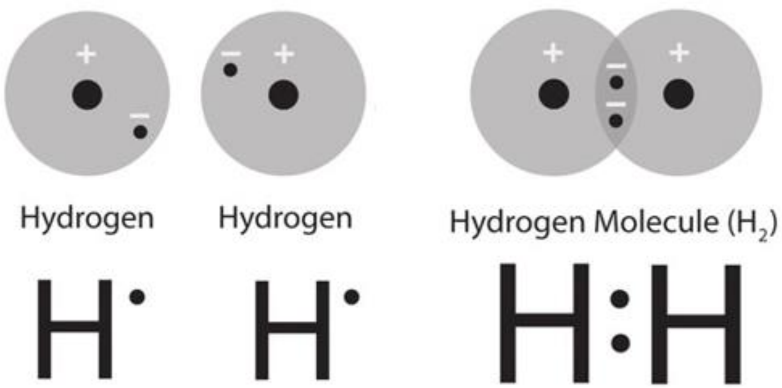
Mean-field description of skyrmion phases in frustrated antiferromagnets

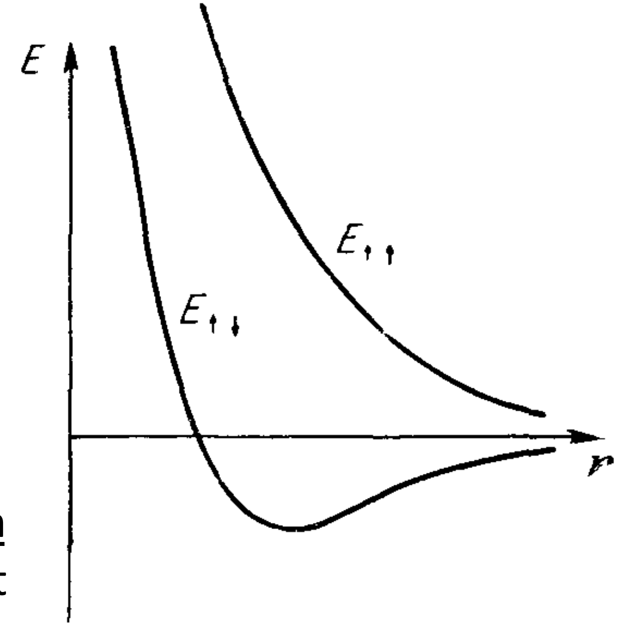
O.I. Utesov

Part I

Modulated Spin Structures

Exchange interaction





Symmetric coordinate part of wave-function – <u>spin singlet</u>, antisymmetric – <u>triplet</u>. When integrating out spatial degrees of freedom one arrives to effective spin Hamiltonian

$$\mathcal{H}_{eff} = E_0 - J\vec{S}_1 \cdot \vec{S}_2$$

In hydrogen $J < 0$; generalization to solids with magnetic **d** (transition metals) and **f** (rare earth elements) electrons reads

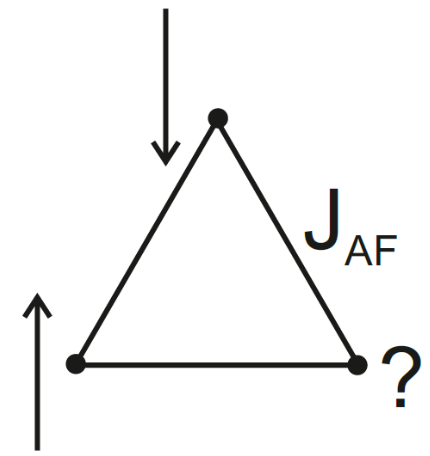
$$\mathcal{H} = -\sum_{\langle i,j \rangle} J_{ij}\vec{S}_i \cdot \vec{S}_j$$

Magnetic frustration

When energies of all exchange couplings cannot be minimized simultaneously, then the magnetic system is called frustrated

Simple example – Ising triangle with AF coupling
(in real life we need strong easy axis anisotropy)

$$\mathcal{H} = \frac{J}{2} \sum_{\langle i,j \rangle} S_i^z S_j^z$$



If we place two spins in opposite directions, the remaining spin can point up or down – energy will be the same.

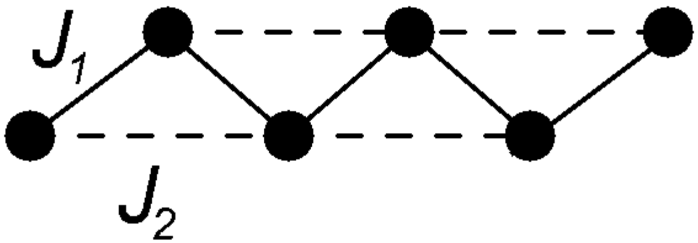
Interesting physics: spin ice (residual entropy, magnetic monopoles), reduced dimensionality, (quantum) spin liquids, etc.

We will focus on **3D** systems, where well-defined magnetically ordered phases are usually observed experimentally

J_1-J_2 model

The simplest Heisenberg model with frustration includes AF next-nearest neighbors interaction

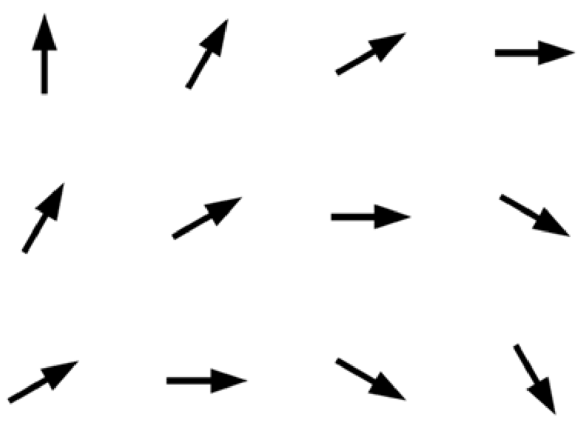
$$\mathcal{H} = -J_1 \sum_n \vec{S}_n \cdot \vec{S}_{n+1} + J_2 \sum_n \vec{S}_n \cdot \vec{S}_{n+2}$$



To avoid complications with **1D** one can think about ordered array of such chains with interchain exchange interaction.

What is the ground state of the system?

$$\vec{S}_n = S(\hat{x}\cos qn + \hat{y}\sin qn)$$
$$\varepsilon = -S^2(J_1 \cos q - J_2 \cos 2q)$$
$$\cos q = \frac{J_1}{4J_2},\ J_1 \le 4J_2$$



1. For large enough **nnn** coupling noncollinear spiral order is preferable in comparison with collinear FM one
2. Spiral plane is still arbitrary (one needs small anisotropic interactions)

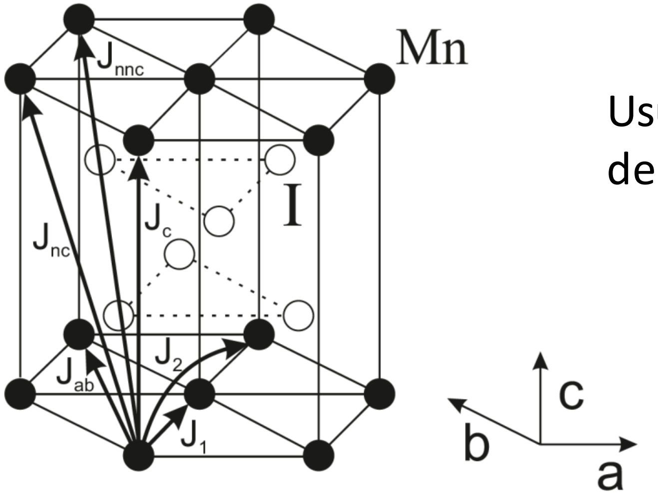
General case

$$\mathcal{H} = -\sum_{\langle i,j \rangle} J_{ij}\vec{S}_i \cdot \vec{S}_j \Leftrightarrow \mathcal{H} = -\sum_{\vec{q}} J_{\vec{q}}\vec{S}_{\vec{q}} \cdot \vec{S}_{-\vec{q}}$$

One should minimize the Fourier transform of the exchange interaction $J_{\vec{q}}$

Particular cases:

- Ferromagnetic order $\vec{k} = (0,0,0)$
- Antiferromagnetic (Neel) order $\vec{k} = (\pi,\pi,\pi)$
- Incommensurate structure, e.g., $\vec{k} \approx (0.36\pi, 0, 0.88\pi)$



Usually several exchange couplings are needed to properly describe modulation vectors in real compounds

Modulated spin structures 1

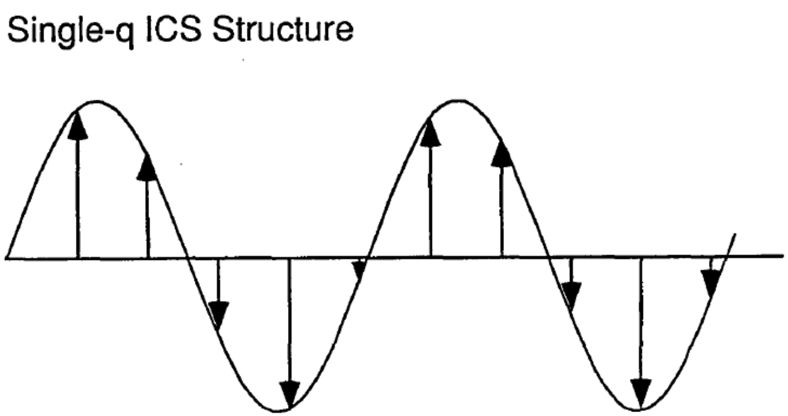
Due to magnetic anisotropy, magnetodipolar intreraction, and Zeeman energy various types of modulated spin structures can be observed experimentally

$$\mathcal{H}_{an} = -\sum_i \left[Z_1 (S_i^z)^2 + Z_2 (S_i^y)^2\right], \quad \mathcal{H}_z = -\mathbf{h}\cdot\left(\sum_i \mathbf{S}_i\right), \quad \mathcal{H}_d = \frac{1}{2}\sum_{i,j} \mathcal{D}_{ij}^{\alpha\beta} S_i^\alpha S_j^\beta$$

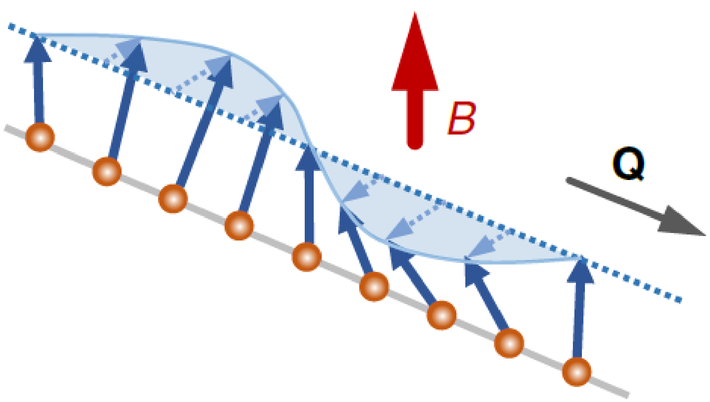
$$\mathcal{D}_{ij}^{\alpha\beta} = \omega_0 \frac{v_0}{4\pi}\left(\frac{\delta^{\alpha\beta}}{R_{ij}^3} - \frac{3R_{ij}^\alpha R_{ij}^\beta}{R_{ij}^5}\right), \quad \omega_0 = 4\pi\frac{(g\mu_B)^2}{v_0}$$

In the reciprocal space, dipolar forces provide momentum-dependent biaxial anisotropy

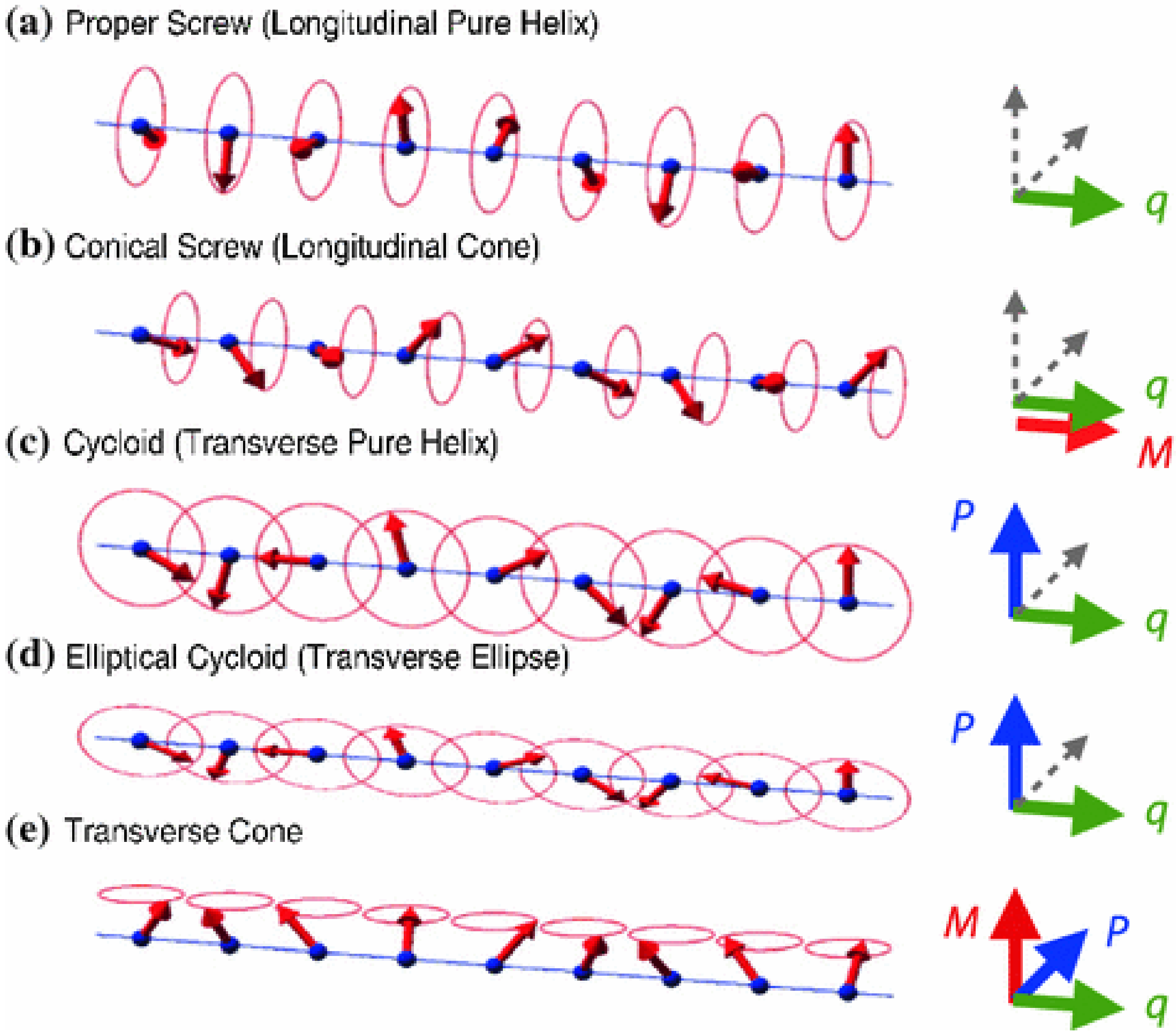
At high T simple **SDW** is typical



At large fields **fan** structures are usually stabilized



Modulated spin structures 2

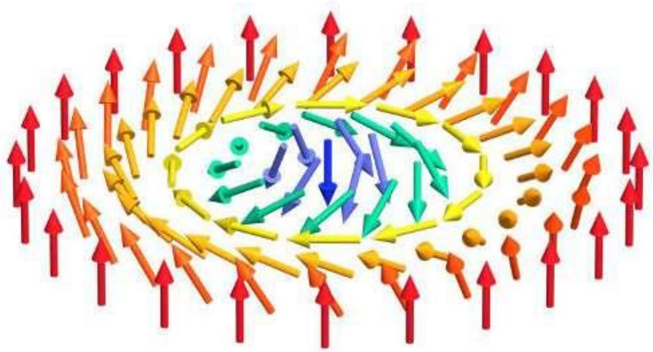


Skyrmions

- Topologically-nontrivial field configurations in non-linear field theories (T. Skyrme, 1962)
- In condensed matter first appear as metastable configurations in 2D ferromagnets (A. Belavin and A. Polyakov, 1975)
- Stable soliton-like solutions due to Lifshitz invariants (A.N. Bogdanov and D. Yablonskii, 1989)

What is special about skyrmions?

- Topologically protected configurations
- Topological Hall effect, emergent field
- Possibility to write/delete single skyrmion
- Possibility to move skyrmions by, e.g., electrical currents
- Multiferroic order in dielectrics stemming from noncollinear spin texture
- Racetrack memory
- Unconventional computing
- ...



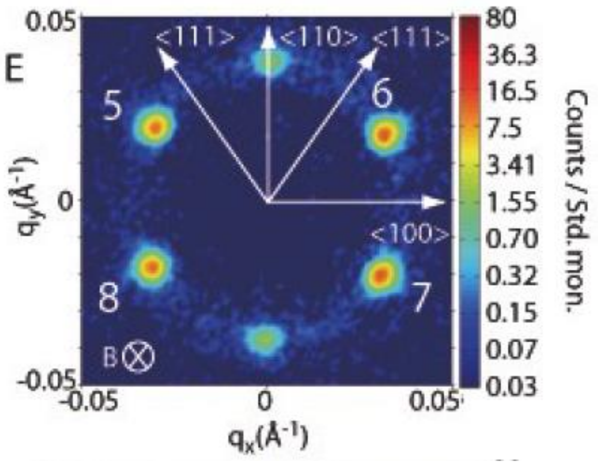
Skyrmion lattice/crystal - SkL

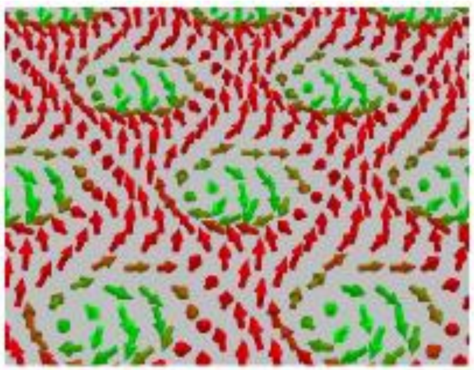
Paper by S. Mühlbauer, *et al*., *Science* **323**, 915 (2009) stimulates upsurge of interest to skyrmions, **SkL**, and various other topological structures in magnetic materials

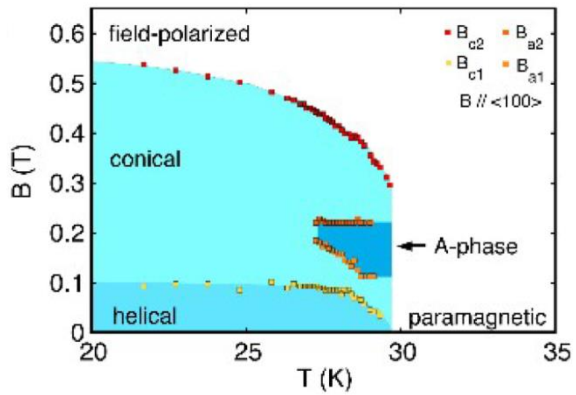
In cubic **B20** helimagnets the **SkL** is hexagonal tight packing of skyrmions due to **DMI**
Important scale J/D is of the order of a skyrmion size, thus the period of **SkL** is large and the density of topological charge is rather small

$$E_{\mathrm{DM}} = D\int \mathbf{M}\cdot(\nabla\times\mathbf{M})\mathrm{d}^3\mathbf{r}$$

$$Q = \frac{1}{4\pi}\int \mathbf{n}\cdot[\partial_x\mathbf{n}\times\partial_y\mathbf{n}]\,dxdy$$

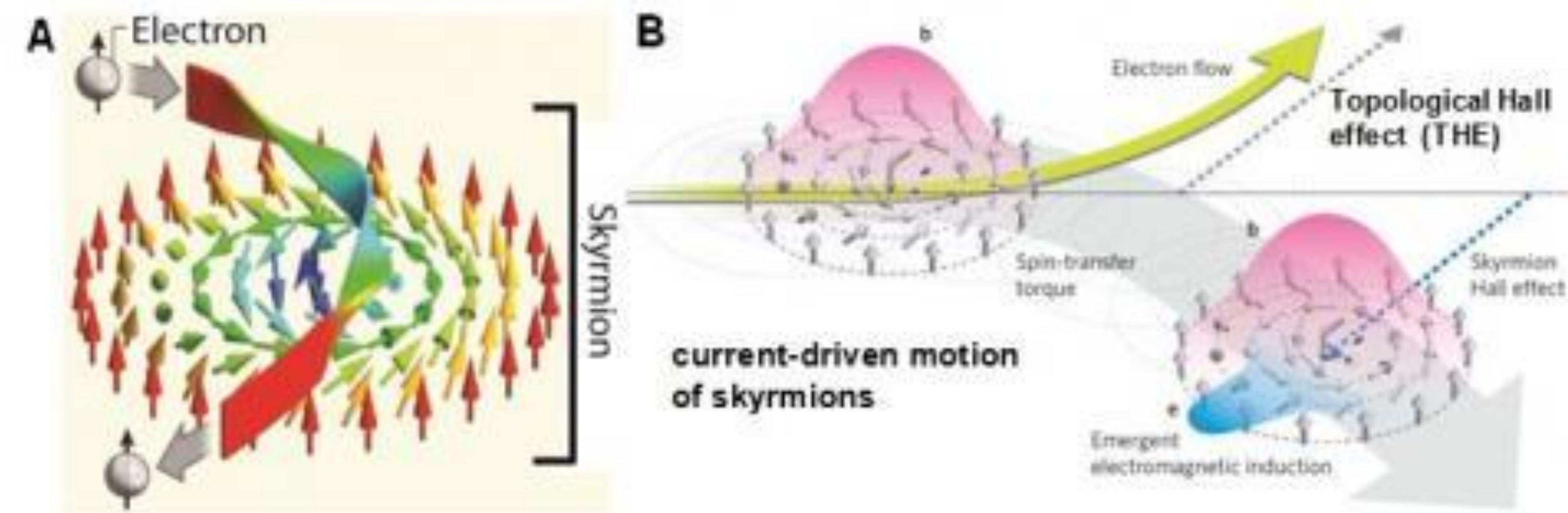


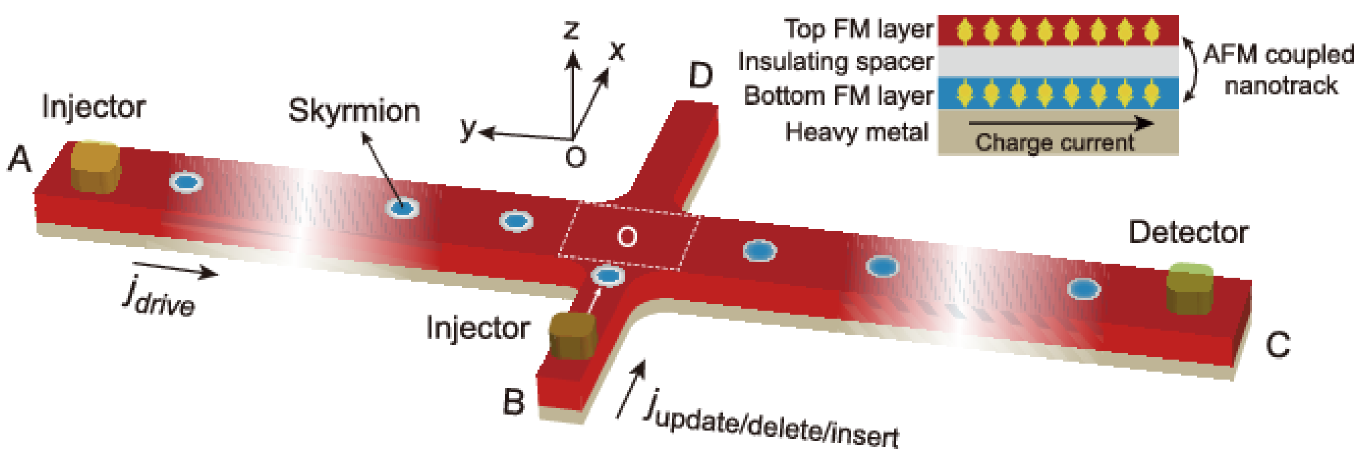




Topological Hall effect and racetrack memory

Skyrmion nontrivial topology leads to unusual electron transport (connected with the Berry phase) and to the possibility to move isolated skyrmions

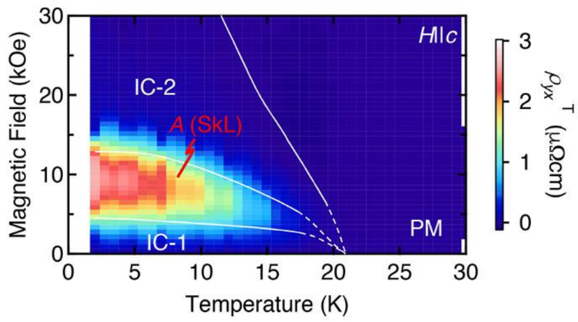


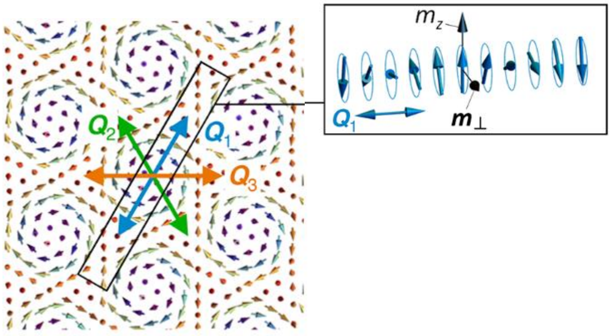


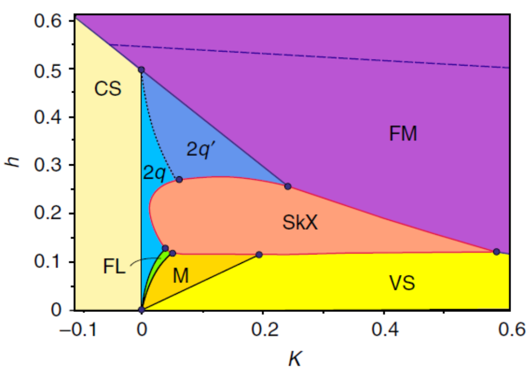
Frustrated antiferromagnets

Skyrmions and skyrmion lattices can be observed in centrosymmetric helimagnets!

- Popular triangular lattice can host topologically nontrivial structures.
  Frustration + easy axis anisotropy
  (Theory by A. Leonov and M. Mostovoy, *Nat. Commun.* **6**, 8275 (2015))
- Short-period magnetic textures
- **Giant** topological Hall effect
- **SkL** – can be considered as superposition of three short-period helices plus higher harmonics
- Large density of topological charge
- Experimentally observed in Gd_2PdSi_3 [see T. Kurumaji, *et al.*, *Science* **365**, 914 (2019)]

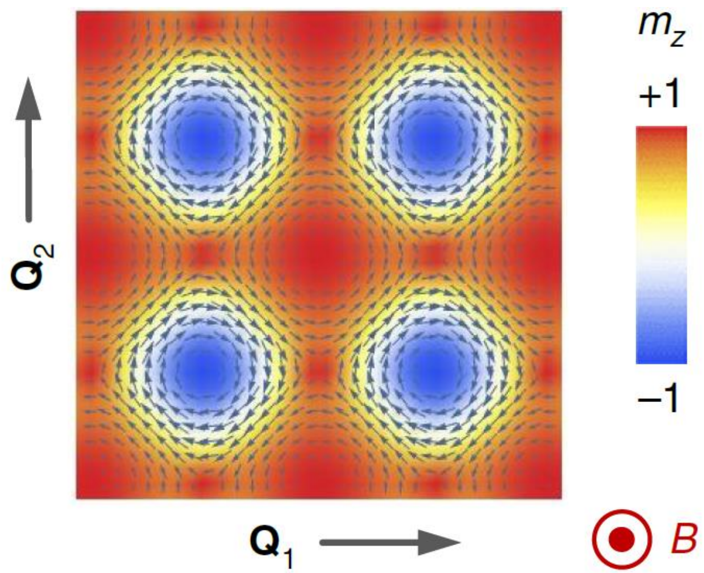


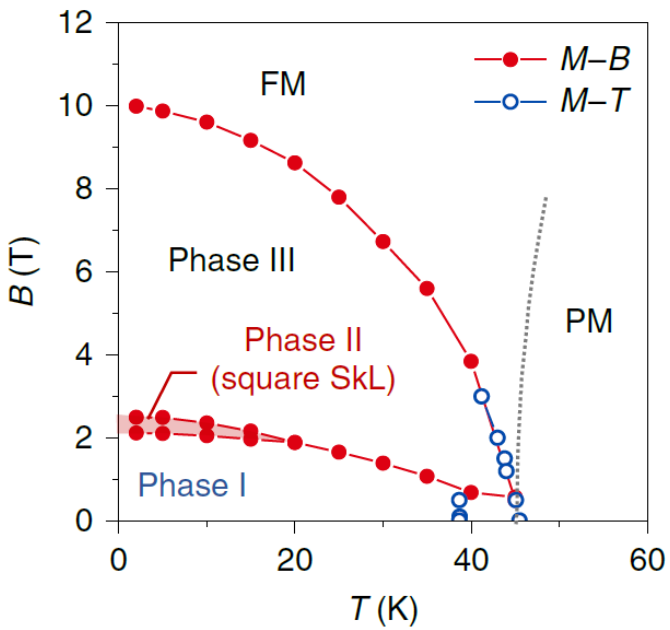




One more experiment

SkL was observed in the recent study devoted to properties of frustrated tetragonal compound $GdRu_2Si_2$ [Khanh *et al.*, *Nat. Nanotechnol.* **15**, 444 (2020)]

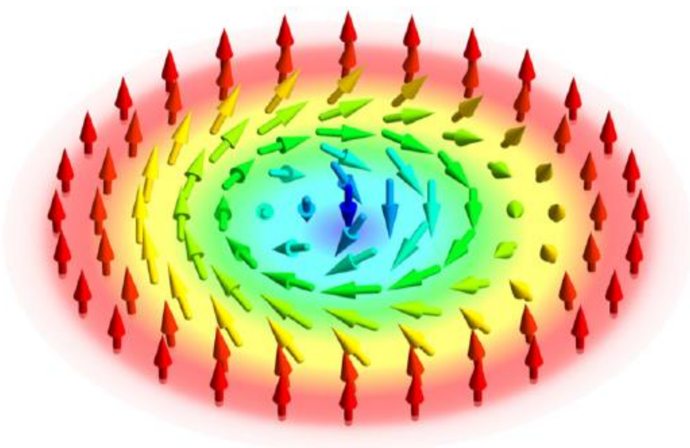




Here the **SkL** is roughly a superposition of two screw helicoids – <u>square skyrmion lattice</u>.
At zero field it corresponds to meron-antimeron lattice (half of skyrmions)

Part II

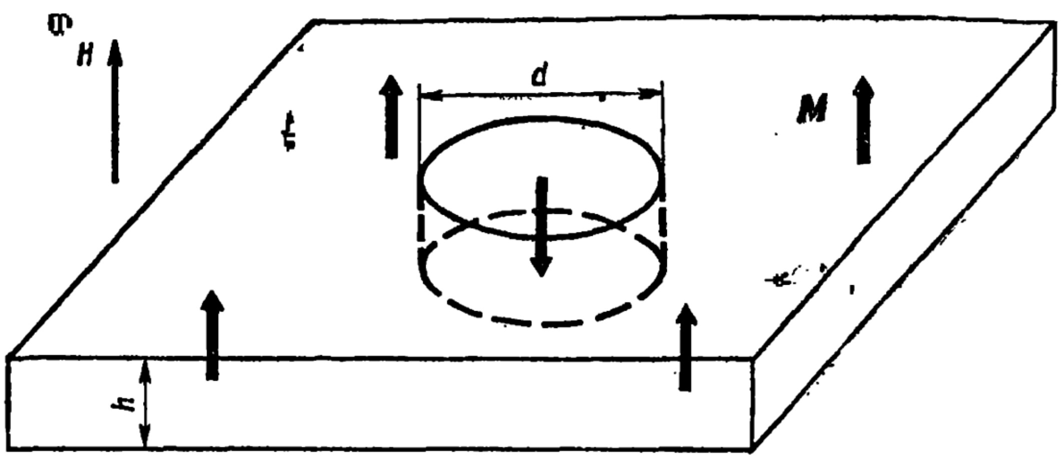
Skyrmions and Skyrmion Lattices



Bubble domains

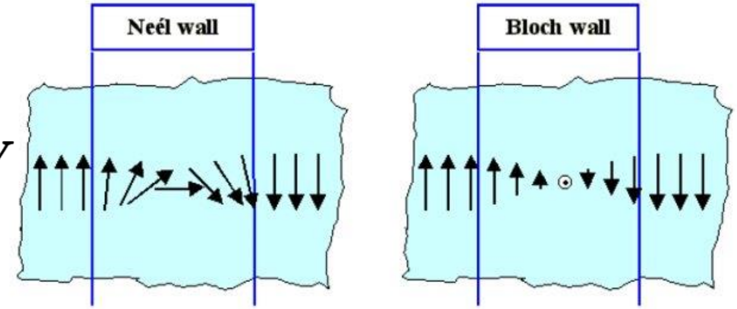
Under certain conditions cylindrical magnetic domains emerge in ferromagnetic films. Their size is of the same order with the size of usual domain wall which is about 1 μm.

Magnetic bubble memory was used in 1970s and 1980s



Domain walls in systems with DMI

Let's consider a magnet with Cnv symmetry



$$E = \int \left[\frac{\alpha}{2} (\nabla \mathbf{M})^2 - \frac{\beta}{2} M_z^2 - \mathbf{H} \cdot \mathbf{M} - \frac{1}{2} \mathbf{H}_d \cdot \mathbf{M} + L \right] dV$$

Lifshitz invariant

$$L = \gamma [M_z \partial_x M_x - M_x \partial_x M_z + M_z \partial_y M_y - M_y \partial_y M_z]$$

One can discuss Bloch and Neel domain walls. For the Bloch wall problem is equivalent to a usual easy-axis ferromagnet

$$\sigma_B = 2M^2 \sqrt{\alpha\beta}$$

Neel wall:

$$M_x = M \sin\theta,\ M_z = M\cos\theta,\ H_{dx} = -4\pi M_x,\ \beta' = \beta + 4\pi$$

$L = \gamma M^2 \theta'$ does not change equations of motion!

$\sigma_N = M^2 \left(2\sqrt{\alpha\beta'} - \pi|\gamma| \right)$ can be negative! "Vortex" structure?

Single Neel skyrmion

We parameterize the magnetization by two angles, azimuth is the same with the polar angle. Far from the center magnetization is collinear (e.g., up)

The energy functional:

$$E = 2\pi M^2 \int \rho d\rho \left\{ \frac{\alpha}{2} \left[(\theta')^2 + \frac{\sin^2\theta}{\rho^2} \right] + \gamma \left[\theta' + \frac{\sin\theta\cos\theta}{\rho} \right] - \frac{H}{M}\cos\theta - \frac{\beta}{2}\cos^2\theta \right\}$$

We subtract the energy of homogeneous state and turn to dimensional units related to the cycloid period and its energy density.

$$R = \frac{\alpha}{\gamma},\ \tilde{H} = \frac{hR^2}{M\alpha},\ \tilde{\beta} = \frac{\beta R^2}{\alpha}$$

$$E = 2\pi M^2 \alpha \int r dr \left\{ \frac{1}{2} \left[(\theta')^2 + \frac{\sin^2\theta}{r^2} \right] + \left[\theta' + \frac{\sin\theta\cos\theta}{r} \right] + \tilde{H}(1-\cos\theta) + \frac{\tilde{\beta}}{2}\sin^2\theta \right\}$$

A.N. Bogdanov, D.A. Yablonskii, *JETP* **95** 178-182 (1989)

Trial functions

One can consider functions with one scale, for example:

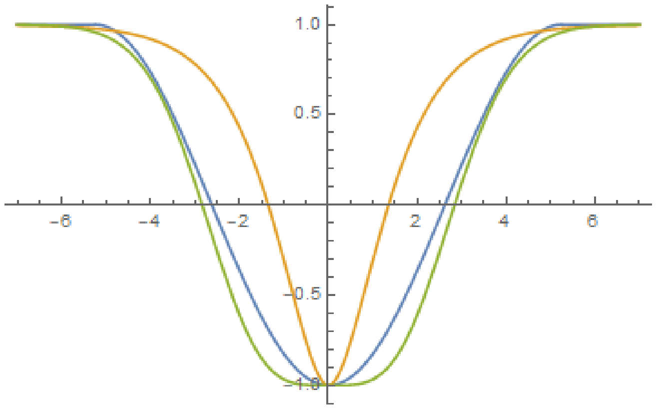
$$\theta = \pi\left(1 - \frac{r}{r_0}\right),\ \theta = \pi \exp\left(-\frac{r}{r_0}\right),\ \theta = \pi \exp\left(-\frac{r^2}{r_0^2}\right)$$

After integration one has

$$E_{EX} = c_0, \quad E_{DM} = -c_1 r_0, \quad E_Z + E_{AN} = c_2 r_0^2; \quad c_0, c_1, c_2 > 0$$

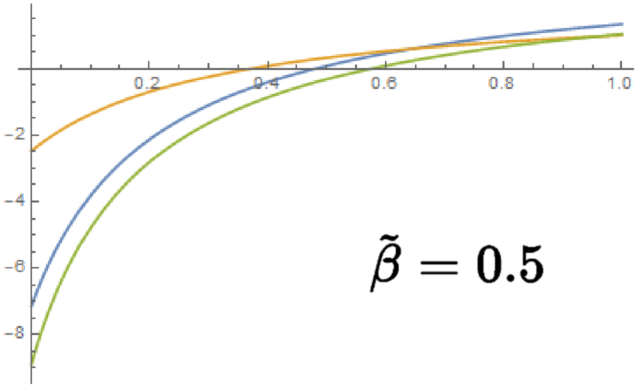
The scale parameter should be chosen to minimize the energy.

$M_z(x)$



$\tilde{H} = 0.3,\ \tilde{\beta} = 0.5$

$E(\tilde{H})$

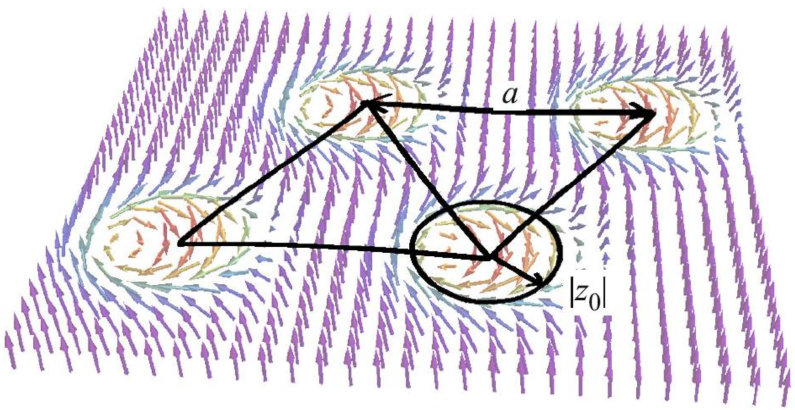


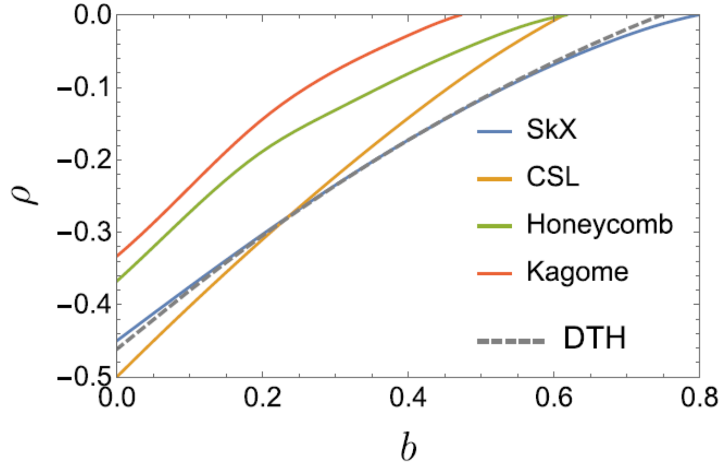
$\tilde{\beta} = 0.5$

It can be shown that the skyrmion consists of a core and exponentially decaying tail

How to construct skyrmion lattice?

1. Due to exponential tails one can take two skyrmions and calculate interaction energy: skyrmion repulsion (there is also important non-pair interaction)
2. Take some lattice and optimize the total energy per unit cell by a proper choose of the skyrmion size and lattice parameter
3. To check the stability we need to compare the energy with other possible structures, e.g., (conical) helicoids
4. Remarkably, at strong enough magnetic field one can "melt" the skyrmion crystal. Single skyrmions can be observed as metastable solitons at stronger fields.
5. The similar program can be realized for high-symmetry frustrated helimagnets with small modulation vectors

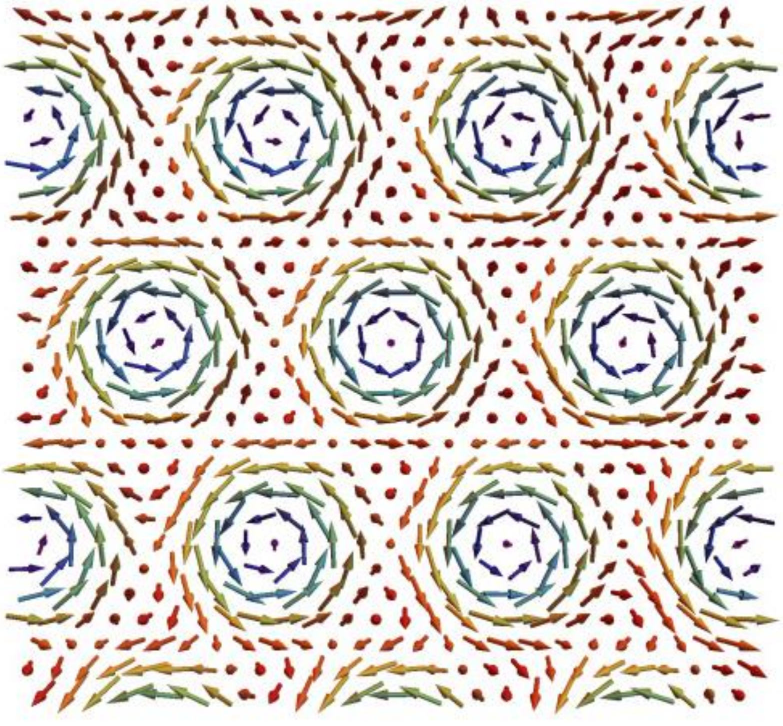




V.E. Timofeev, A.O. Sorokin, D.N. Aristov, *JETP Letters* **109** 207-212 (2019)
V.E. Timofeev, A.O. Sorokin, D.N. Aristov, *PRB* **103** 094402 (2021)
S.-Z. Lin and S. Hayami, *PRB* **93** 064430 (2016)

Part III

High-T simple mean-field approach for **SkL**



Theoretical concepts

The common wisdom is that everything is quite **complicated** theoretically:

- In **B20** helimagnets to describe the A-phase stability thermal fluctuations were taken into account
- At low temperatures spin modulus saturation is demanded, so multiple higher-order harmonics arise
- In the external magnetic field, one needs to fight with conical helices, so additional complicated anisotropies are usually taken into account

The present study:

1. In two mentioned above experiments on frustrated magnets the magnetic ions are in $L=0$ spherically-symmetrical state. So the **magnetodipolar interaction** should be of prime importance among other possible anisotropies
2. It is well-known to be responsible for complicated sequences of phase transitions and phase diagrams. Moreover, it is always present in real systems
3. We show that dipolar forces and frustrated exchange are sufficient to stabilize **multiple-Q** magnetic structures (at least at high temperatures)
4. Magnetodipolar interaction lifts degeneracy between Neel and Bloch skyrmions.
5. The proposed a framework which allows rather simple analytical treatment, where SkL can be described and "touched by hands"

Dipolar forces in tetragonal systems

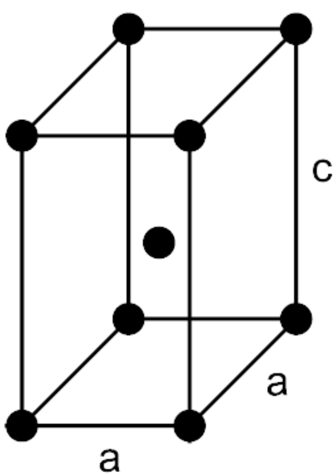
In our model we have frustrated exchange, Zeeman term, and dipolar forces

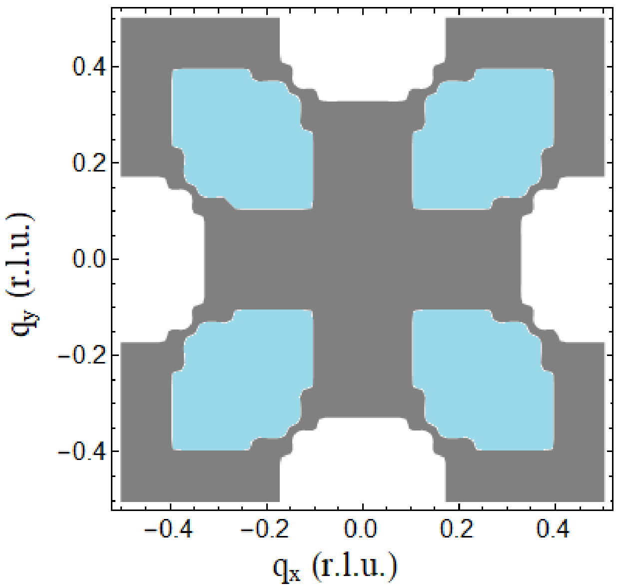
In reciprocal space

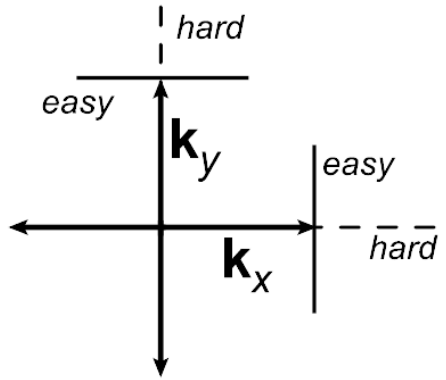
$$\mathcal{H}_d = \frac{1}{2}\sum_{\mathbf{q}} \mathcal{D}^{\alpha\beta}_{\mathbf{q}} S^{\alpha}_{\mathbf{q}} S^{\beta}_{-\mathbf{q}}$$ - momentum-dependent biaxial anisotropy

Its strength is governed by $\omega_0 = 4\pi\frac{(g\mu_B)^2}{v_0}$, which is of the order of $0.1 \div 1$K.

In tetragonal lattice, axis **c** is the easy one in blue regions and middle in gray region







Screw helicoids are favorable for modulation vectors from the most of the Brillouin zone

Mean-field approach

$\mathbf{S}_i$ - spin averaged over thermal fluctuations

$$\mathcal{F} = -\sum_{\mathbf{q}} \mathcal{H}_{\mathbf{q}}^{\alpha\beta} s_{\mathbf{q}}^{\alpha} s_{-\mathbf{q}}^{\beta} - \sqrt{N}\mathbf{h}\cdot\mathbf{s}_0 + AT\sum_i s_i^2 + BT_c\sum_i s_i^4$$

Tensor $\mathcal{H}_{\mathbf{q}}^{\alpha\beta}$ has three eigenvalues $\lambda_1(\mathbf{q}) \geqslant \lambda_2(\mathbf{q}) \geqslant \lambda_3(\mathbf{q})$ and three eigenvectors.

Ordering temperature $T_c = \lambda_1(\mathbf{k}_x)/A$ corresponds to largest eigenvalue (approximately maximum of exchange interaction Fourier transform, whereas dipolar tensor determines spin polarization). Below we assume that λ_1 has four equivalent maxima (due to tetragonal symmetry)

Small S expansion parameters are given by [R. Gekht, *JETP* **60**, 1210 (1984)]

$$A = \frac{3}{2S(S+1)},$$

$$B = \frac{9[(2S+1)^4 - 1]}{20(2S)^4(S+1)^4}$$

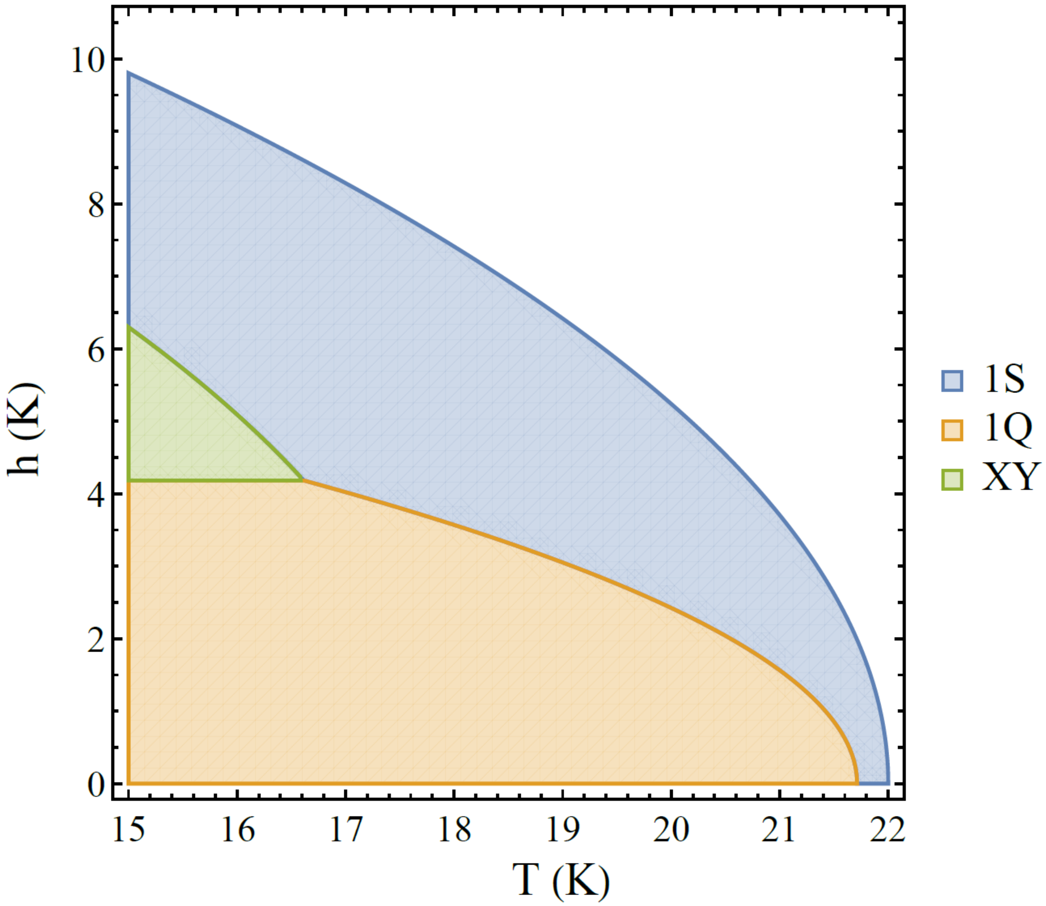
For $S = 7/2$ one has $A \approx 0.095$ and $B \approx 0.002$.

We begin analysis with the case where easy axes are in-plane, and the middle one is along **c**, which is relevant to $GdRu_2Si_2$ where two modulation vectors along $\hat{x}$ and $\hat{y}$ are equal to 0.22 r.l.u.

Standard phase diagram for high temperatures

Here:

- Middle axis and magnetic field are along **c**
- 1*S* phase includes transverse modulated spin component and uniform magnetization
- 1*Q* phase is helicoid with spins rotating in plane, which includes easy and middle axes
- XY phase is a conical helicoid, spins rotate in plane, which includes middle and hard axes



<u>**Multiple-*Q*** and commensurate structures are not considered here</u>

Zero field. 1*S* vs. 2*S*

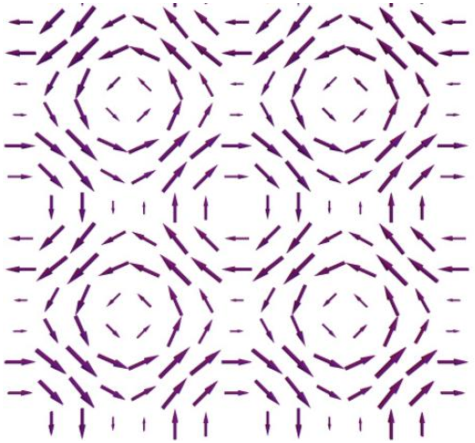
Simple sinusoidal spin density wave (SDW, 1*S*)

$$\mathbf{s}_i = s\mathbf{e}_y \cos \mathbf{k}_x \mathbf{R}_i$$

$$\frac{\mathcal{F}}{N} = -\frac{s^2\lambda_1}{2} + \frac{s^2 AT}{2} + \frac{3s^4 BT_c}{8}$$

$$\frac{\mathcal{F}_{1S}}{N} = -\frac{(\lambda_1 - AT)^2}{6BT_c}$$

Double SDW (vortex-like structure, 2*S*)



$$\mathbf{s}_i = s(\mathbf{e}_y \cos \mathbf{k}_x \mathbf{R}_i + \mathbf{e}_x \cos \mathbf{k}_y \mathbf{R}_i)$$

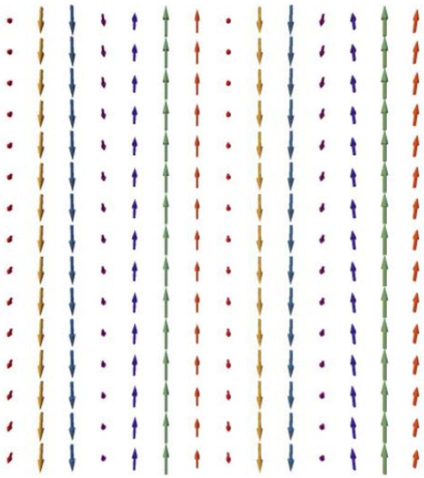
$$\frac{\mathcal{F}}{N} = -s^2\lambda_1 + s^2 AT + \frac{5s^4 BT_c}{4}$$

$$\frac{\mathcal{F}_{2S}}{N} = -\frac{(\lambda_1 - AT)^2}{5BT_c}$$

Modulated in two perpendicular directions coplanar 2*S* structure has lower free energy, than simple SDW! T_c corresponds to continuous transition between PM and 2*S*

Zero field. 1Q vs. 2Q

Elliptical screw helicoid (1Q)



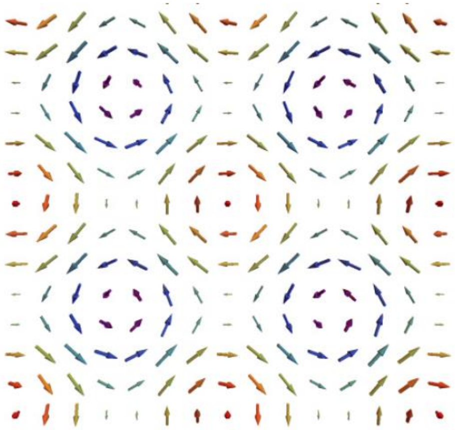
$$\mathbf{s}_i = s_1 \mathbf{e}_y \cos \mathbf{k}_x \mathbf{R}_i + s_2 \mathbf{e}_z \sin \mathbf{k}_x \mathbf{R}_i$$

$$\frac{\mathcal{F}_{1Q}}{N} = -\frac{4(\lambda_1 - AT)^2 - 4(\lambda_1 - AT)(\lambda_1 - \lambda_2) + 3(\lambda_1 - \lambda_2)^2}{16BT_c}$$

Emerges from 1S at

$$T < T_{1Q} = T_c - 3(\lambda_1 - \lambda_2)/2A$$

Double-Q elliptical phase (2Q)



$$\mathbf{s}_i = s_1(\mathbf{e}_y \cos \mathbf{k}_x \mathbf{R}_i + \mathbf{e}_x \cos \mathbf{k}_y \mathbf{R}_i) + s_2 \mathbf{e}_z(\sin \mathbf{k}_x \mathbf{R}_i + \sin \mathbf{k}_y \mathbf{R}_i).$$

$$\frac{\mathcal{F}_{2Q}}{N} = -\frac{8(\lambda_1 - AT)^2 - 4(\lambda_1 - AT)(\lambda_1 - \lambda_2) + 5(\lambda_1 - \lambda_2)^2}{36BT_c}$$

Emerges from 2S at

$$T < T_{2Q} = T_c - 5(\lambda_1 - \lambda_2)/2A$$

2Q structure consists of alternating merons and antimerons (charge $\pm\, ^1/_2$), however the total topological charge is zero

Sequence of phase transitions at zero field

We introduce parameters $t = \lambda_1 - AT$, $\Lambda = \lambda_1 - \lambda_2$, and compare the free energies:

$$f_{2S} = -\frac{t^2}{5}, \quad \frac{5\Lambda}{2} \geqslant t > 0,$$

$$f_{1Q} = -\frac{4t^2 - 4\Lambda t + 3\Lambda^2}{16}, \quad t > \frac{3\Lambda}{2},$$

$$f_{2Q} = -\frac{8t^2 - 4\Lambda t + 5\Lambda^2}{36}, \quad t > \frac{5\Lambda}{2}.$$

As a result, one has the following sequence of phase transitions

$$\mathrm{PM} \leftrightarrow 2S \leftrightarrow 2Q \leftrightarrow 1Q$$

The temperature of the third transition (first order one) reads

$$t_S = \frac{5 + 3\sqrt{2}}{2}\Lambda \approx 4.6\Lambda$$

So, $2Q$ phase is <u>intermediate at zero field</u>

Nonzero magnetic fields

Taking into account nonzero field along the **c** axis is rather easy. Assuming that the system is far from ferromagnetic instability one has Curie-Weiss law, where susceptibility can be taken as a constant

$$\delta \mathbf{s}_i = m\hat{c},$$

$$m = \chi(T)h = \frac{h}{2(AT - \lambda_0)} \approx \chi h, \qquad \lambda_0 = (J_0 - \omega_0 \mathcal{N}_{zz})/2$$

$$\chi \equiv \chi(T_c)$$

Nonlinear terms $\propto Bm^2$ can be taken into account by proper renormalization of t and Λ

$$t \to t' = t - 2BT_c(\chi h)^2, \; \Lambda' = \Lambda + 4BT_c(\chi h)^2$$

Conical XY phase with spins rotating in the ab-plane should be also considered

$$\mathbf{s}_i = s_1 \mathbf{e}_y \cos \mathbf{k}_x \mathbf{R}_i + s_2 \mathbf{e}_x \sin \mathbf{k}_x \mathbf{R}_i + m\mathbf{e}_z$$

$$f_{XY} = -\frac{4t^2 - 4\Lambda'' t + 3\Lambda''^2}{16}, \quad t > \frac{3\Lambda''}{2}. \quad \Lambda'' = \lambda_1 - \lambda_3 > \Lambda$$

In the external field Λ'' stays intact. Finally, in the present framework one can analytically determine the phase boundaries and the topology of the corresponding phase diagram

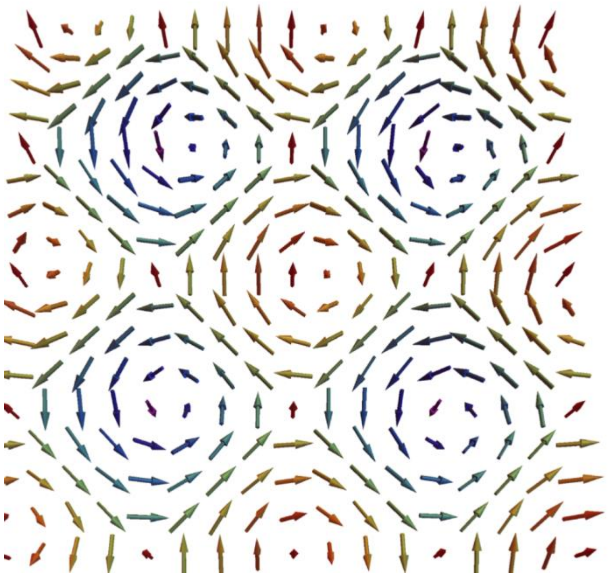
2Q phase topology

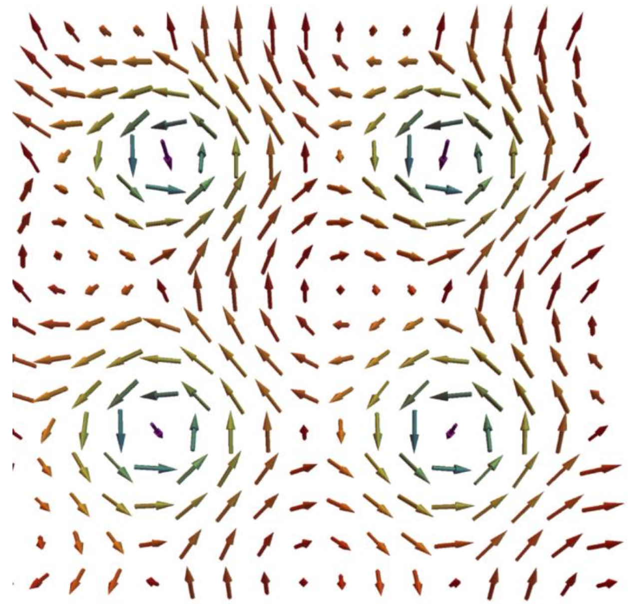
2Q structure can be either topologically trivial or nontrivial. Taking for definiteness particular spin ordering (chiralities and phases of two helicoids can be chosen "by hands")

$$\mathbf{s}(x,y)=\begin{pmatrix} s_1\sin ky \\ -s_1\sin kx \\ s_2[\cos kx+\cos ky]+m \end{pmatrix}$$

one can see that at $m=0$ $\mathbf{s}(x,y)=-\mathbf{s}(x\pm\pi/k,y\pm\pi/k)$ and $\langle n_{sk}\rangle=0$

Even at infinitesimal h at points with coordinates $(\pi/k,0),(0,\pi/k)$ additional merons emerge and $n_{sk}=-1$ per magnetic unit cell. At moderate fields the structure can be considered as a square SkL. However, at yet <u>larger fields</u> when $m^2\geq 4s_2^2$ the structure becomes <u>topologically trivial</u> ($\hat{c}$-component of all spins is along the field).





$GdRu_2Si_2$ parameters and first type of phase diagram

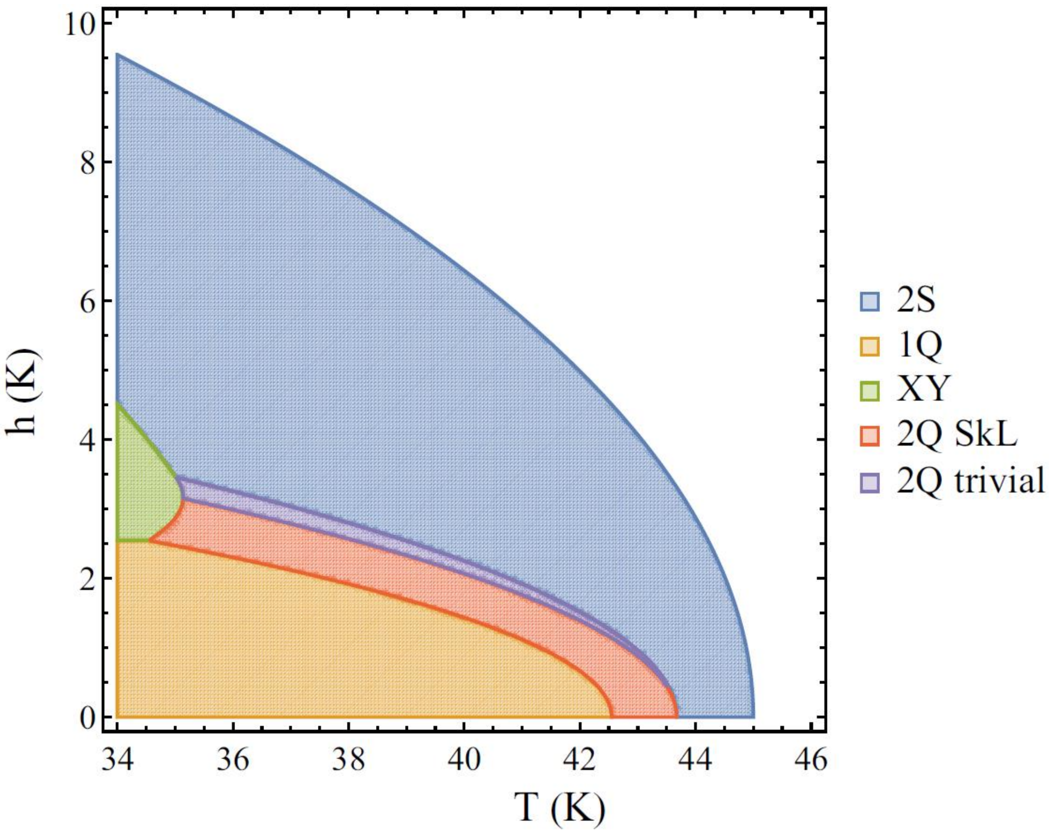
Dipolar tensor for $\mathbf{k}_x$ and $\mathbf{k}_y$ depends only on lattice parameters; for demagnetization tensor component we assume cylindrical shape of the sample. Relevant exchange interactions can be calculated using T_c (determining $J_{\mathbf{k}}$) and the saturation field at zero temperature $H_{sat} \approx S(J_{\mathbf{k}} - J_{\mathbf{0}})$. As a result we have (all values are in kelvins)

$$\lambda_1 \approx 4.3, \quad J_{\mathbf{0}} \approx 4.6,$$
$$\lambda_1 - \lambda_2 \approx 0.05, \quad \lambda_1 - \lambda_3 \approx 0.20$$

Note, that at temperatures where conical phase is present in figure, average order parameter is not small. The question "whether this phase really appears or not?" requires additional research.

Variation of model parameters (upon restrictions $\Lambda > \Lambda'' > 0$) does not change the PD topology

O.I. Utesov, *PRB* **103**, 064414 (2021)

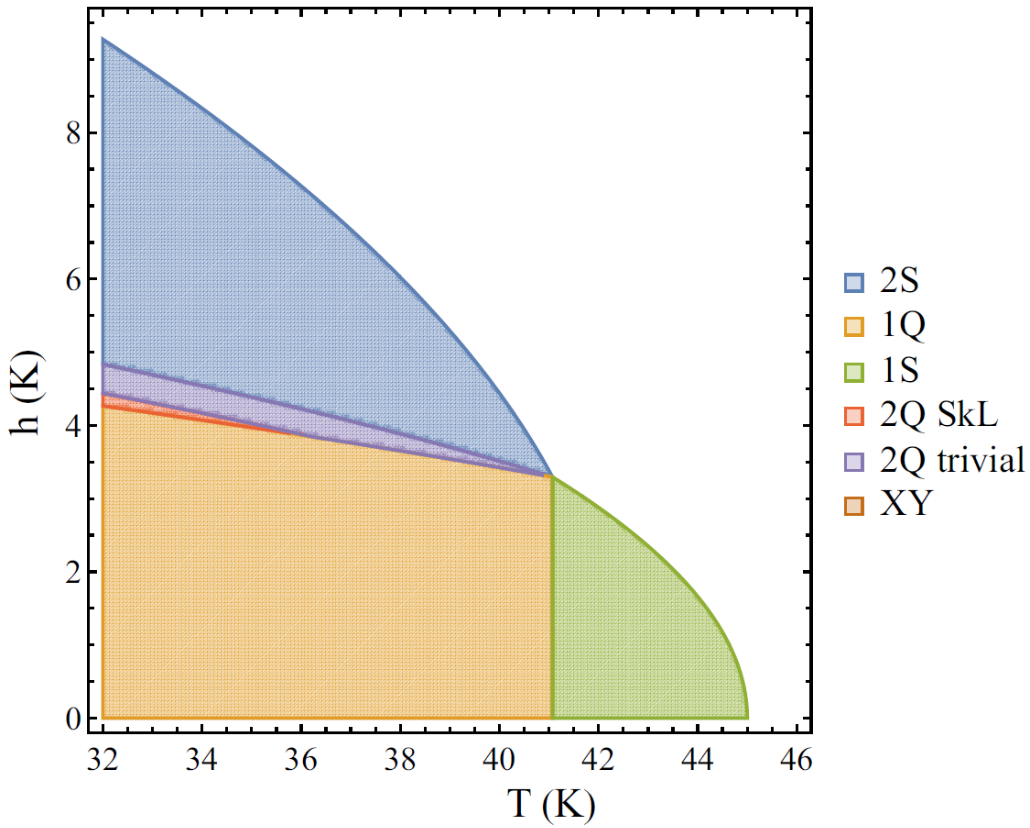


Another type of phase diagram: easy axis **c**

Tetragonal axis **c** can be the easy axis of the system, e.g. for modulation vectors $||(1,1,0)$ and $(1,-1,0)$. Also by adding easy-axis anisotropy to the previous case one can swap easy direction to **c**

<u>Main properties</u>:

- simple SDW is stable at small h
- <u>polycritical</u> point (5 phases in equilibrium)
- vortex-like double-fan 2*S* phase is the pre-saturation one. It can be also proved for T=0 using method from O. I. Utesov and A. V. Syromyatnikov, *JMMM* **527**, 167732 (2021)
- Conical XY phase appears only in the region out of the approach validity
- 2*Q* SkL structure is stabilized as a small wedge in the phase diagram
- These type of PD reproduces main experimental findings for $GdRu_2Si_2$

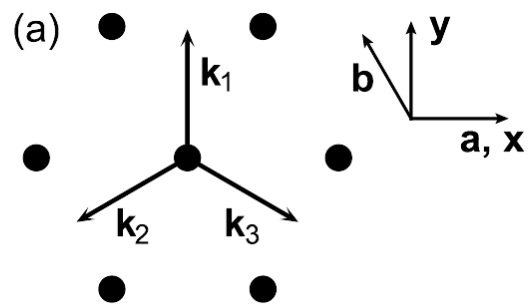


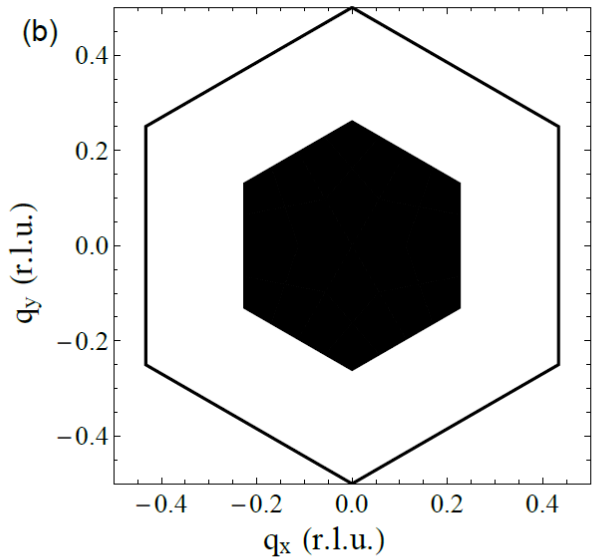
Intermediate remarks

- ✓ It is shown that magnetodipolar interaction, which is always present in real magnets, can stabilize nanometer-sized skyrmions in frustrated tetragonal antiferromagnets
- ✓ Two different types of phase diagrams are obtained. Analytical expressions for phase boundaries are derived. The theory can be used for corresponding experimental data interpretation
- ✓ Certain additional anisotropic interactions (e.g., compass anisotropy or single-ion anisotropy) can be easily included into the proposed scheme
- ✓ Complementary theory for low temperatures is a challenging problem both analytically (many additional harmonics) and numerically (long-range nature of dipolar forces)
- ✓ Accounting for thermal fluctuations (beyond the present mean-field approach) is also important issue. Evidently, when the ordered spin on each site is not close to saturated value S, the fluctuations can locally destroy topological order, thus making $|n_{sk}| < 1$ per magnetic unit cell

Hexagonal systems

c axis is the middle one for in-plane modulation vectors inside black region, an easy one outside. Dipolar forces favors screw helicoids





Stabilization of the 3Q phase here stems from specific term in the free energy, which favors combination of three right (or left) helicoids

$$\mathcal{F}_{3Q} = -\frac{t}{2}s^2 - \frac{t-\Lambda}{2}p^2 - hm - (t-\Lambda_0)m^2 + b\left[m^4 + m^2\left(s^2+3p^2\right) + \frac{9s^4+10s^2p^2+15p^4}{24} - \frac{mp\left(2p^2+s^2\right)}{\sqrt{3}}\right]$$

(s – in-plane helicoid component, p – out-of-plane) At nonzero magnetic fields this term makes 1S and 3S phases unstable towards transition to 3Q phase for in-plane easy axes.

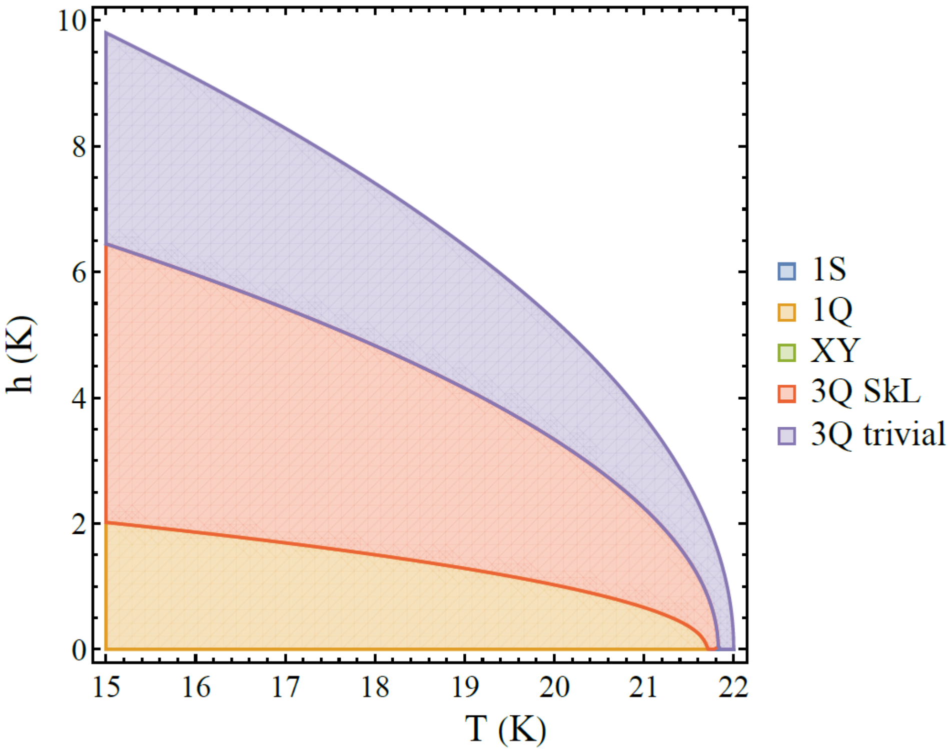
Order parameters s, p can be found from the cubic equation using Cardano's formula

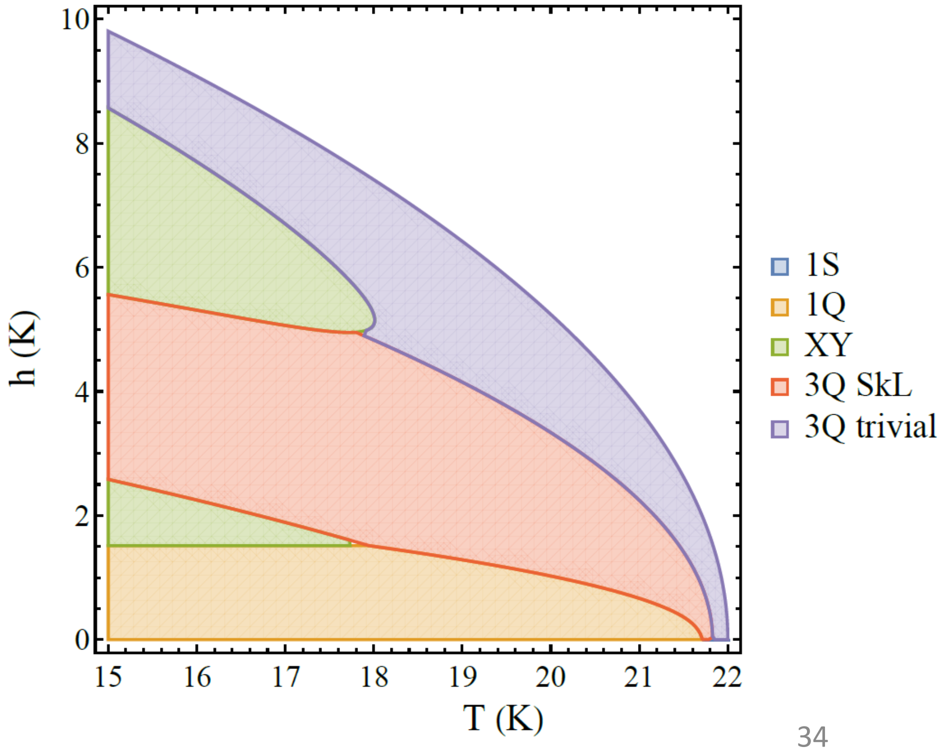
O.I. Utesov, *PRB* **105**, 054435 (2022)

Phase diagram for in-plane easy axis

Parameters estimated for Gd_2PdSi_3 are used here.

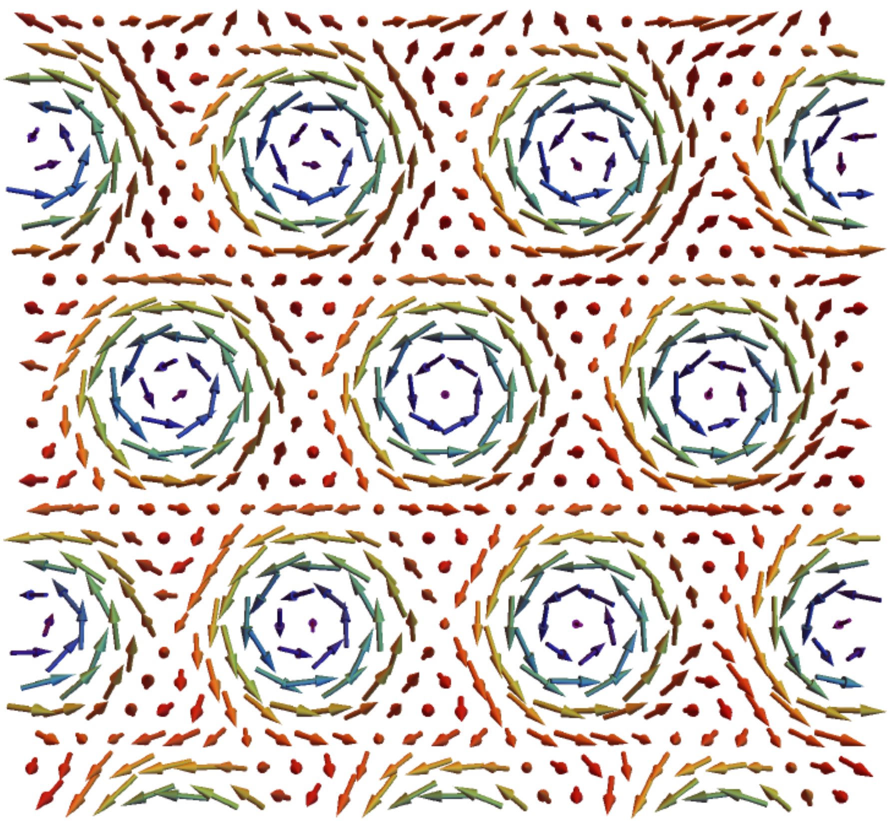
- obtained phase diagram is very similar with the one observed experimentally
- conical XY phase does not appear at all (even in low-temperature region)
- making parameter $\lambda_1 - \lambda_3$ to be smaller by hands (0.05K) we observe phase diagram shown in the right figure

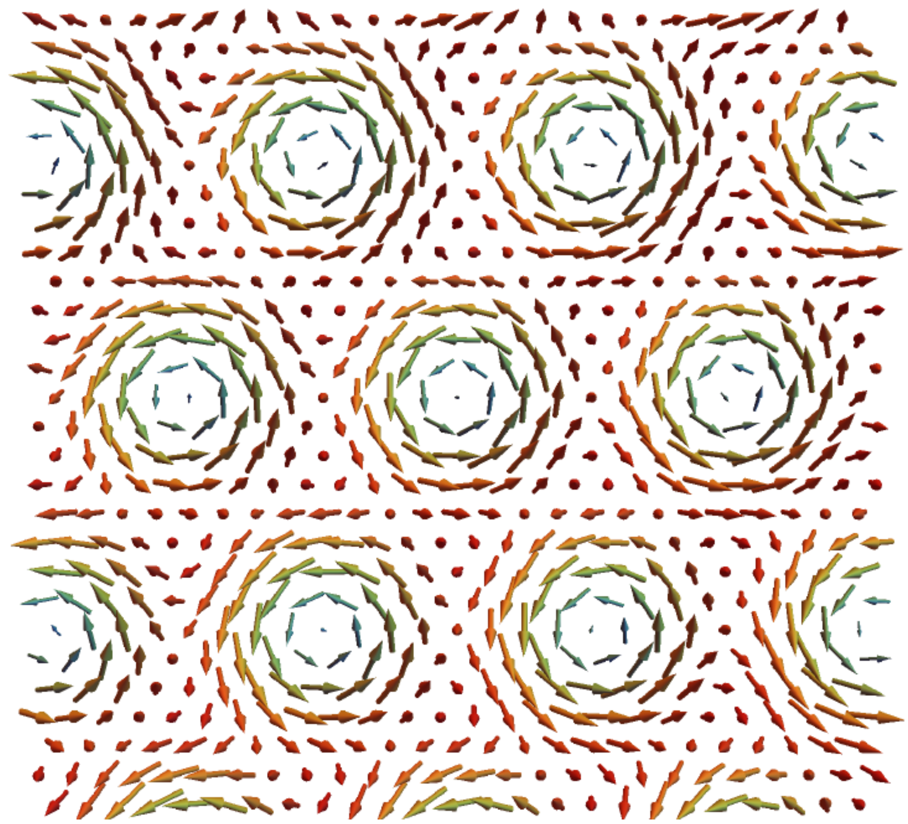




3*Q* SkL and 3*Q* trivial

Under magnetic field increase <u>Bloch-type skyrmions</u> transform into topologically trivial "<u>vortexes</u>" (however, noncoplanar)

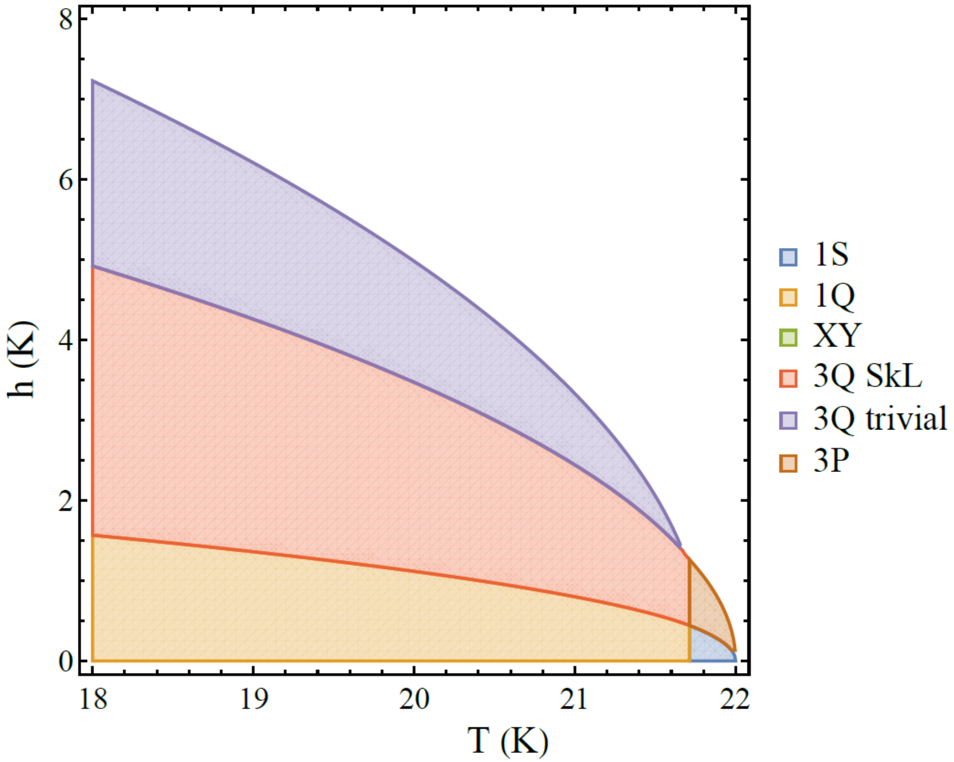


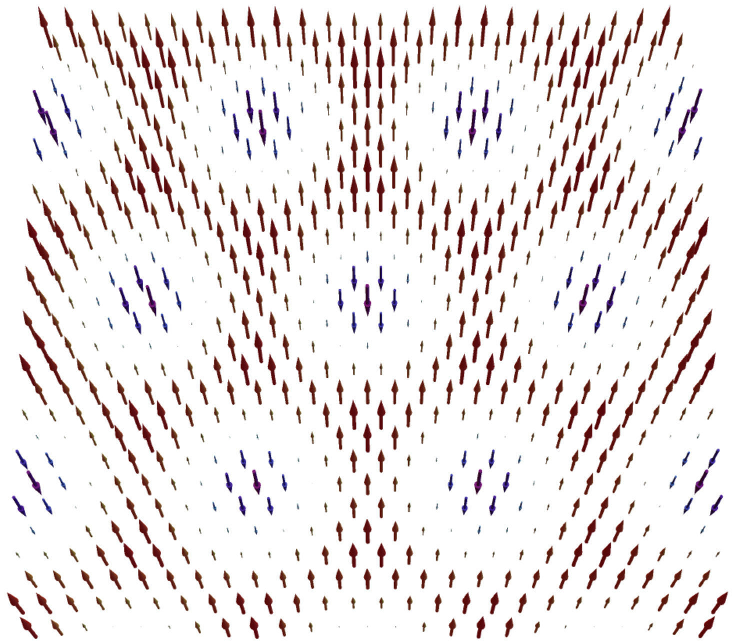


Phase diagram for out-of-plane easy axis

The same parameters were used, except for modulation vector magnitude.

- triple-modulated collinear 3*P* phase appears at high temperatures
- magnetic field-induced phase transitions between 3*P* and PM as well as 3*Q* SkL and PM are discontinuous first order ones
- there is first order magnetic field-induced phase transition between 3*Q* SkL and 3*Q* at high temperatures, which becomes smooth crossover at lower temperatures

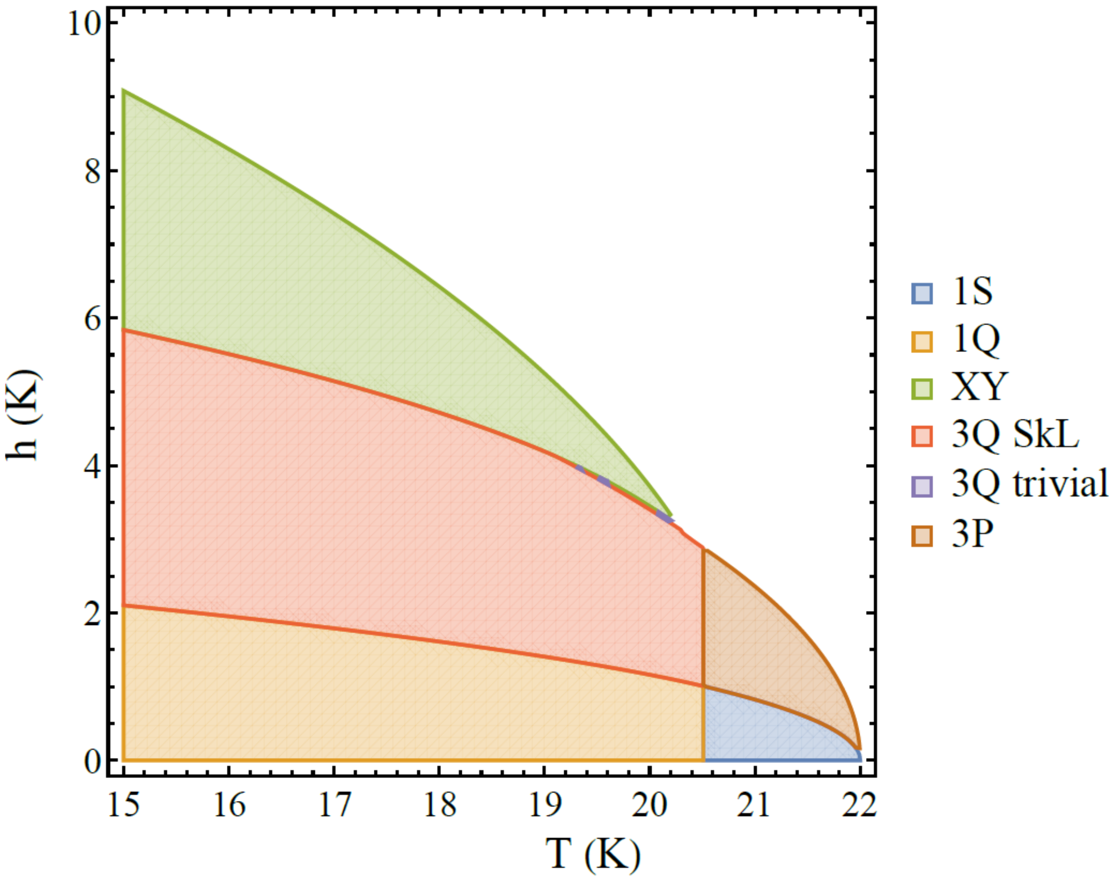




Phase diagram for easy-axis anisotropy

For illustration purposes we show phase diagram in the presence of conventional single-ion easy-axis anisotropy without dipolar forces (in opposite case of easy-plane anisotropy the whole phase diagram is a simple combination of XY and PM phases)

Note, that due to the symmetry of ab-plane, in this case pre-saturation phase is the standard conical spin structure. Nevertheless, the 3Q SkL phase dominates in the intermediate fields region



Conclusions

- ✓ We show that frustrated exchange and magnetodipolar interaction are sufficient to stabilize SkL with nanometer-sized skyrmions in high-symmetry lattices
- ✓ Simple analytical mean-field approach is developed
- ✓ Dipolar forces-induced anisotropy leads to effective combining of single-modulated spin structures into multiple-Q ones
- ✓ Several types of high-temperature phase diagrams with square and hexagonal SkL are obtained
- ✓ Good correspondence with phase diagrams of Gd_2PdSi_3 and $GdRu_2Si_2$, where magnetic ions are in spherically-symmetrical state with $L=0$, can be reported
- ✓ Additional anisotropic interactions can be included into consideration in a simple way
- ✓ Obtained phase diagrams can be used for experimental data interpretation

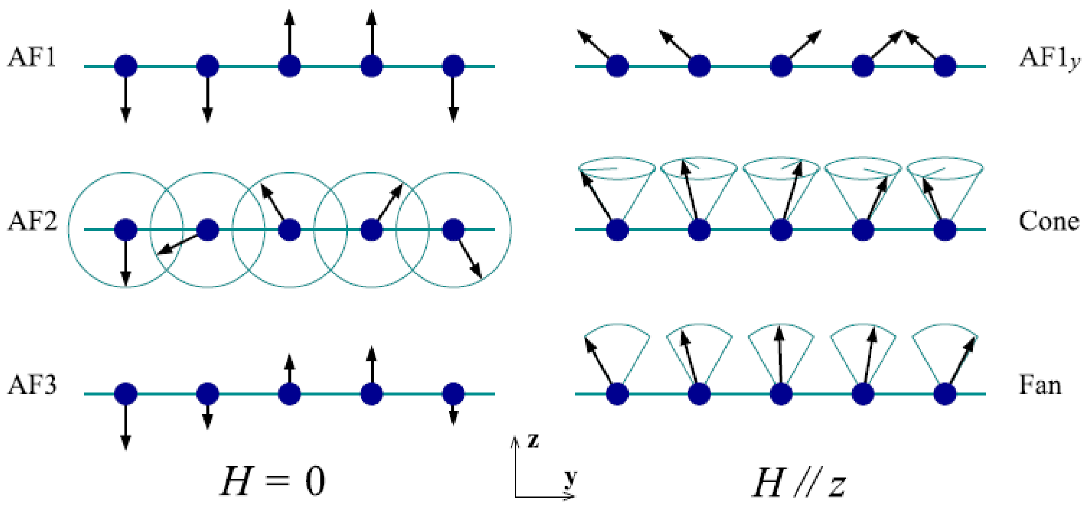
O.I. Utesov, *PRB* **103**, 064414 (2021)
O.I. Utesov, *PRB* **105**, 054435 (2022)

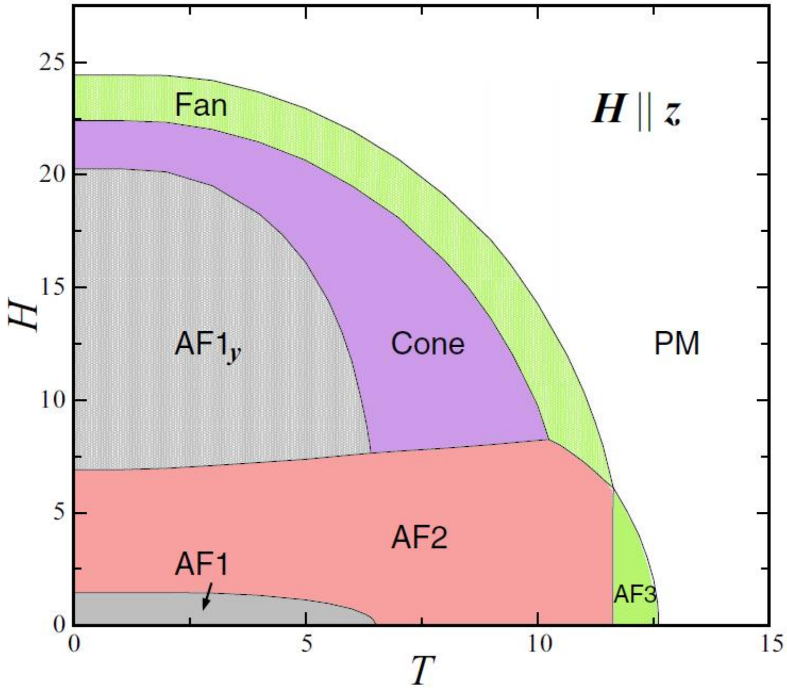
Thank you for attention!

Заголовок слайда

Example of phase diagram: $MnWO_4$

Numerical results for anisotropic next-nearest-neighbors Heisenberg model



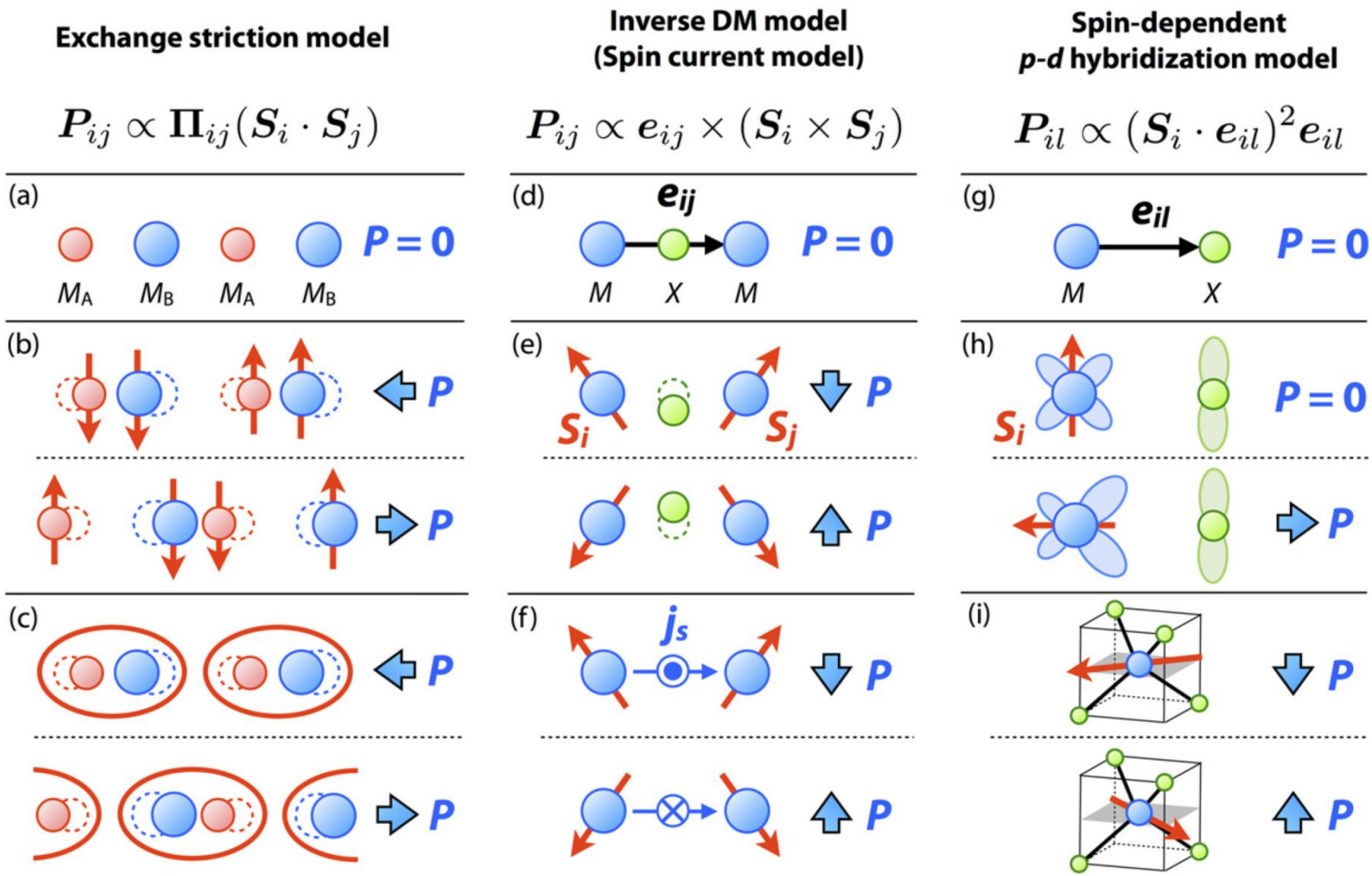


Analytical theory for low-temperatures, which is based on smallness of the biaxial anisotropy (or dipolar forces):

*O.I. Utesov and A. V. Syromyatnikov, Phys. Rev. B **100**, 054439 (2019)*

*O.I. Utesov, A.V. Syromyatnikov, J. Magn. Magn. Mater. **527**, 167732 (2021)*

Multiferroics of spin origin



Yoshinori Tokura, Shinichiro Seki and Naoto Nagaosa, Rep. Prog. Phys. ***77*** *(2014) 076501*

Frustration → <u>noncollinear</u> spin ordering