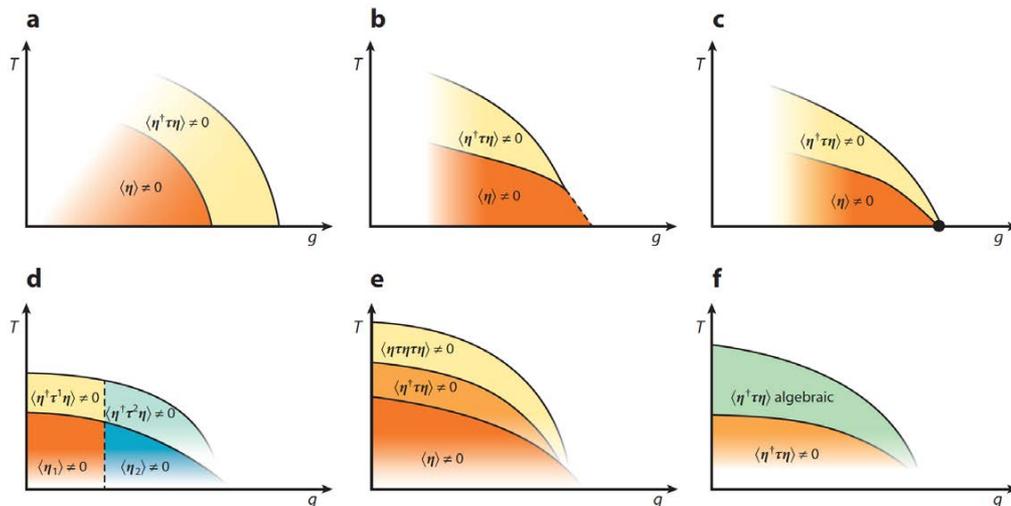


Intertwined vestigial order in quantum materials: nematicity and beyond

Peter P. Orth (Iowa State University)

Condensed Matter Seminar, LANL, May 20, 2019



Reference:

R. M. Fernandes, PPO, J. Schmalian
Annu. Rev. Cond. Mat. **10**,133 (2019).

Collaborators



R. M. Fernandes
(Minnesota)



M. H. Christensen
(Minnesota)



P. Chandra
(Rutgers)



P. Coleman
(Rutgers)



J. Schmalian
(Karlsruhe)



B. Jeevanesan
(Munich)

Experimental collaborators:



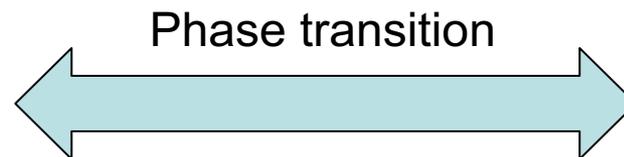
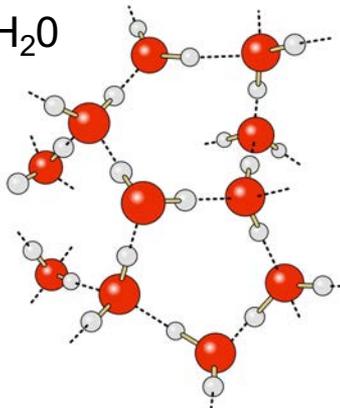
P. C. Canfield (Iowa)
& his group

States of matter: symmetry, order and topology

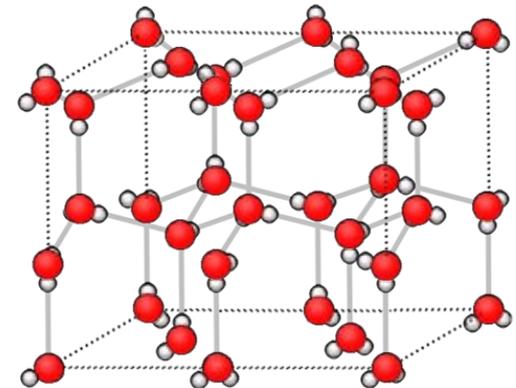
- Condensed matter physics investigates **states of matter = phases**
 - Distinguish states by **symmetry**: Landau paradigm
 - Distinguish states by topology



Water: H_2O



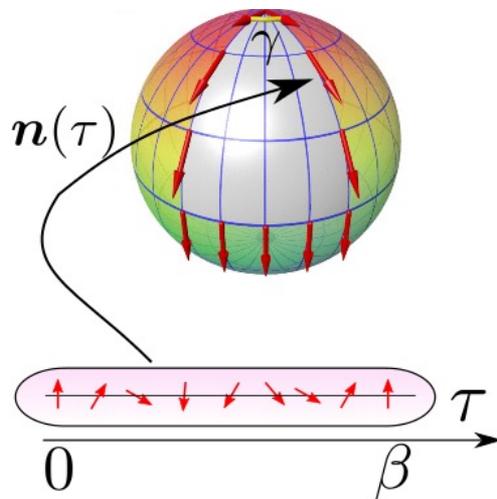
Phase transition
Breaking of continuous translational symmetry



States of matter: symmetry, order and topology

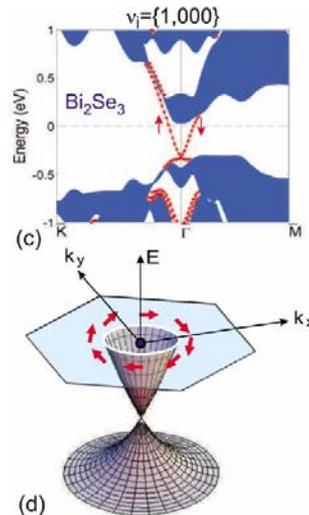
- Condensed matter physics investigates **states of matter = phases**
 - Distinguish states by **symmetry**: Landau paradigm
 - Distinguish states by **topology**: Topological properties of electronic wavefunction

Geometric Berry phase

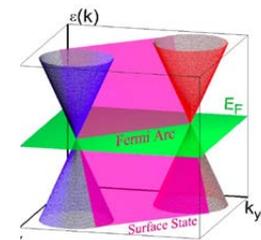
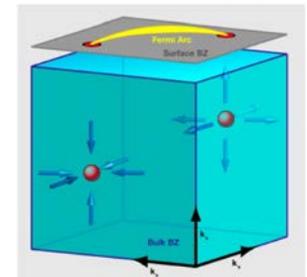


Topological insulators and metals

TI
 Bi_2Se_3



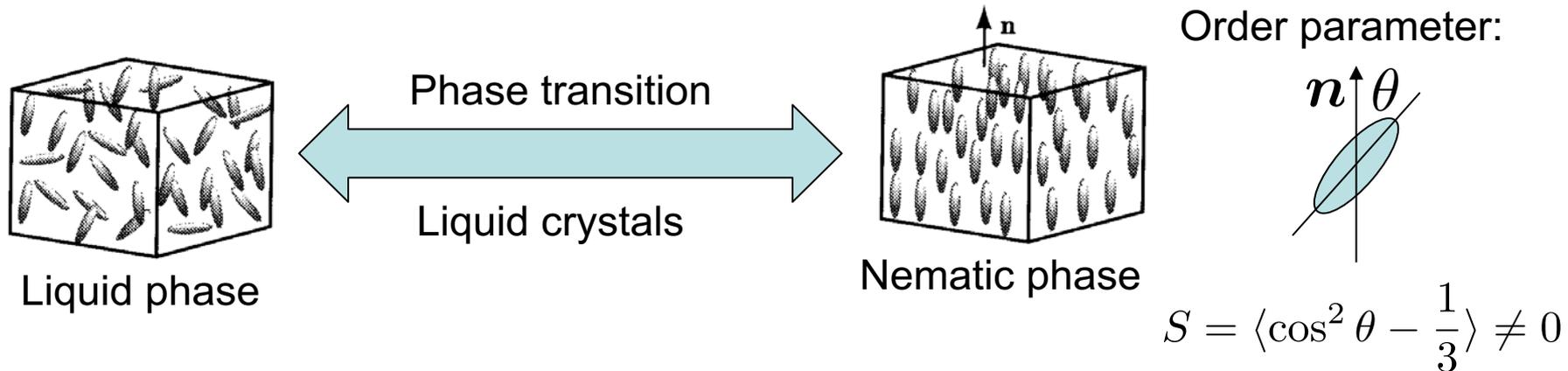
Weyl SM



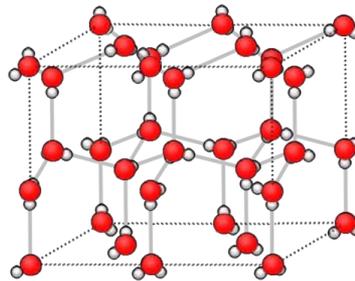
[1] M. Z. Hasan, C. L. Kane, RMP **82** 3045 (2010); N. P. Armitage *et al.*, arXiv:1705:01111 (2017).

States of matter: symmetry and order

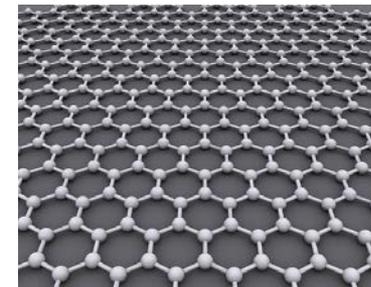
- Condensed matter physics investigates **states of matter = phases**
 - Liquids → Solids: translational symmetry breaking by crystalline order
 - Liquids → Nematics, Smectics: rotational symmetry breaking



- Solids break both continuous translational and rotational symmetries:
 - Discrete symmetries remain: 230 space groups, 32 point groups (in 3D)
 - Rigidity to shear
 - Goldstone modes
 - Quasi-crystals



Water ice: 3D crystal



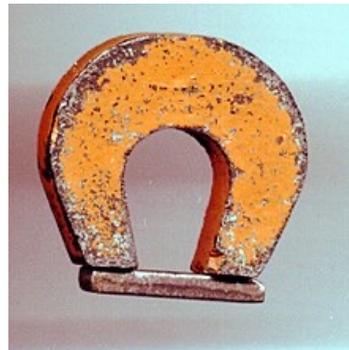
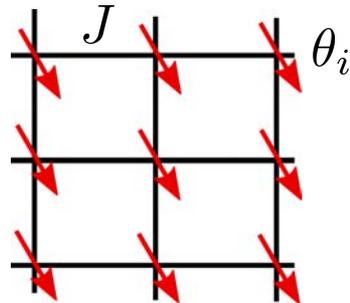
Graphene: 2D crystal

[1] Wikipedia; [2] P. M. Chaikin, T. C. Lubensky
 "Principles of Condensed Matter Physics"

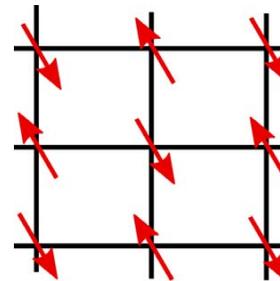
States of matter: symmetry and order

- Condensed matter physics investigates **states of matter = phases**
 - Spatial symmetry-breaking: crystals, amorphous solids, nematics
 - Internal symmetry-breaking:
 - Spin space $SU(2)$: magnetic order

Ferromagnet



Antiferromagnet



Chromium

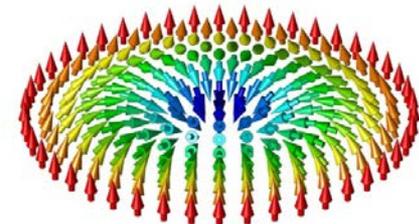


Order parameters:

$$\text{FM Magnetization: } \langle \mathbf{S} \rangle = \frac{1}{N} \sum_{i=1}^N \mathbf{S}_i$$

$$\text{AFM Magnetization: } \langle \mathbf{S} \rangle_{\mathbf{Q}=(\pi,\pi)} = \frac{1}{N} \sum_{i=1}^N e^{i\mathbf{Q} \cdot \mathbf{r}_i} \mathbf{S}_i$$

Skyrmion spin structure

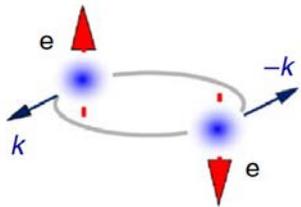


[1] Wikipedia;

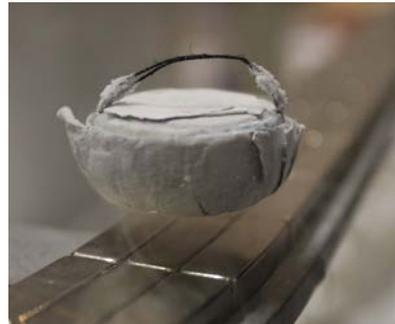
States of matter: symmetry and order

- Condensed matter physics investigates **states of matter = phases**
 - Spatial symmetry-breaking: crystals, amorphous solids, nematics
 - Internal symmetry-breaking:
 - Spin space $SU(2)$: magnetic order
 - Particle conservation global $U(1)$: superconductivity

Superconductivity



Cooper pair

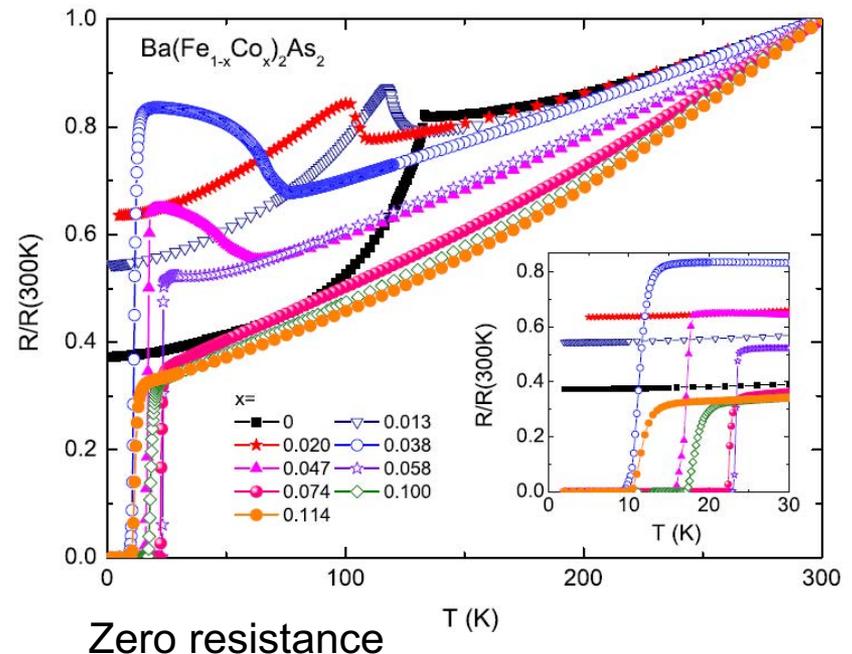


Meissner effect

Order parameter

$$\Delta = -V_0 \sum_{\mathbf{k}} \langle c_{-\mathbf{k},\downarrow} c_{\mathbf{k},\uparrow} \rangle$$

Superconducting gap function (s-wave singlet pairing state)



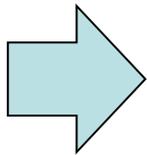
[1] Wikipedia; [2] N. Ni *et al.*, PRB **78**, 214515 (2008).

States of matter: symmetry and order

- Condensed matter physics investigates states of matter = phases
 - Spatial symmetry-breaking: crystals, amorphous solids, nematics
 - Internal symmetry-breaking: magnets, superconductors

In all examples discussed so far:

Order occurs in elementary degrees of freedom: charge, spin.



Order can also occur in composite objects such as higher order correlation functions (of charge and spin):

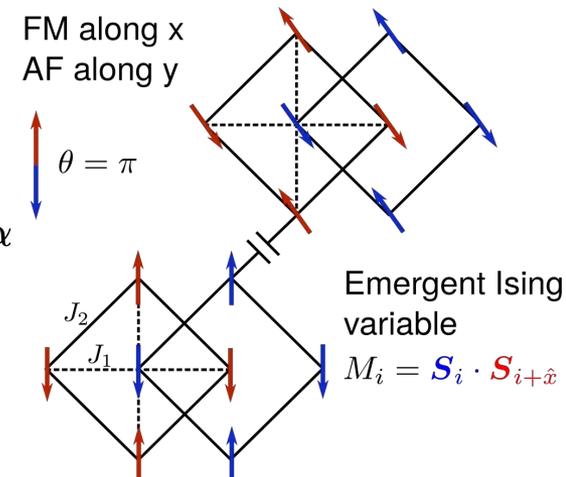
Composite order

$$\langle \eta_\alpha^* \eta_\beta \rangle \neq 0$$

- Composite order then relative spin order
- But not all combinations break a symmetry

For example, primary magnetic order

$$\eta_\alpha = (\langle \mathbf{S}_{Q_1} \rangle, \langle \mathbf{S}_{Q_2} \rangle)_\alpha$$

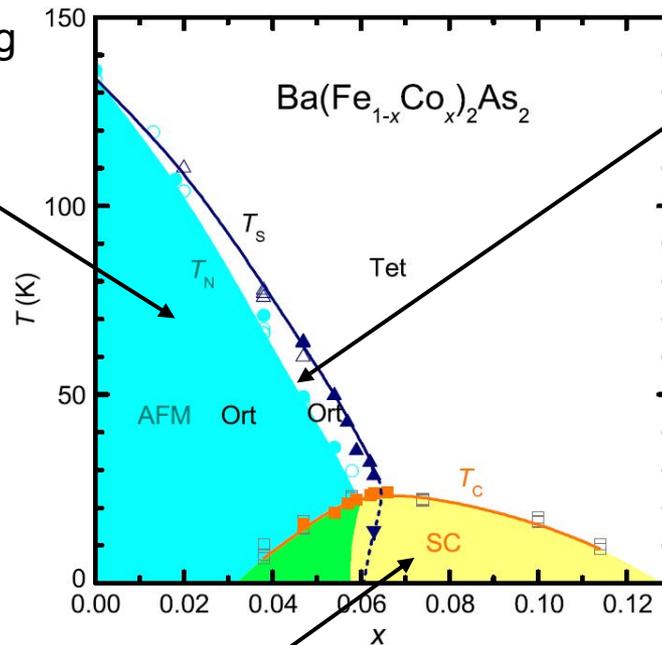
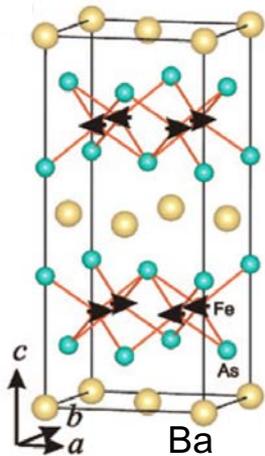


[1] R. M. Fernandes, PPO, J. Schmalian, Annu. Rev. Cond. Mat. **10**,133 (2019).

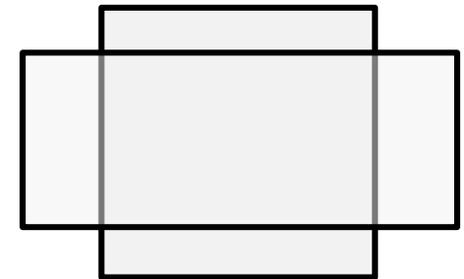
Example: iron-based superconductors

- Primary orders: magnetic and superconducting
- Vestigial order: nematic (122) and spin-vorticity density wave (1144) orders

Magnetic order (breaking of **spin rotational symmetry**)



Nematic order (**rotational symmetry** breaking from tetragonal C_4 to orthorhombic C_2)



Superconductivity (breaking of **global $U(1)$ symmetry**)

Definition of vestigial order

- In the ordered phase, we always find composite order

$$\langle \eta_\alpha \rangle \neq 0 \implies \langle \eta_\alpha \eta_\beta \rangle \neq 0 \quad (\text{trivial})$$

- Vestigial phase: **composite order without primary order**

$$\langle \eta_\alpha \rangle = 0 \quad \text{yet} \quad \langle \eta_\alpha \eta_\beta \rangle \neq 0$$

vestige noun

ves·tije | \ 've-stij  \

Definition of vestige

- 1 a (1)** : a trace, mark, or visible sign left by something (such as an ancient city or a condition or practice) vanished or lost
- (2)** : the smallest quantity or trace

Vestigial order

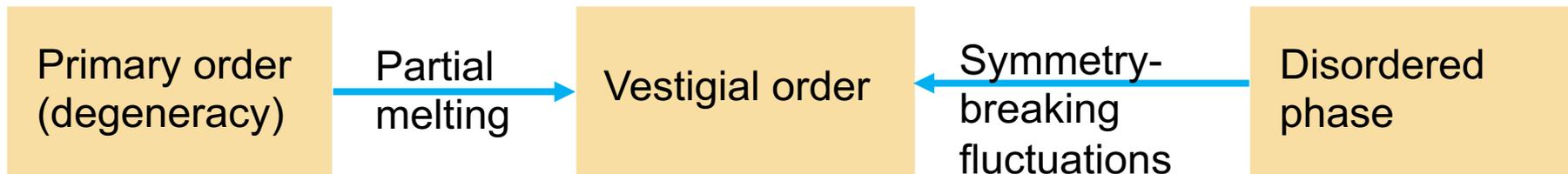
- In the ordered phase, we always find composite order

$$\langle \eta_\alpha \rangle \neq 0 \implies \langle \eta_\alpha \eta_\beta \rangle \neq 0 \quad (\text{trivial})$$

- Vestigial phase: composite order without primary order

$$\langle \eta_\alpha \rangle = 0 \quad \text{yet} \quad \langle \eta_\alpha \eta_\beta \rangle \neq 0$$

General idea: a “mother phase” from which several different vestigial orders with similar energy scales emerge.

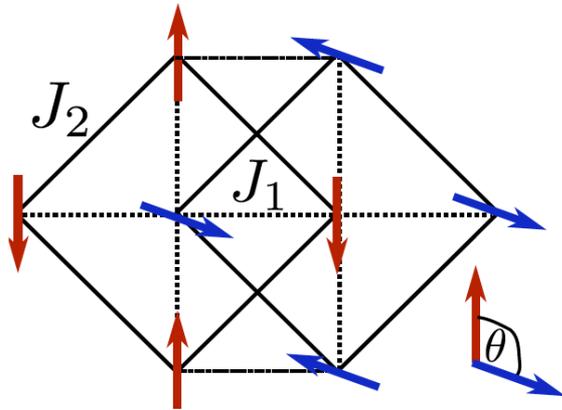


➤ Similar to the phenomenon of “order by disorder” in frustrated magnets

[1] Nie et al, PNAS (2014); [2] Villain, J. Phys. France (1977); Henley, PRL (1989); Chandra, Coleman, Larkin, PRL (1990).

Example of vestigial order in antiferromagnet

- Frustrated J1-J2 antiferromagnet on square lattice



$$H = J_1 \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

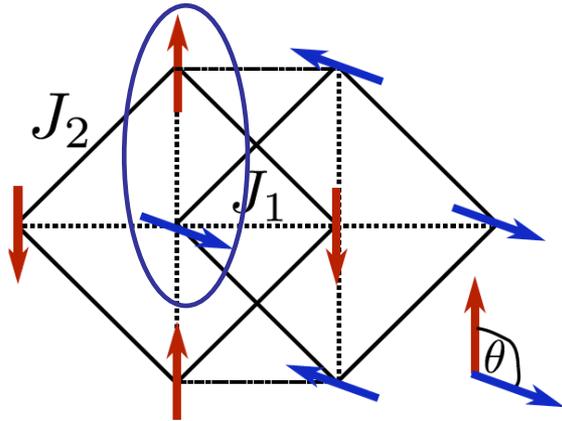
Consider $J_2 > J_1$:

- Interpenetrating square lattices with dominant Neel-order fluctuations
- At $T > 0$, magnetic correlation length finite (Mermin-Wagner): $\langle \eta_\alpha \rangle = 0$
- Sublattices only coupled by fluctuations $\mathbf{S}_i = \langle \mathbf{S}_i \rangle + \delta \mathbf{S}_i$

[1] Villain, J. Phys. France (1977); Henley, PRL (1989); Chandra, Coleman, Larkin, PRL (1990).

Example of vestigial order in antiferromagnet

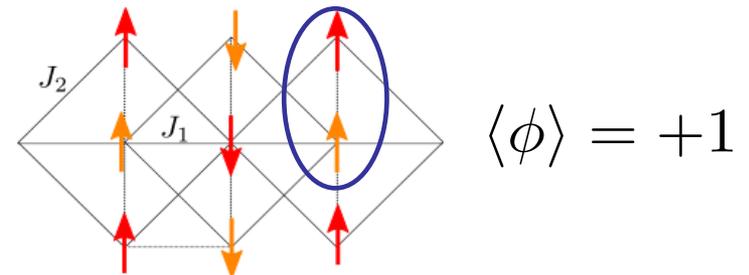
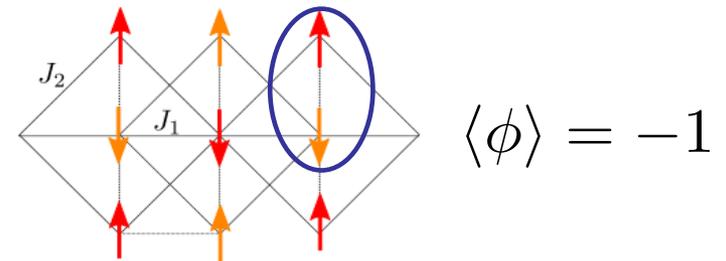
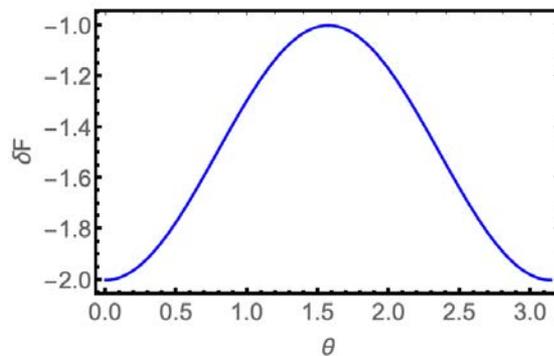
- Frustrated J1-J2 antiferromagnet on square lattice



Composite order parameter:

$$\langle \phi \rangle \equiv \langle \eta_\alpha \eta_\beta \rangle = \langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle$$

Fluctuation free-energy minima at $\theta = 0, \pi$

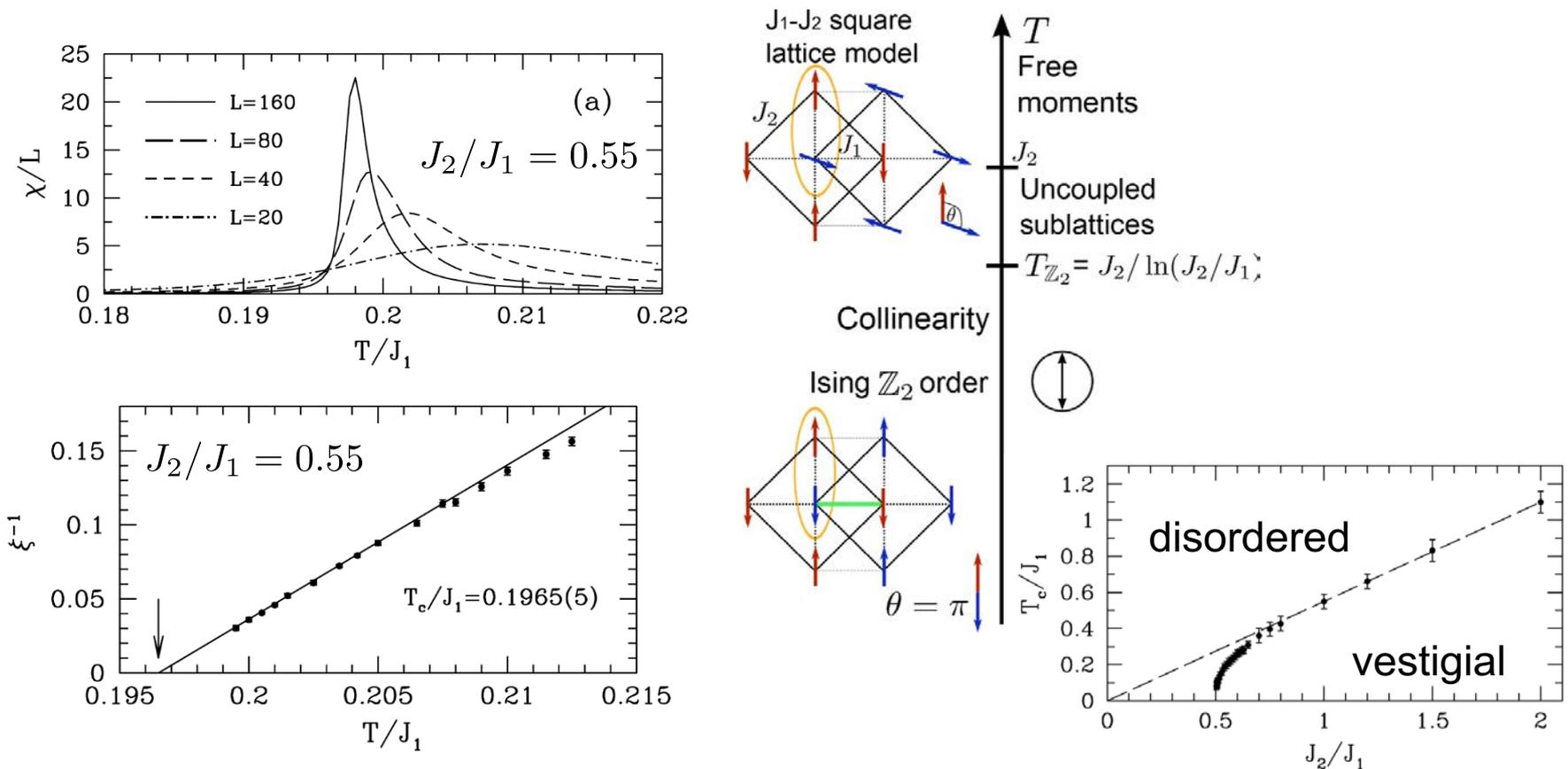


From spin-wave analysis. Entropy maximized \rightarrow “Order by Disorder”.

[1] Chandra, Coleman, Larkin, PRL (1990).

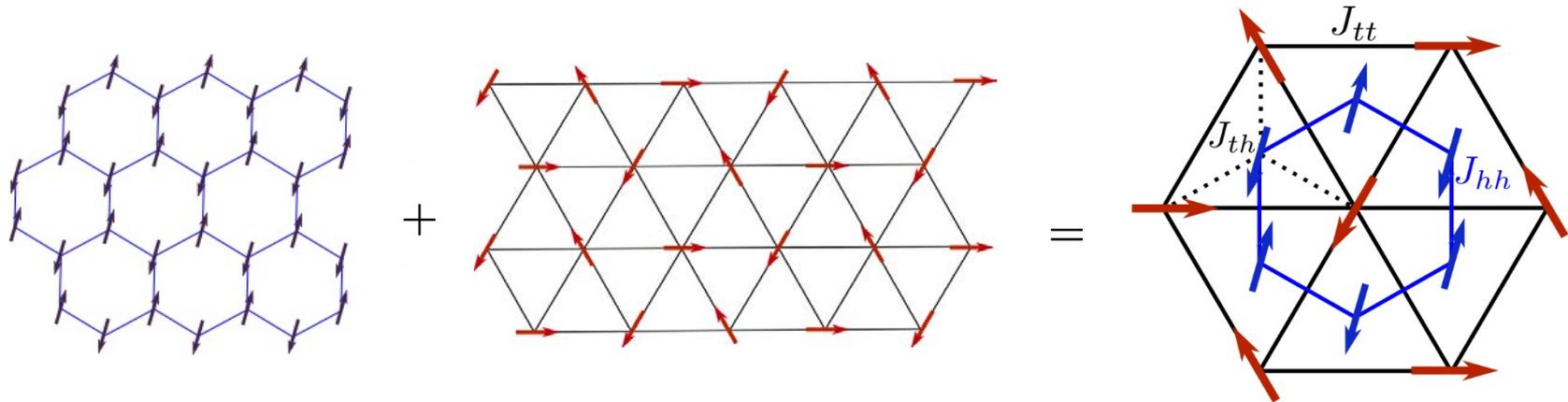
Ising phase transition at finite temperature

- Finite T phase transition into phase with finite vestigial order
- Classical Monte-Carlo results



[1] P. Chandra, P. Coleman, A. I. Larkin, PRL **64**, 88 (1990); [2] C. Weber et al., PRL **91**, 177202 (2003);

2D Heisenberg windmill antiferromagnet



- Honeycomb + triangular lattice sites
- Heisenberg spins $\mathbf{S}_t(r_j)$, $\mathbf{S}_A(r_j)$, $\mathbf{S}_B(r_j)$
- Antiferromagnetic nearest-neighbor coupling

$$H = H_{tt} + H_{AB} + H_{tA} + H_{tB}$$

$$H_{ab} = J_{ab} \sum_{j=1}^{N_L} \sum_{\delta_{ab}} \mathbf{S}_a(r_j) \cdot \mathbf{S}_b(r_j + \delta_{ab})$$

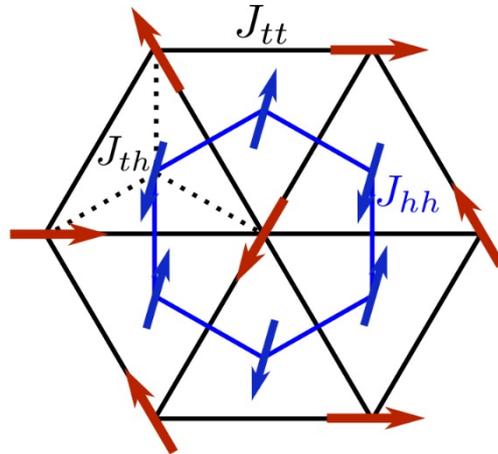
$a, b \in \{t, A, B\}$



Windmill in Strängnaes (Sweden)

[1,2] PPO, P. Chandra, P. Coleman, J. Schmalian, PRL (2012); PRB (2014); [3] PPO, B. Jeevanesan, PRB (2014); B. Jeevanesan, P. Chandra, P. Coleman, PPO, PRL (2015).

Ground state of classical spins at small J_{th}



Weak inter-sublattice coupling

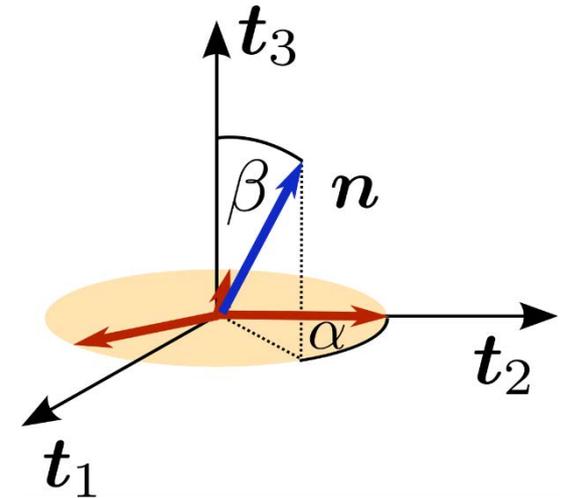
$$J_{th} \ll J_{tt}, J_{hh}$$

Neel order on **honeycomb lattice**

→ $O(3)/O(2)$ order parameter $\mathbf{n}(\mathbf{x})$

120 degree state on **triangular lattice**

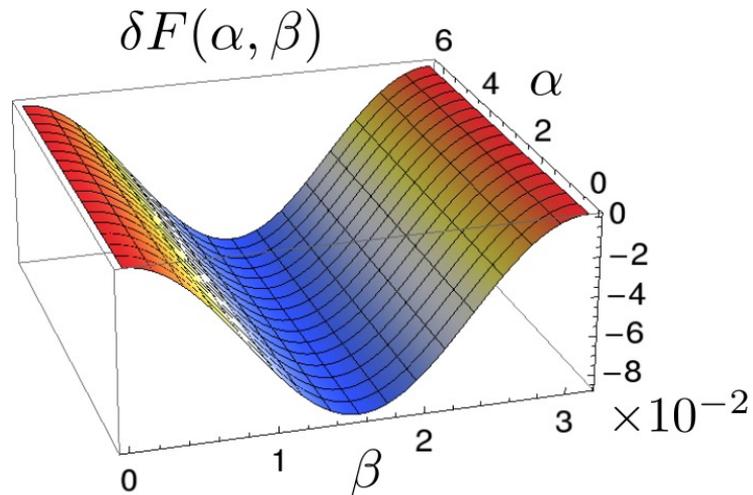
→ $SO(3)$ order parameter $\mathbf{t}(\mathbf{x}) = (t_1, t_2, t_3)$



Classically at $T=0$ decoupled even for $J_{th} > 0$

[1] B. Jeevanesan, PPO, PRB **90**, 144435 (2014).

Fluctuation coupling “order from disorder”



$$J_{th} = 0.4\bar{J}$$

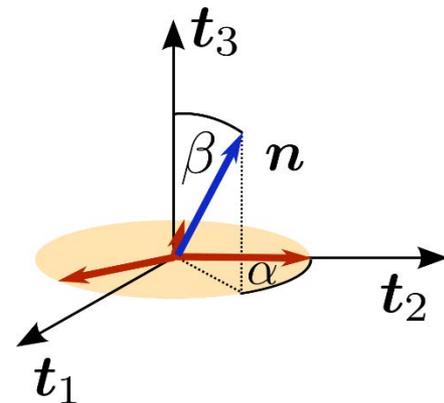
$$\bar{J} = \sqrt{J_{tt}J_{hh}}$$

$$T = 1, S = 1$$

- Fluctuations couple spins on different sublattices
- Spins tend to align perpendicular to fluctuation Weiss field

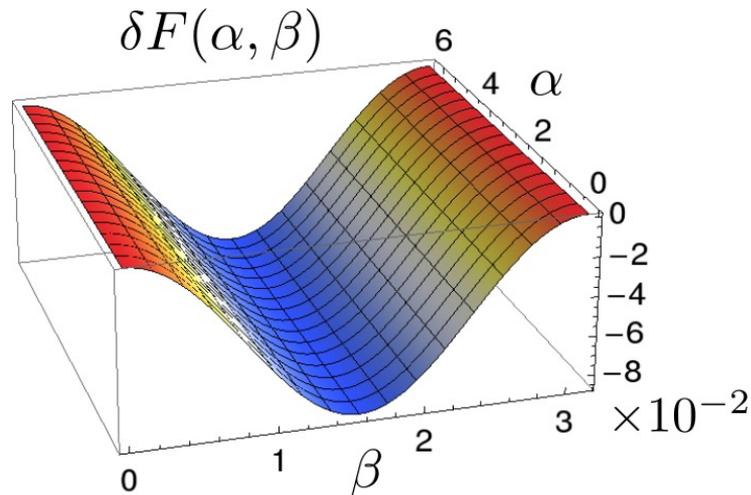
$$S_c = \frac{1}{2} \int d^2x (\gamma \cos^2 \beta)$$

Coplanar: $\gamma = (J_{th}/\bar{J})^2 A_\gamma (J_{tt}/J_{hh}, \bar{J}/T)$



[1] C. L. Henley, PRL **62**, 2056 (1989)

Fluctuation coupling “order from disorder”



$$J_{th} = 0.4\bar{J}$$

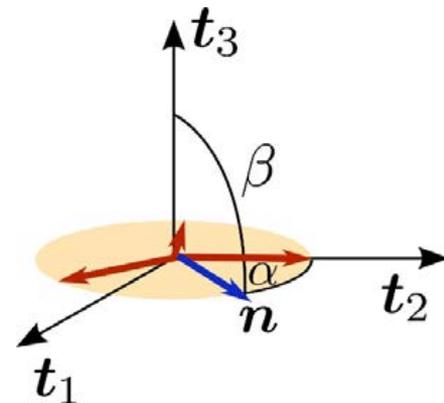
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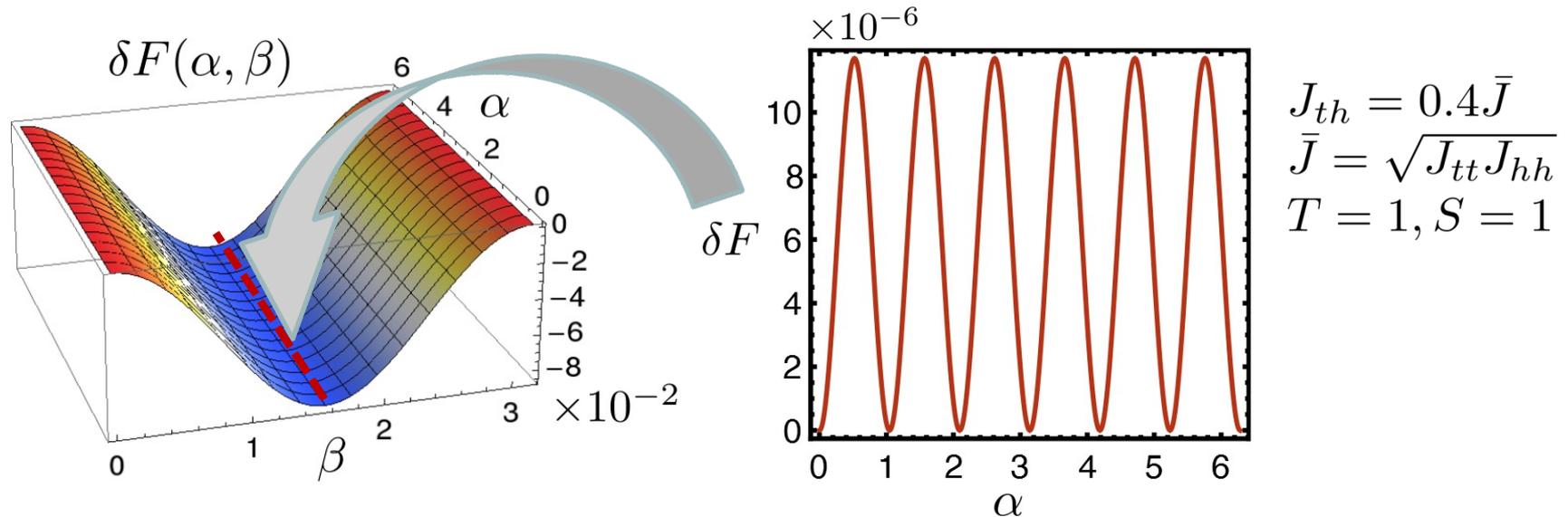
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[1] C. L. Henley, PRL **62**, 2056 (1989)

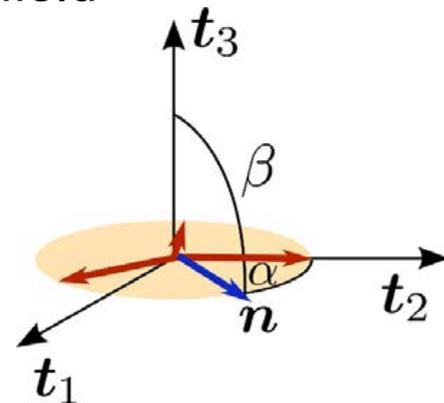
Fluctuation coupling “order from disorder”



- Fluctuations couple spins on different sublattices
- Spins tend to align perpendicular to fluctuation Weiss field

$$S_c = \frac{1}{2} \int d^2x (\gamma \cos^2 \beta + \lambda \sin^6 \beta \sin^2 (3\alpha))$$

Coplanar: $\gamma \propto (J_{th}/\bar{J})^2$ Z_6 : $\lambda \propto (J_{th}/\bar{J})^6$

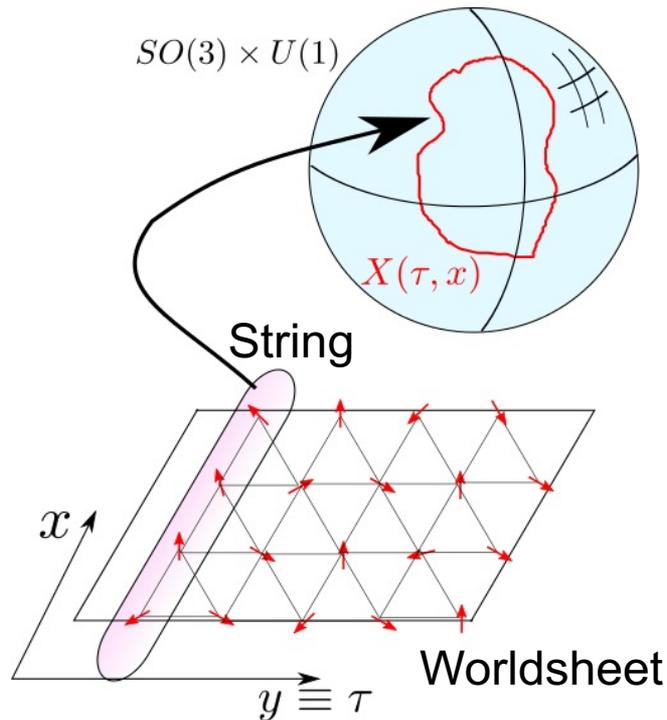


[1] C. L. Henley, PRL **62**, 2056 (1989)

Long-wavelength covariant action

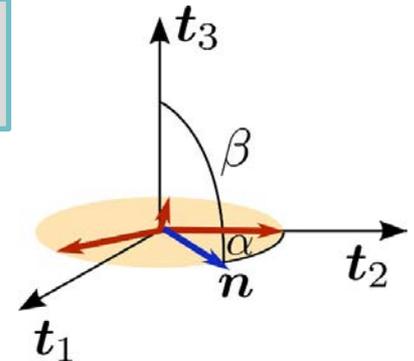
- Long-wavelength action of 2d spin system takes form of (Euclidean) **string theory** [1]

$$S = \frac{1}{2} \int d^2x g_{ij}[X(x)] \partial_\mu X^i(x) \partial_\mu X^j(x) + \frac{\lambda}{2} \int d^2x \sin^2(3\alpha)$$



3 Euler angles and relative phase

$$X(\tau, x) = (\phi, \theta, \psi, \alpha)$$



Magnetization X = displacement of string in $D=4$ (compact) dimensions

[1] D. Friedan, PRL **45**, 1057 (1980)

Magnetism as string theory

- Action of 2D spin system takes form of (Euclidean) string theory [1]

$$S = \frac{1}{2} \int d^2x g_{ij}[X(x)] \partial_\mu X^i(x) \partial_\mu X^j(x) + \frac{\lambda}{2} \int d^2x \sin^2(3\alpha)$$

- Spin stiffnesses define metric tensor**

$$X(\tau, x) = (\phi, \theta, \psi, \alpha)$$

$$g = \begin{pmatrix} g^{SO(3)} & \mathcal{K}^T \\ \mathcal{K} & I_\alpha \end{pmatrix}$$

SO(3) stiffnesses I_1, I_2, I_3

U(1) phase α is coupled to non-Abelian sector U(1) stiffness

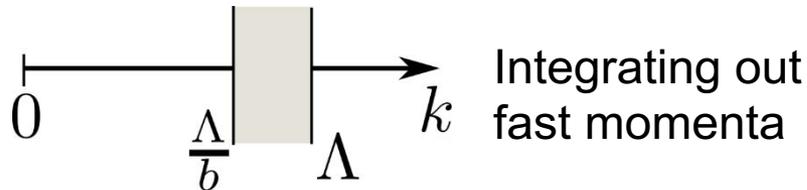
Geometric curvature of manifold (Riemann tensor) determined by spin stiffnesses.

[1] D. Friedan, PRL **45**, 1057 (1980);

[2, 3] PPO, P. Chandra, P. Coleman, J. Schmalian, PRL (2012); PRB (2014)

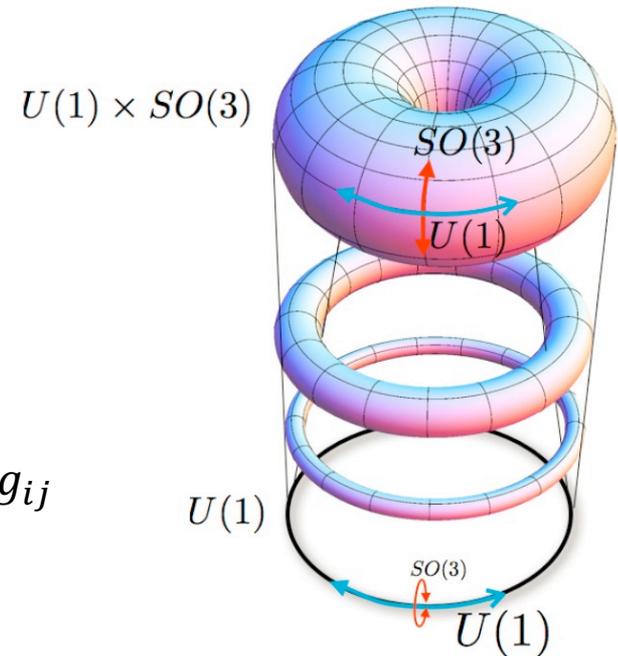
Magnetism and gravity: RG flow = Ricci flow

- Action is covariant with stiffness metric tensor
- Covariance is preserved during RG scaling [1]
- **RG flow of the metric is given by the Ricci flow** [1,2] (two loops)



$$\frac{dg_{ij}}{dl} = -\frac{1}{2\pi} R_{ij} - \frac{1}{8\pi^2} R_i{}^{klm} R_{jklm}$$

Ricci and Riemann tensor determined by g_{ij}



[1] D. Friedan, PRL **45**, 1057 (1980); [2] R. S. Hamilton, J. Differential Geom. **17**, 255 (1982)

Compactification and magnetism

$$\frac{dg_{ij}}{dl} = -\frac{1}{2\pi} R_{ij} - \frac{1}{8\pi^2} R_i{}^{klm} R_{jklm}$$

- One-dimensional U(1) part of manifold decouples from 3D non-Abelian SO(3) part
- Ricci scalar grows like

$$R = R^{SO(3)} - \frac{1}{2\pi I'_\alpha} \beta_\alpha$$

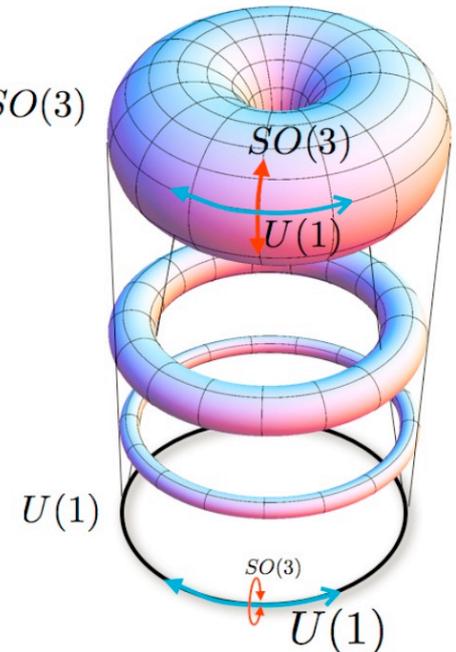
$$R^{SO(3)} \sim 1/\bar{I}$$

$$\beta_\alpha = \frac{(I_1 - I_2)^2 r^2}{4\pi I_1 I_2}$$

SO(3) part curls up

U(1) becomes flat

$U(1) \times SO(3)$



Toy model for compactification

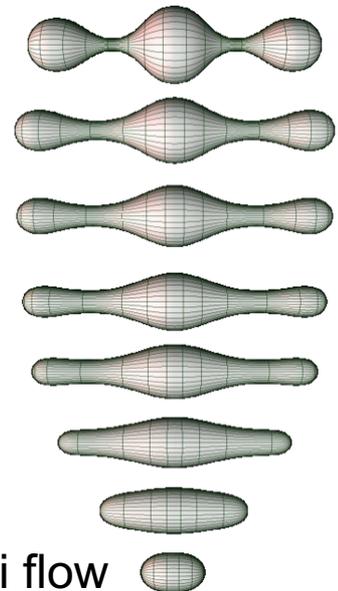
[1] M. Gell-Mann and B. Zwiebach, Phys. Lett. B **141**, 333 (1984);
 [2] L. Randall and R. Sundrum, PRL **83**, 4690 (1999)
 [3, 4] PPO, P. Chandra, P. Coleman, J. Schmalian, PRL (2012); PRB (2014);

Experimental proof of Poincare conjecture

- **Poincare conjecture** (1904), proven by Perelman in 2006
- “Every simply connected, closed 3-manifold is homeomorphic to a 3-sphere”
- Two-loop perturbative Ricci flow experiences singularities (false Landau poles). Not present in exact Ricci flow.
- **Use classical magnet to simulate exact Ricci flow. Experimental proof of Poincare conjecture.**
- Protocol:
 - Suitable magnet realizes given metric
 - Cool system
 - Measure spin correlation functions at various temperatures
 - Extract metric tensor
 - Obtain “surgery-free” generalized Ricci flow of manifold



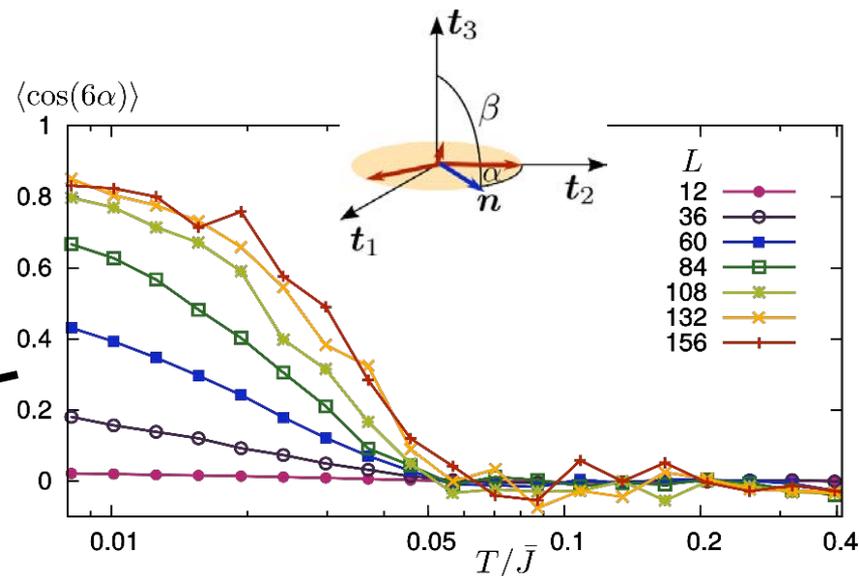
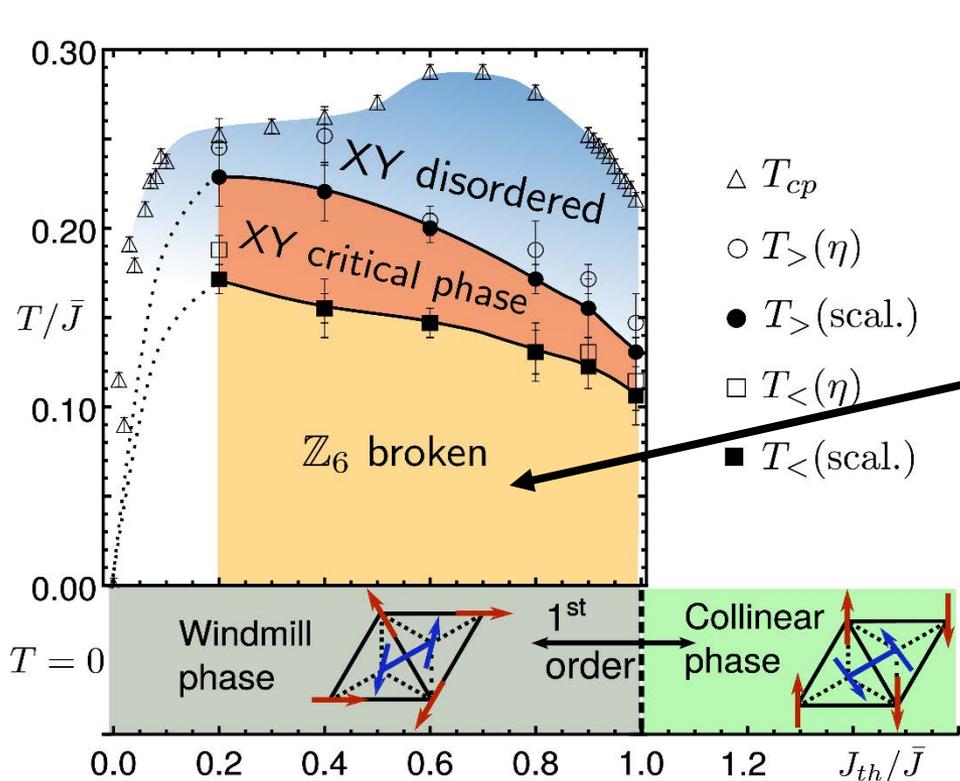
G. Perelman (2006)
H. Poincare



Ricci flow

[1] P. Coleman, A. Tselik (private communication)

Classical Monte-Carlo simulation: phase diagram

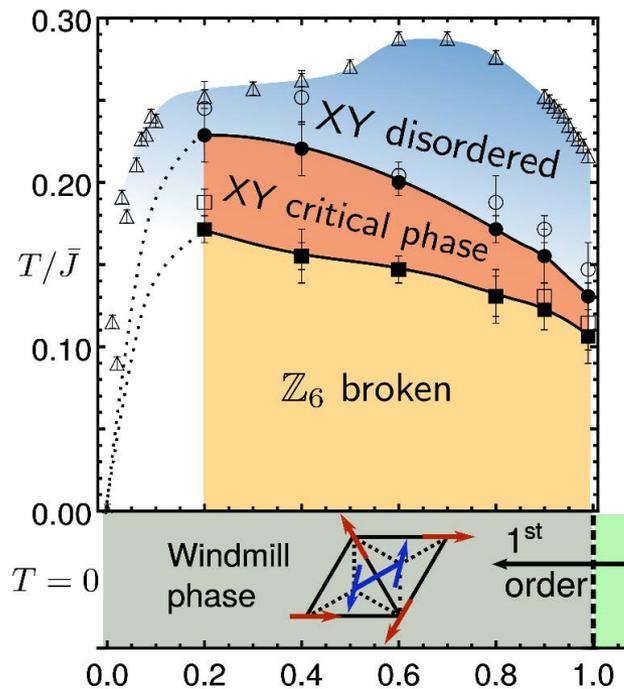


System falls into one of the six minima
Long-range discrete order occurs.

- Large-scale parallel-tempering classical Monte-Carlo simulations
- Proof of Polykov's conjecture that critical phase can exist in Heisenberg system (due to topological vacuum degeneracy).

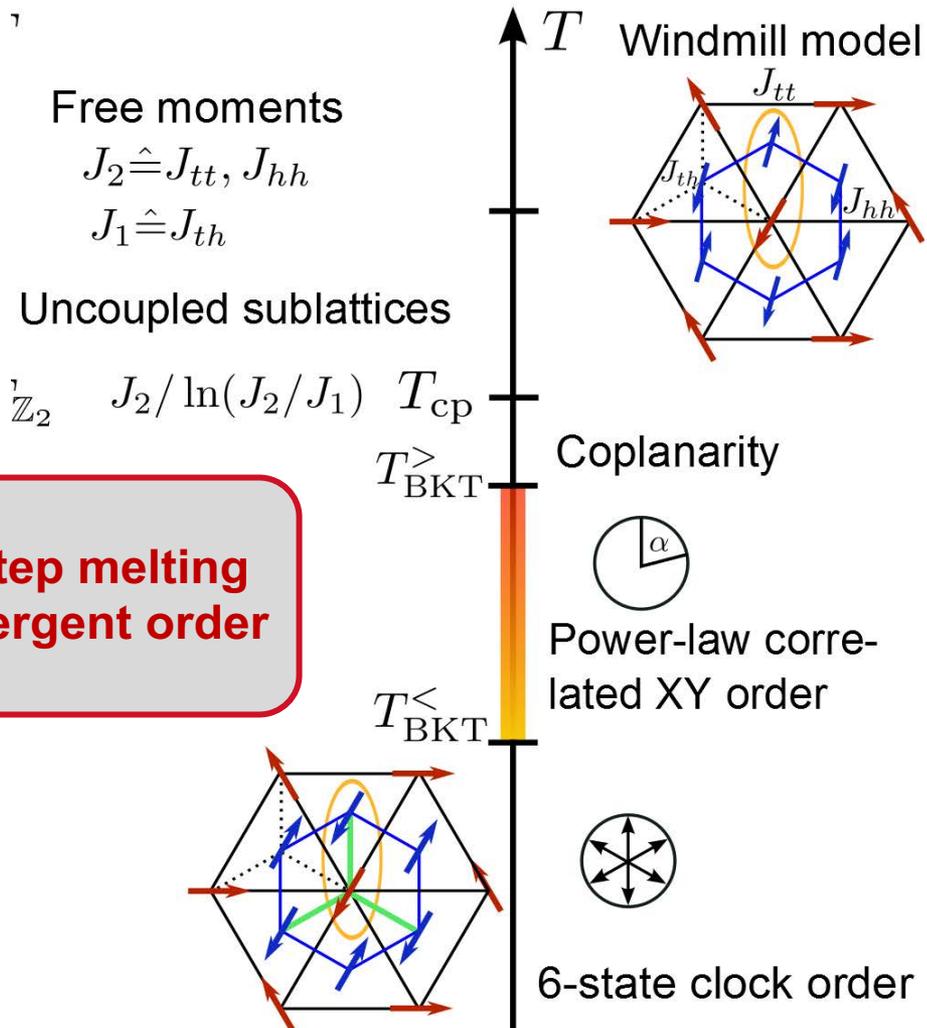
[1] B. Jeevanesan, P. Chandra, P. Coleman, PPO, PRL (2015).

Phase diagram of windmill antiferromagnet



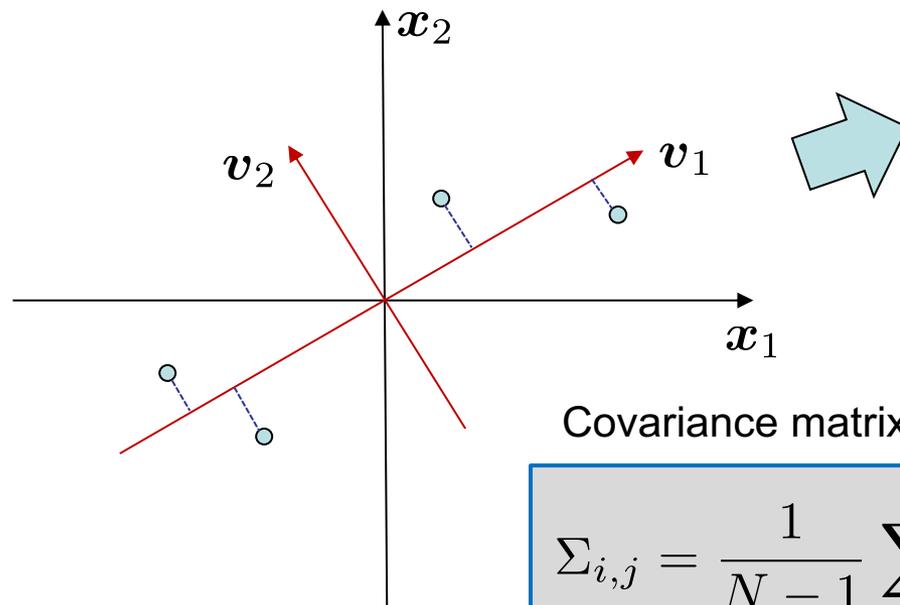
- [1,2] PPO, P. Chandra, P. Coleman, J. Schmalian
 PRL (2012); PRB (2014);
 [3] B. Jeevanesan, P. Chandra, P. Coleman, PPO
 PRL (2015).

Two-step melting of emergent order

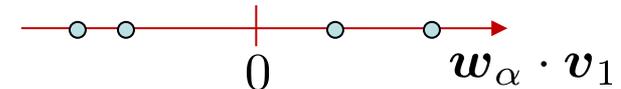


Interlude: Can machine-learning find vestigial order

- Unsupervised machine learning algorithm
- Principal Component Analysis (PCA)
 - Linear orthogonal transformation to basis with decreasing data variance (maximal projections)



v_1 corresponds to maximal eigenvalue λ_1 of covariance matrix



Projection of data along v_1 maximal
➤ **Strongest correlations in the data**
➤ Minimal data loss

Covariance matrix:

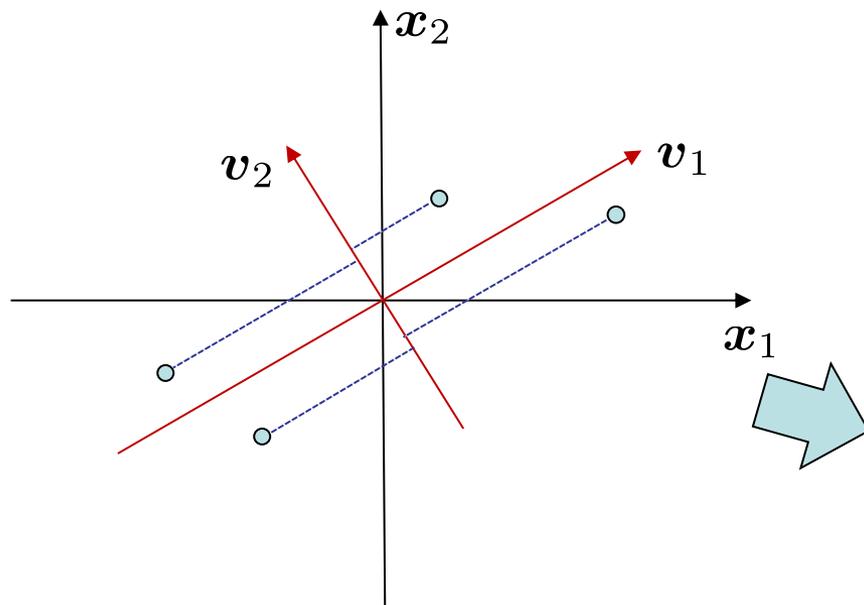
$$\Sigma_{i,j} = \frac{1}{N-1} \sum_{\alpha=1}^N (w_{\alpha})_i (w_{\alpha})_j$$

Work in progress with Mathias S. Scheurer (Harvard).

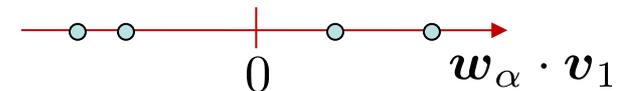
Rescaled data to zero mean and equal standard-deviations along axes.

Interlude: Can machine-learning find vestigial order

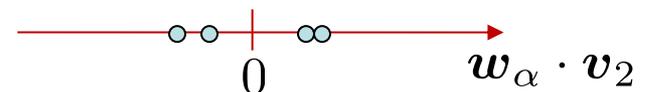
- Unsupervised machine learning algorithm
- Principal Component Analysis (PCA)
 - Linear orthogonal transformation to basis with decreasing data variance (maximal projections)



v_1 corresponds to maximal eigenvalue λ_1 of covariance matrix



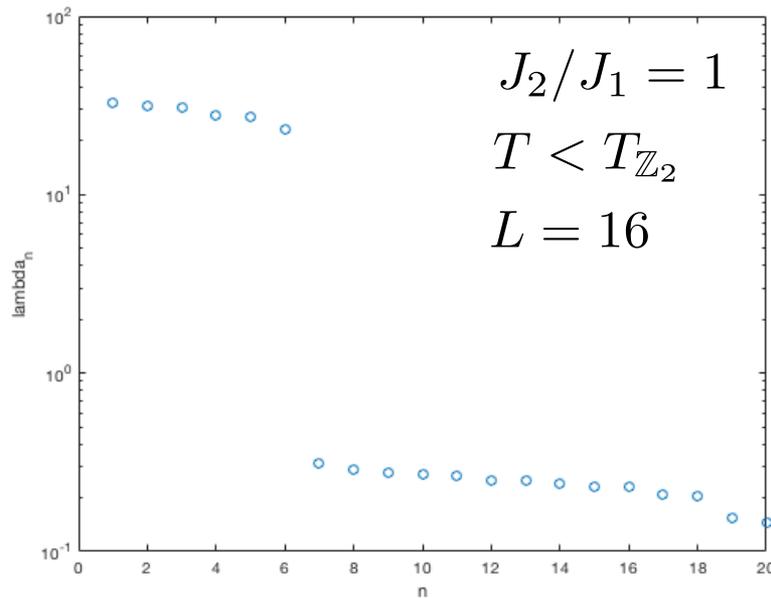
v_2 corresponds to next largest eigenvalue λ_2 of covariance matrix



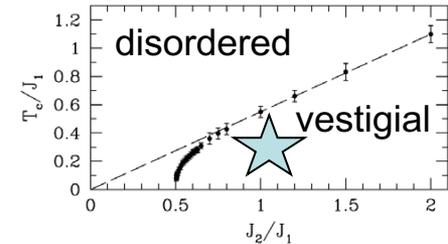
Interlude: Can machine-learning find vestigial order

- Unsupervised machine learning algorithm
- Principal Component Analysis (PCA)
 - Linear orthogonal transformation to basis with decreasing data variance
 - Feed spin snapshot data obtained in classical Monte-Carlo simulation

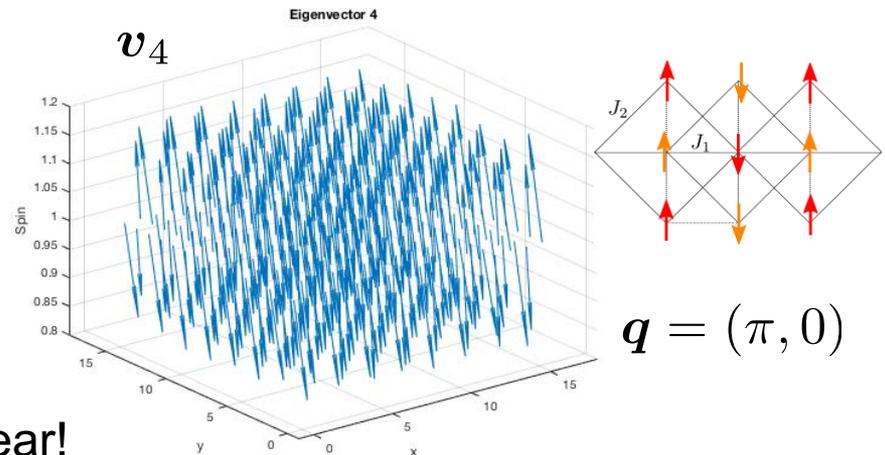
$$\mathbf{x} = (S_1^x, S_1^y, S_1^z, \dots, S_N^z)$$



No sign of vestigial order as PCA is linear!



- Six principal modes $\lambda_1, \dots, \lambda_6$
- Correspond to
 - 3 spin polarizations at
 - 2 wavevectors $(\pi, 0)$ and $(0, \pi)$



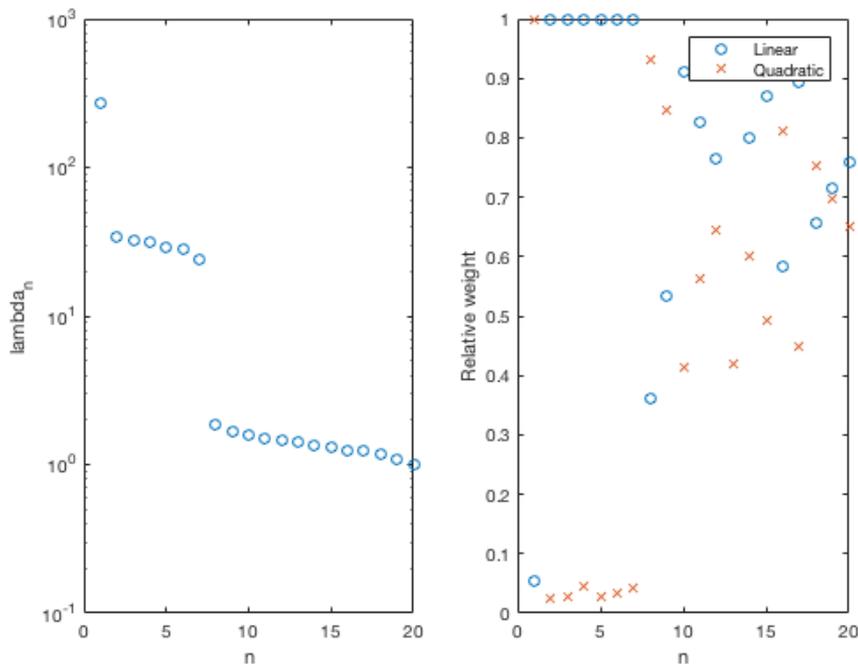
Interlude: Can machine-learning find vestigial order

- Feed in addition bond expectation values of spin snapshot data

$$\mathbf{x} = (S_1^x, S_1^y, S_1^z, \dots, S_N^z, S_1 \cdot S_2, S_1 \cdot S_{1+L}, \dots, S_L \cdot S_1)$$

Linear “spin” sector

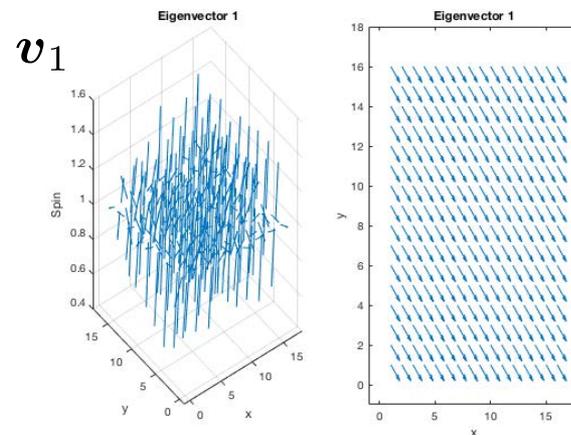
Quadratic “bond” sector



$$J_2/J_1 = 1$$

$$T < T_{\mathbb{Z}_2} \quad L = 16$$

- One dominant mode λ_1 appears now
 - Mode lies entirely in bond sector
- 6 sub-leading modes $\lambda_2, \dots, \lambda_7$ as before



“Spin” sector:
no correlations

“Bond” sector: vestigial order

$$\mathbf{v}_1 = S_i \cdot S_{i+1} - S_i \cdot S_{i+L}$$

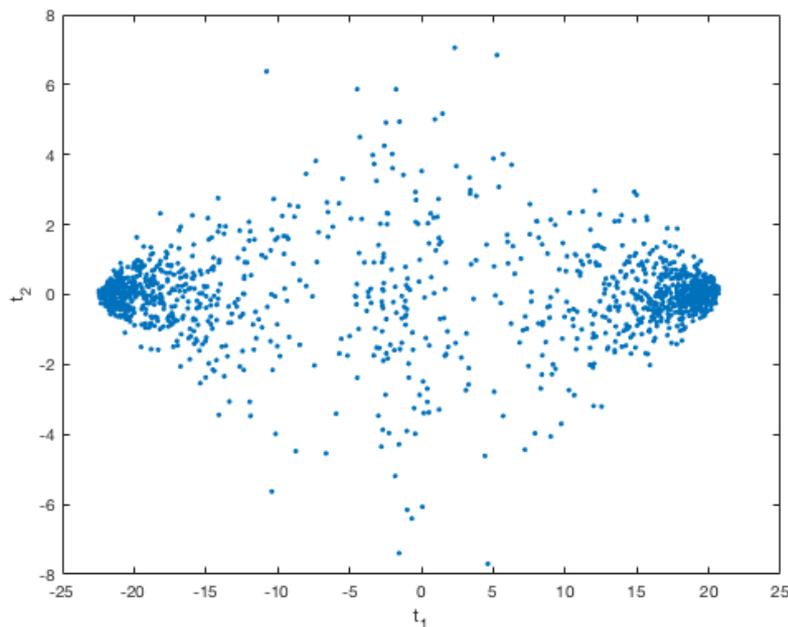
Interlude: Can machine-learning find vestigial order

- Feed in addition bond expectation values of spin snapshot data

$$\mathbf{x} = (S_1^x, S_1^y, S_1^z, \dots, S_N^z, S_1 \cdot S_2, S_1 \cdot S_{1+L}, \dots, S_L \cdot S_1)$$

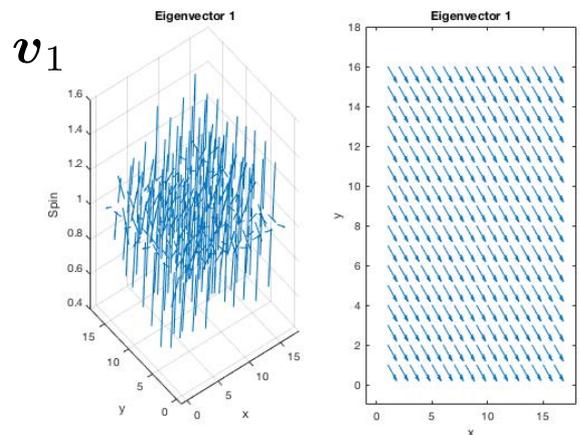
Linear “spin” sector

Quadratic “bond” sector



Two clusters along v_1 direction
 $\rightarrow Z_2$ (Ising) vestigial order

- One dominant mode λ_1 appears now
 - Mode lies entirely in bond sector
- 6 sub-leading modes $\lambda_2, \dots, \lambda_7$ as before



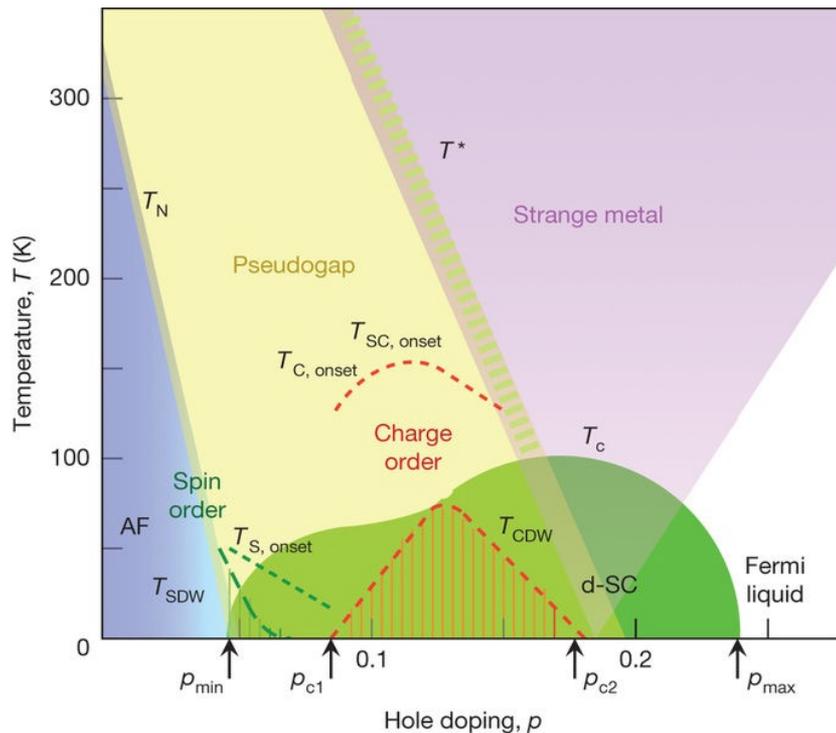
“Spin” sector:
no correlations

“Bond” sector: vestigial order

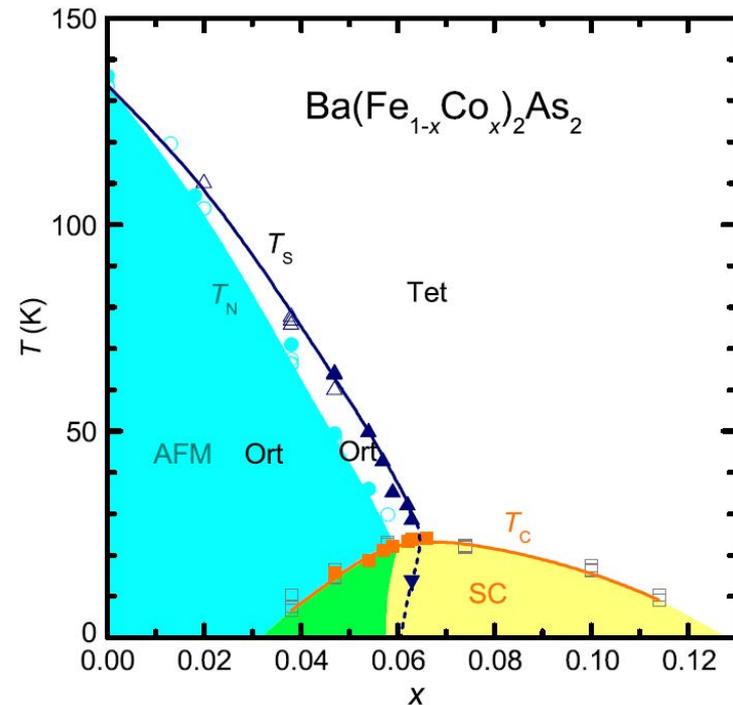
$$\mathbf{v}_1 = S_i \cdot S_{i+1} - S_i \cdot S_{i+L}$$

Vestigial order in complex materials

- Naturally gives rise to complexity observed in phase diagrams across correlated quantum materials



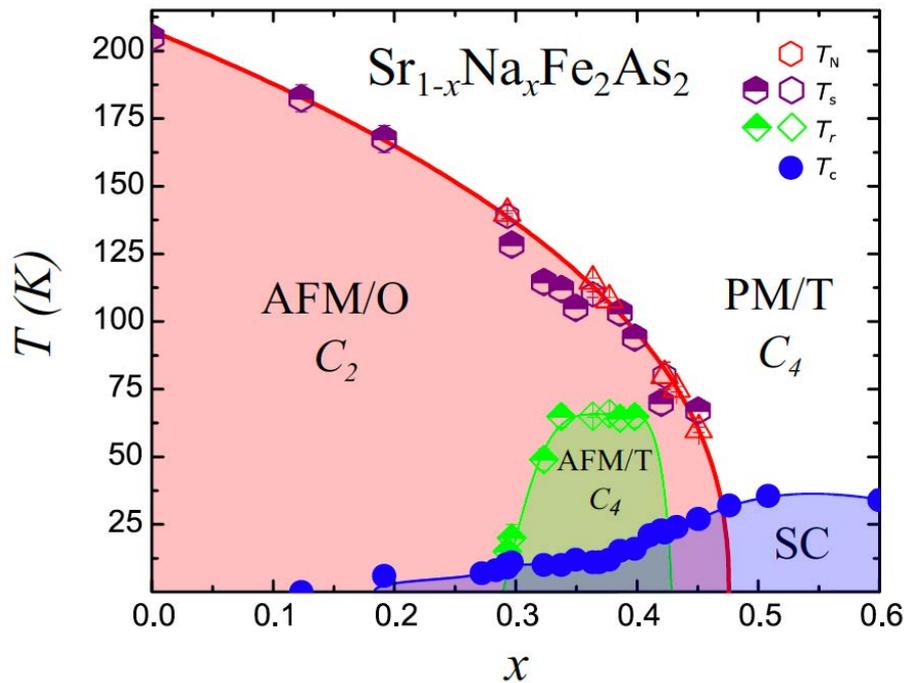
Cuprate Superconductor (YBCO)



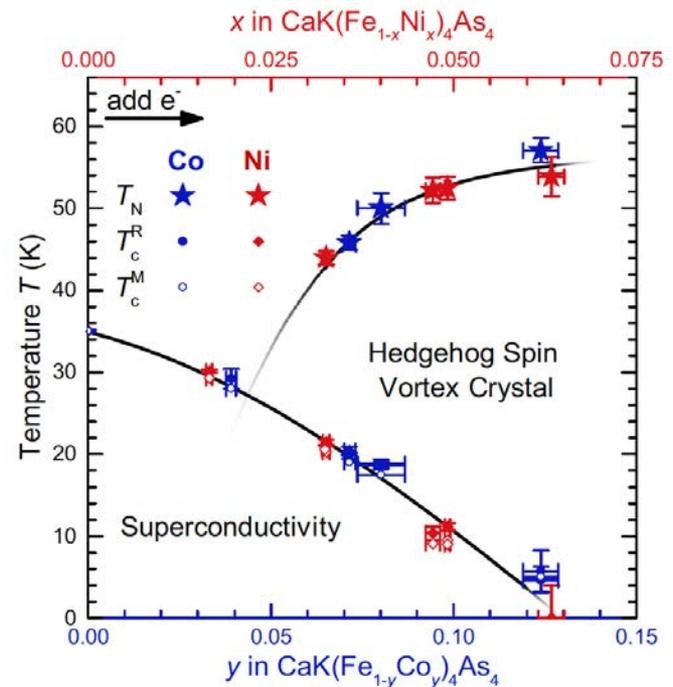
Iron-Based Superconductor
(hole doped Ba-122)

[1] Keimer et al., Nature (2015); [2] S. Nandi *et al.*, PRL **104**, 057006 (2010); [2] P. C. Canfield, S. L. Budko, Annu. Rev. Cond. Mat. **1**, 27 (2010).

Complexity of phase diagrams in correlated materials



Iron-Based Superconductor
(electron doped Sr-122)



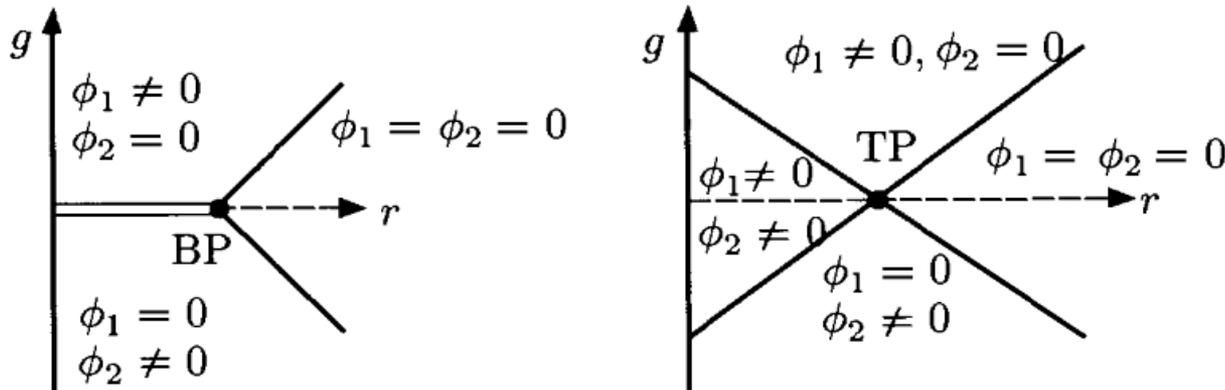
Iron-Based Superconductor
(electron doped 1144)

[1] Taddei et al., PRB (2016); [2] W. R. Meier, ..., PPO, ...P.C. Canfield, npj Quantum Materials (2018).

Complex phase diagrams

- Multiple ordered states that break different symmetries but exhibit comparable energy scales
- Landau theory of competing orders: ϕ_1, ϕ_2

$$f = \frac{1}{2}r(\phi_1^2 + \phi_2^2) - \frac{1}{2}g(\phi_1^2 - \phi_2^2) + u_1\phi_1^4 + u_2\phi_2^4 + 2u_{12}\phi_1^2\phi_2^2.$$

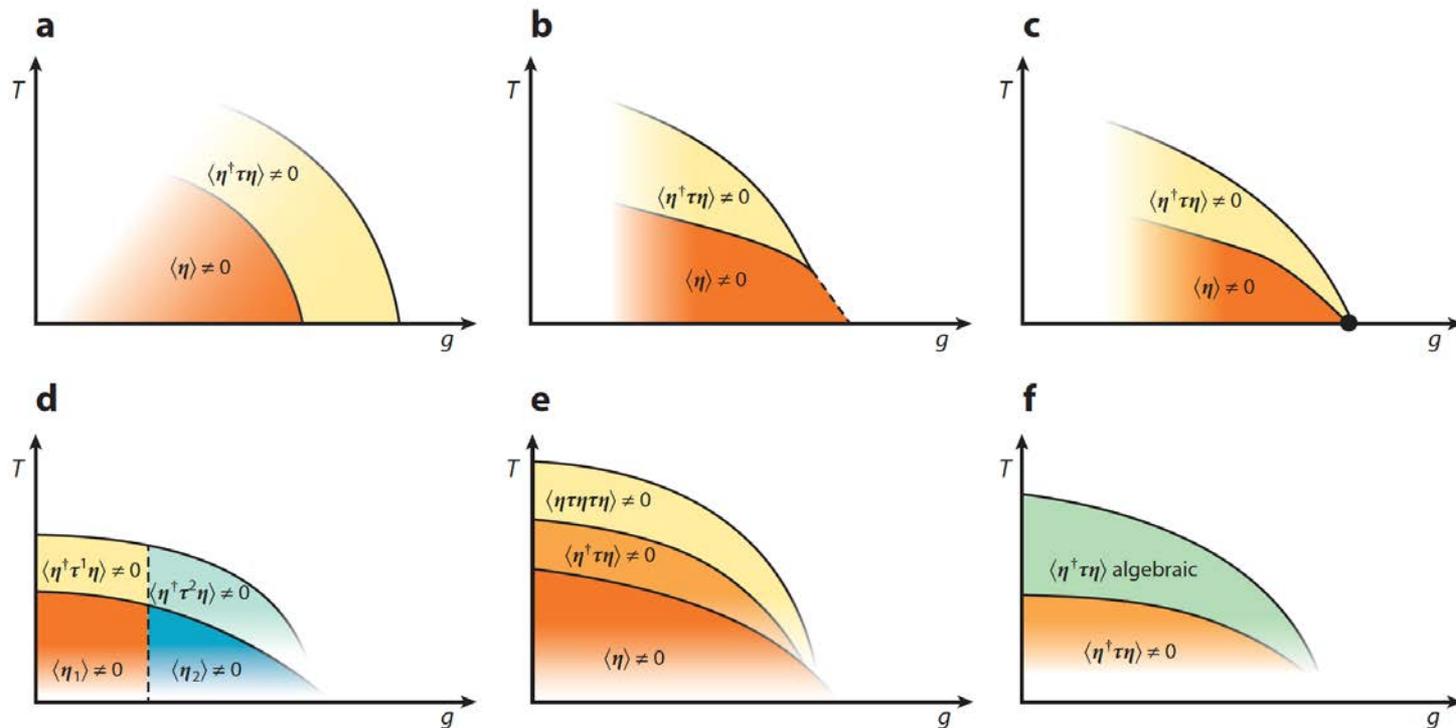


➤ Fine-tuning of multiple coupling constants required to explain complexity (several multicritical points).

[1] P. M. Chaikin, T. C. Lubensky "Principles of Condensed Matter Physics; [2] Kosterlitz, Nelson, Fisher, PRB (1976).

Vestigial order: a natural explanation of complexity

- Fluctuation-driven vestigial orders: powerful framework to describe interplay between **multiple phases with comparable transition temperatures**
- **Based on symmetry alone**, no fine tuning of parameters



[1] R. M. Fernandes, PPO, J. Schmalian, Annu. Rev. Cond. Mat. **10**, 133 (2019); [2] see also Fradkin et al, RMP (2015).

Group theory definition of vestigial order

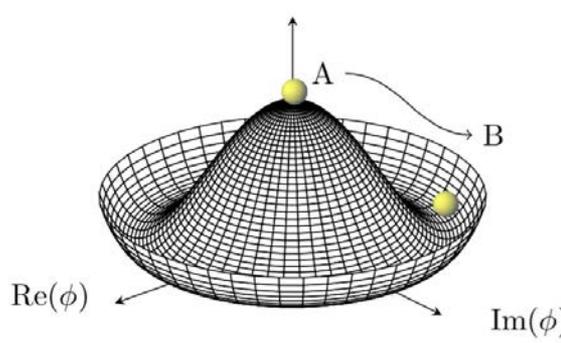
- **Symmetry group** of the system: \mathcal{G} = (spatial) x (internal) symm.
- Complex primary **order parameter** η_α transforms according to an irreducible representation (**irrep**) Γ of \mathcal{G}
- Components $\alpha = 1, \dots, d_\Gamma$, where d_Γ = dimensionality of irrep
- Example: **singlet s-wave superconductivity (l=0)**

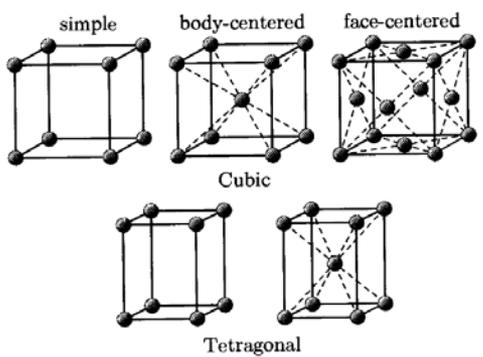
η
 Complex order parameter

$\mathcal{G} = G \otimes U(1)$
 Point group of lattice

$\Gamma = A_1 \otimes e^{ik\varphi}$
 Trivial irrep

Y_{00}
 Basis function

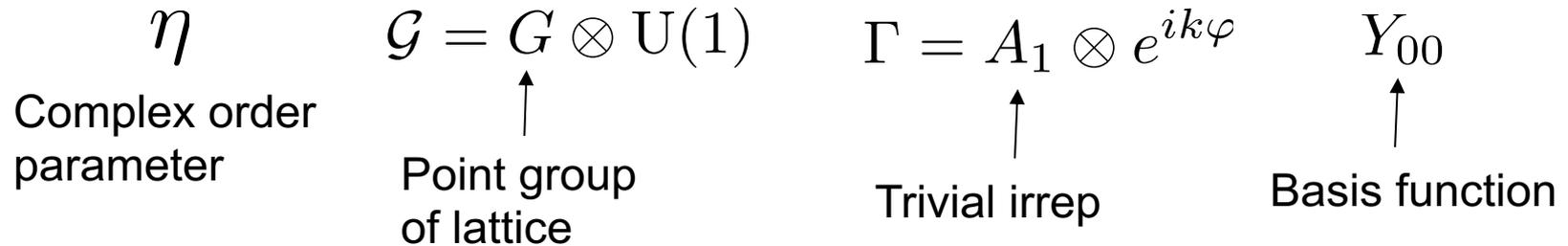




D_{4h} <small>A=16</small>	E	$2C_4$	C_2	$2C_2'$	$2C_2''$	i	$2S_4$	σ_h	$2\sigma_v$	$2\sigma_d$
A_{1g}	1	1	1	1	1	1	1	1	1	1
A_{2g}	1	1	1	-1	-1	1	1	1	-1	-1
B_{1g}	1	-1	1	1	-1	1	-1	1	1	-1
B_{2g}	1	-1	1	-1	1	1	-1	1	-1	1
E_g	2	0	-2	0	0	2	0	-2	0	0
A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1
A_{2u}	1	1	1	-1	-1	-1	-1	-1	1	1
B_{1u}	1	-1	1	1	-1	-1	1	-1	-1	1
B_{2u}	1	-1	1	-1	1	-1	1	-1	1	-1
E_u	2	0	-2	0	0	-2	0	2	0	0

[1] P. M. Chaikin, T. C. Lubensky "Principles of Condensed Matter Physics; [2] Gernot-katzers-spice-pages.com

Primary and vestigial phase



- Primary phase: $\langle \eta \rangle \neq 0$

Here: Breaking of U(1) symmetry, as trivially under point group operations.

- Composite order parameter:

$$\phi_m = \sum_{\alpha, \beta=1}^{d_\Gamma} \eta_\alpha^* \Lambda_{\alpha\beta}^m \eta_\beta$$

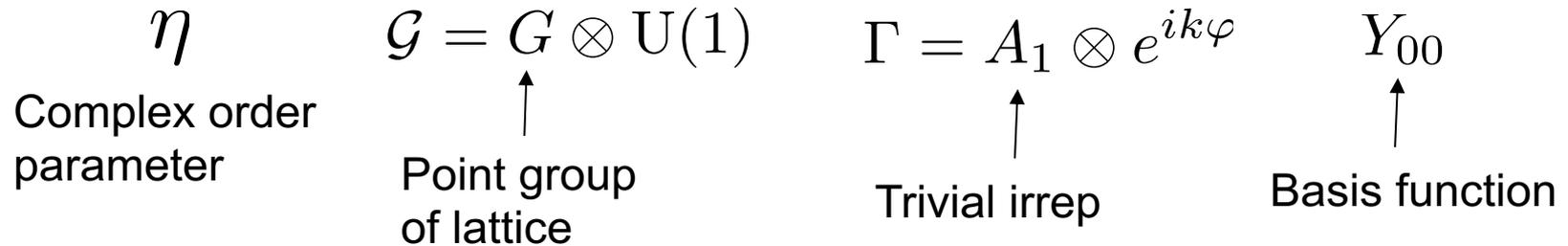
$d_\Gamma \times d_\Gamma$ matrix

➤ Transforms under one of the m irreps Γ^m of the product $\Gamma^* \otimes \Gamma$

➤ Note that $\Gamma^* \otimes \Gamma = A_{1g}$, if $d_\Gamma = 1$ as $(-1)^2 = 1$.

➤ Composite object can transform non-trivially only for $d_\Gamma > 1$

Primary and vestigial phase



- **Primary phase:** $\langle \eta \rangle \neq 0$

Breaking of U(1) symmetry. Transforms trivially under point group operations.

- **Composite order** parameter:

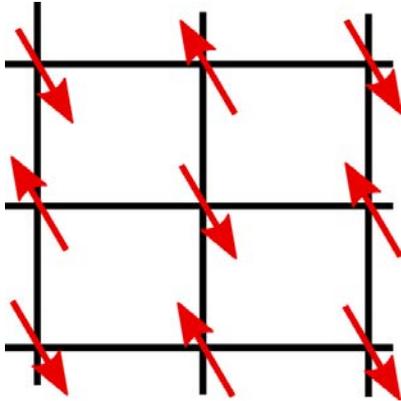
$$\phi_1 = \langle |\eta|^2 \rangle \neq 0$$

- **Transforms trivially as A_{1g}**
- Always non-zero: gap amplitude fluctuations: **No vestigial order!**
- Not all composite objects break a symmetry

[1] P. M. Chaikin, T. C. Lubensky "Principles of Condensed Matter Physics; [2] Gernot-katzers-spice-pages.com

Vestigial order from magnetic primary order

- Neel magnetic order with $Q = (\pi, \pi)$



$$\mathcal{G} = G \otimes \text{SO}(3)$$

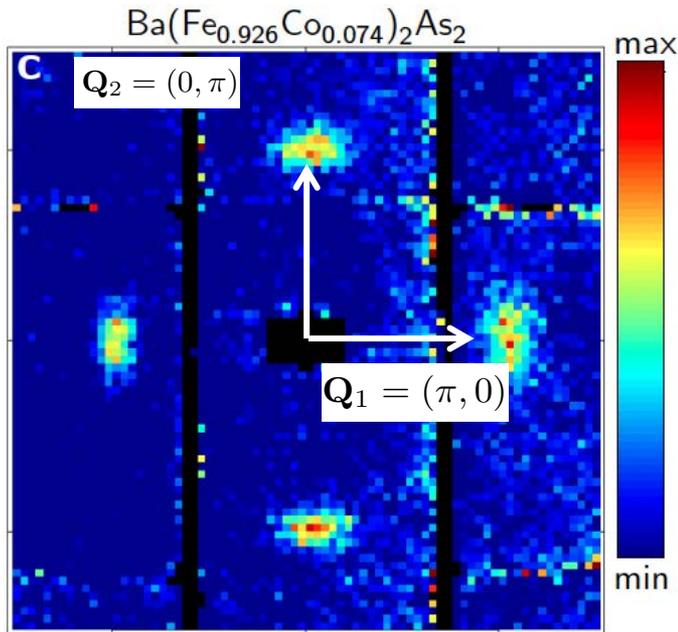
G is, for example, tetragonal point group like D_{4h} or C_{4v} .

- Local spin $\mathbf{S}(\mathbf{r}) = m_{\mathbf{Q}=(\pi,\pi)} \cos(\mathbf{Q} \cdot \mathbf{r})$
- Vestigial order transforms as A_{1g} as $d_{\Gamma} = 1$ in spatial part G: $m_{\mathbf{Q}}$.
→ no vestigial order that breaks lattice symmetries (from G part)
- Need multiple wave-vectors related by lattice symmetry.

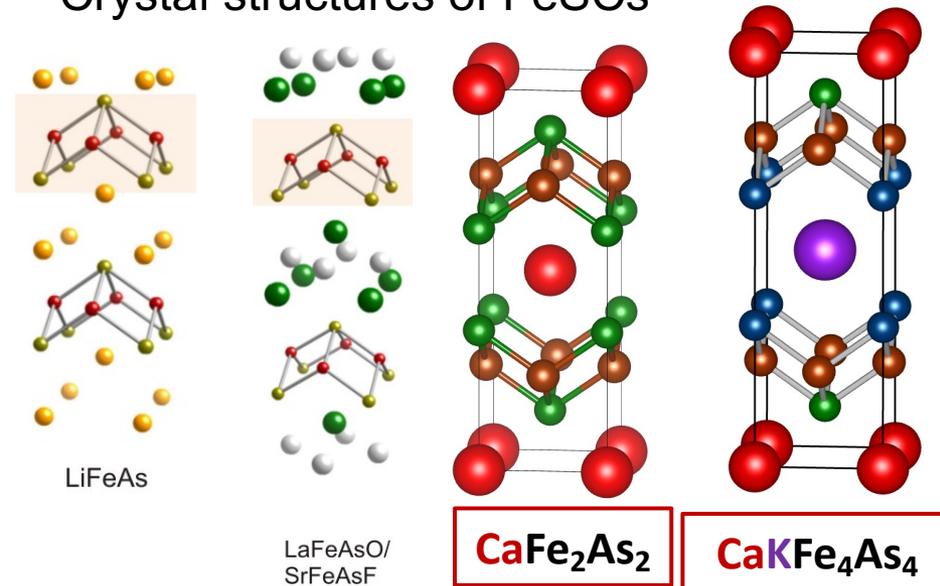
Magnetism in iron-based superconductors

- Magnetic fluctuations peaked at two inequivalent wave-vectors $Q_1 = (\pi, 0)$ and $Q_2 = (0, \pi)$

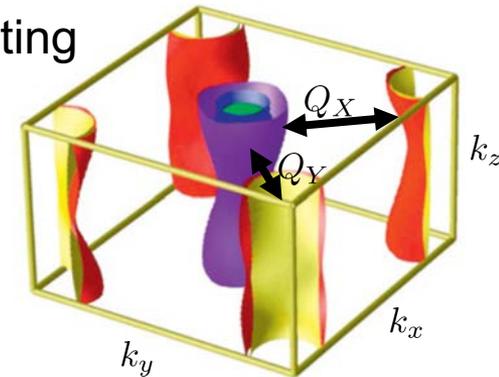
Neutron scattering



Crystal structures of FeSCs



Bandstructure with nesting wavevectors



$$S(\mathbf{r}) = m_1 \cos(\mathbf{Q}_1 \cdot \mathbf{r}) + m_2 \cos(\mathbf{Q}_2 \cdot \mathbf{r})$$

[1] Tucker et al, PRB (2012); [2] J. Paglione and R. Greene Nature Physics 6, 645 (2010); [3] R. M. Fernandes et al., PRB 85, 024534 (2012); [4] Chubukov et al, PRB (2009); [5] W. Meier

Spin-density waves on the square lattice

- Free-energy in tetragonal system and including time-reversal (without spin-orbit coupling)

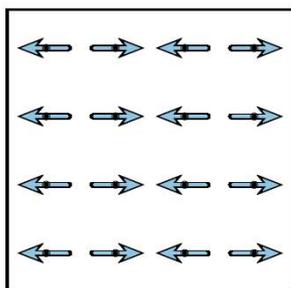
$$S = \int_k r_0(k) (\mathbf{m}_1^2 + \mathbf{m}_2^2) + \frac{u}{2} \int_r (\mathbf{m}_1^2 + \mathbf{m}_2^2)^2 - \frac{g}{2} \int_r (\mathbf{m}_1^2 - \mathbf{m}_2^2)^2 + 2w \int_r (\mathbf{m}_1 \cdot \mathbf{m}_2)^2$$

Second-order coefficient:

$$r_0 = r_0 + k^2 + \gamma |\omega_n|$$

- Three-types of magnetic order minimize free-energy

SSDW



$$g > 0, g > -w$$

Stripe spin-density wave (SSDW)

$$\langle \mathbf{m}_1 \rangle \neq 0$$

$$\langle \mathbf{m}_2 \rangle = 0$$

$$\mathbf{Q}_1 = (\pi, 0)$$

Spin-density waves on the square lattice

- Free-energy in tetragonal system and including time-reversal (without spin-orbit coupling)

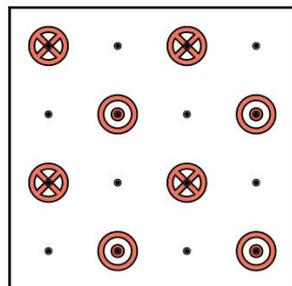
$$S = \int_k r_0(k) (\mathbf{m}_1^2 + \mathbf{m}_2^2) + \frac{u}{2} \int_r (\mathbf{m}_1^2 + \mathbf{m}_2^2)^2 - \frac{g}{2} \int_r (\mathbf{m}_1^2 - \mathbf{m}_2^2)^2 + 2w \int_r (\mathbf{m}_1 \cdot \mathbf{m}_2)^2$$

Second-order coefficient:

$$r_0 = r_0 + k^2 + \gamma |\omega_n|$$

- Three-types of magnetic order minimize free-energy

CSDW



$$w < 0, |w| > g$$

Charge-spin density wave (CSDW)

$$\langle m_1 \rangle = \langle m_2 \rangle \neq 0$$

$$\langle \mathbf{m}_1 \rangle \parallel \langle \mathbf{m}_2 \rangle$$

Collinear double-Q

Spin-density waves on the square lattice

- Free-energy in tetragonal system and including time-reversal (without spin-orbit coupling)

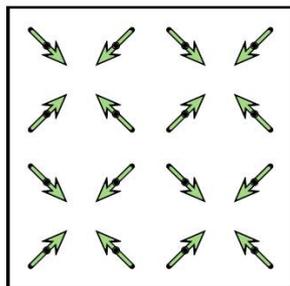
$$S = \int_k r_0(k) (\mathbf{m}_1^2 + \mathbf{m}_2^2) + \frac{u}{2} \int_r (\mathbf{m}_1^2 + \mathbf{m}_2^2)^2 - \frac{g}{2} \int_r (\mathbf{m}_1^2 - \mathbf{m}_2^2)^2 + 2w \int_r (\mathbf{m}_1 \cdot \mathbf{m}_2)^2$$

Second-order coefficient:

$$r_0 = r_0 + k^2 + \gamma |\omega_n|$$

- Three-types of magnetic order minimize free-energy

SVC



Spin-vortex crystal (SVC)

$$\langle m_1 \rangle = \langle m_2 \rangle \neq 0$$

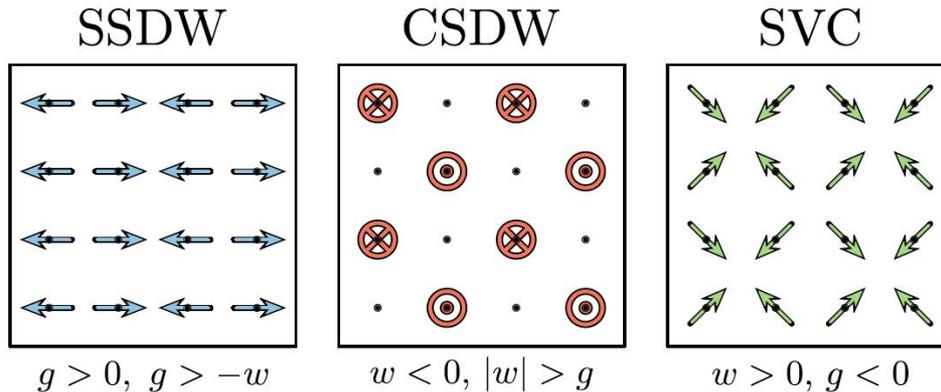
$$\langle \mathbf{m}_1 \rangle \perp \langle \mathbf{m}_2 \rangle$$

Non-collinear double-Q

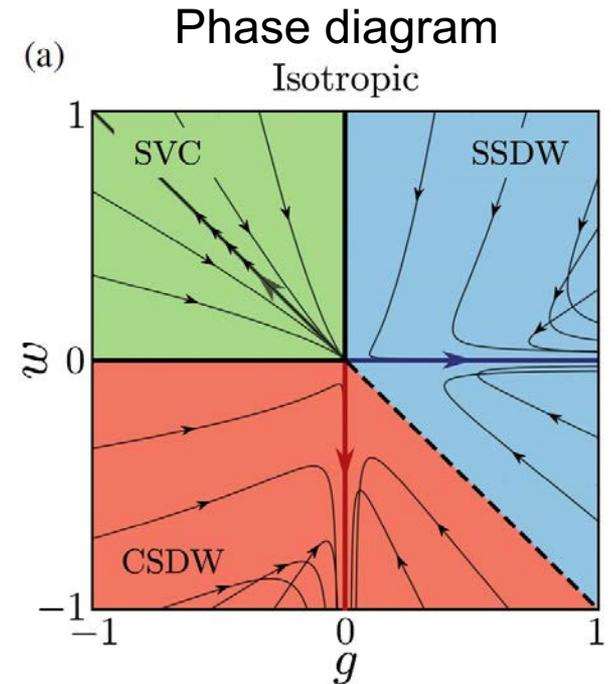
$$w > 0, g < 0$$

Spin-density waves on the square lattice (primary orders)

- Three-types of **magnetic order** minimize free-energy



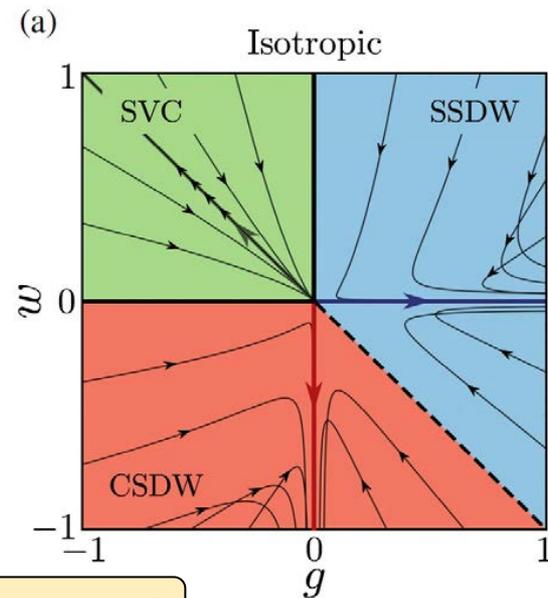
- All states break spatial symmetries in addition to $SO(3)$



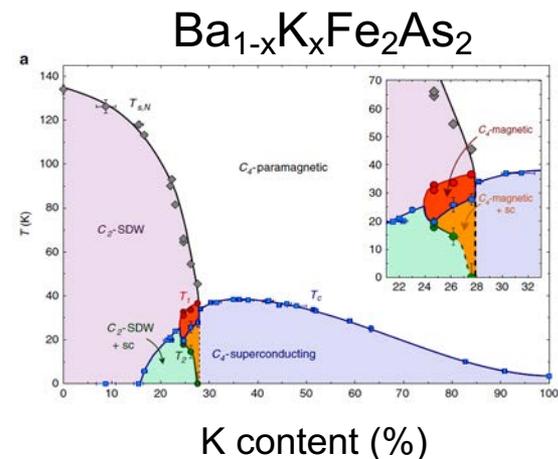
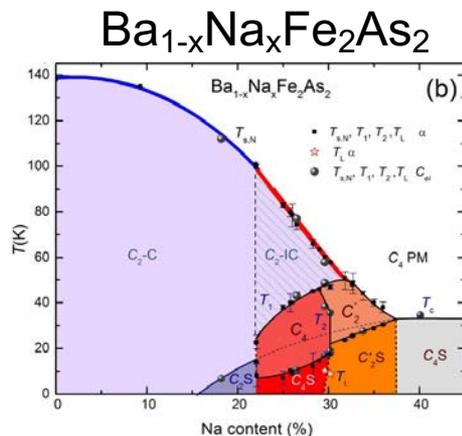
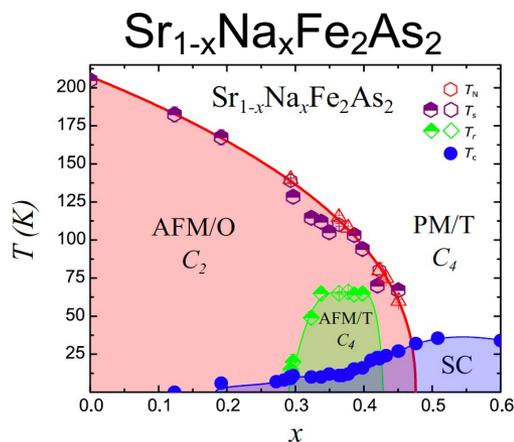
[1] Lorenzana et al, PRL (2008); [2] Eremin et al, PRB (2010); [3] Brydon et al, PRB (2011); [4] Giovannetti et al, Nat. Commun. (2011); Wang et al., PRB (2015), M. H. Christensen, PPO, B. Andersen, R. M. Fernandes, PRL (2018).

Interlude: complexity from universality

- Mean-field analysis so far
- Interactions are relevant as system is at upper critical dimension ($d=2, z=2$)
- Perform renormalization group analysis
- Find mean-field phases are stable with respect to interactions
- Transitions become first-order

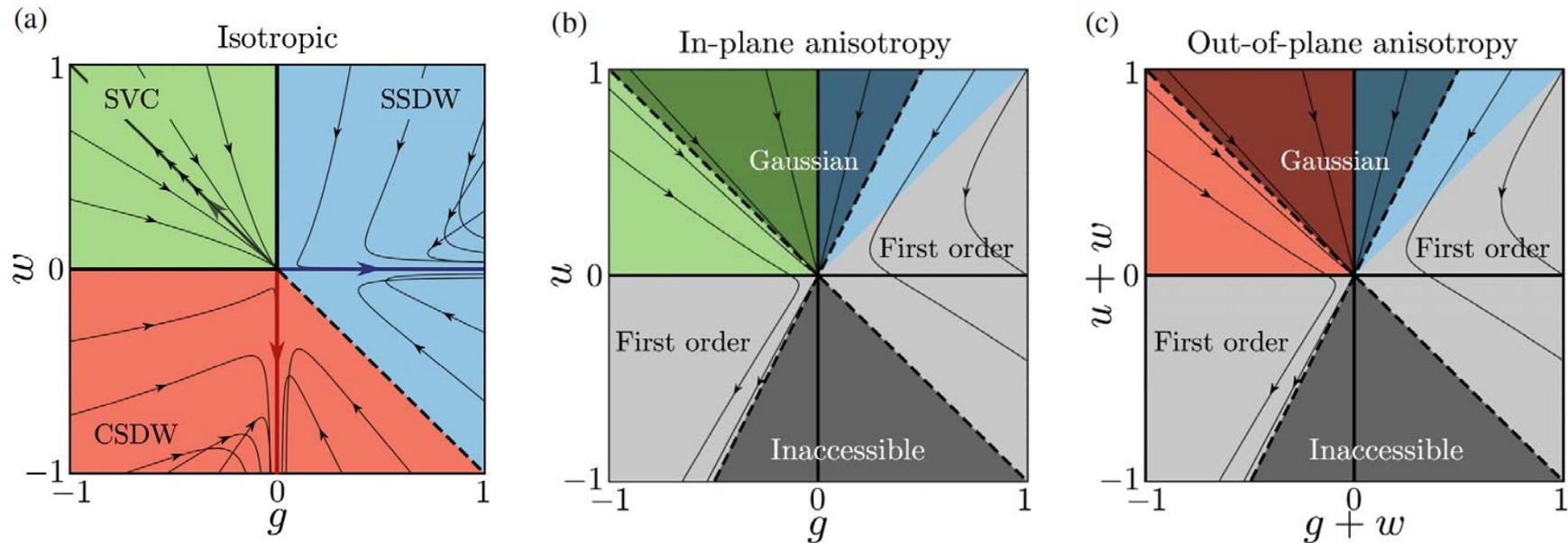


Complexity of magnetic phases close to SC dome fine tuned?



Böhmer et al., Nat. Commun. (2015); Tadei et al, PRB (2015).

Emergent magnetic degeneracy from spin-orbit



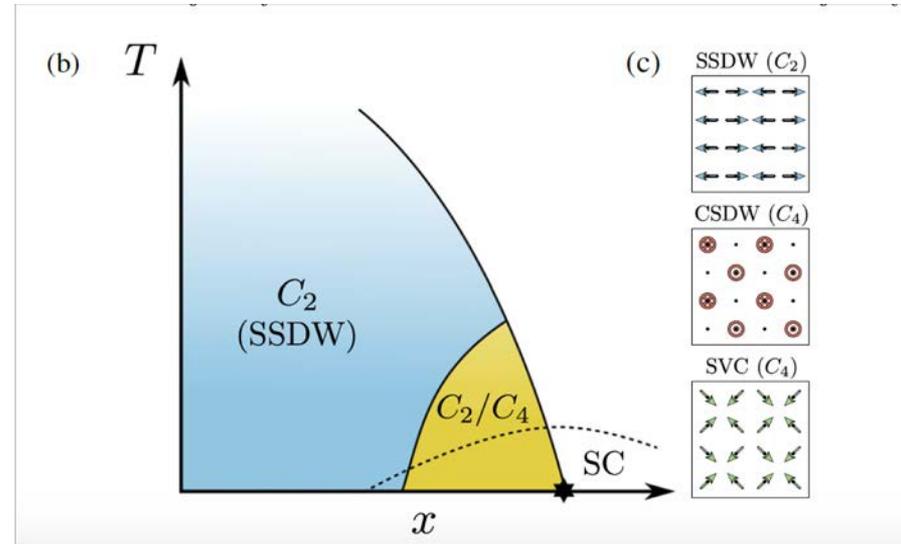
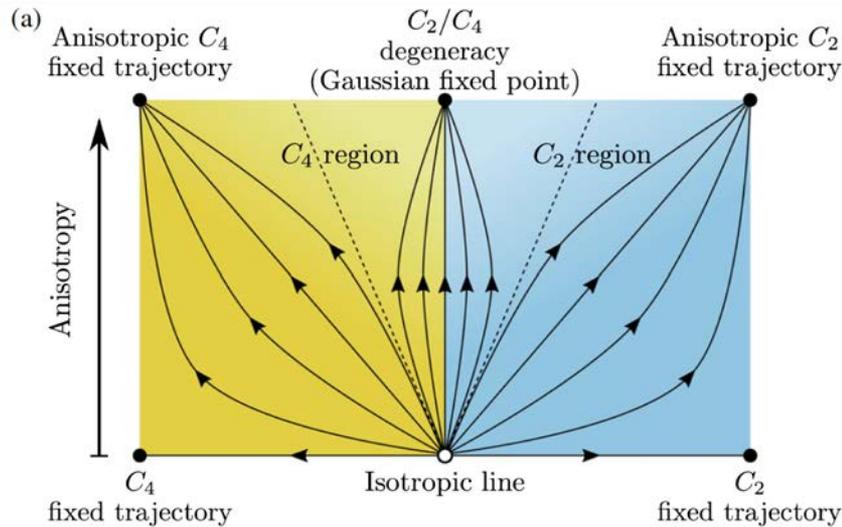
Spin-orbit coupling amplified by interactions (in RG flow):

$$S_{\text{SOC}}^{(2)} = \int_k r_0(k) (\mathbf{M}_1^2 + \mathbf{M}_2^2) + \alpha_1 \int_k (M_{x,1}^2 + M_{y,2}^2) + \alpha_2 \int_k (M_{x,2}^2 + M_{y,1}^2) + \alpha_3 \int_k (M_{z,1}^2 + M_{z,2}^2)$$

- New Gaussian fixed point emerges at finite spin-orbit coupling
- Magnetic phases become degenerate at low energies
- Proliferation of new magnetic phases expected at QCP

M. H. Christensen, PPO, B. Andersen, R. M. Fernandes, PRL (2018), PRB (2018).

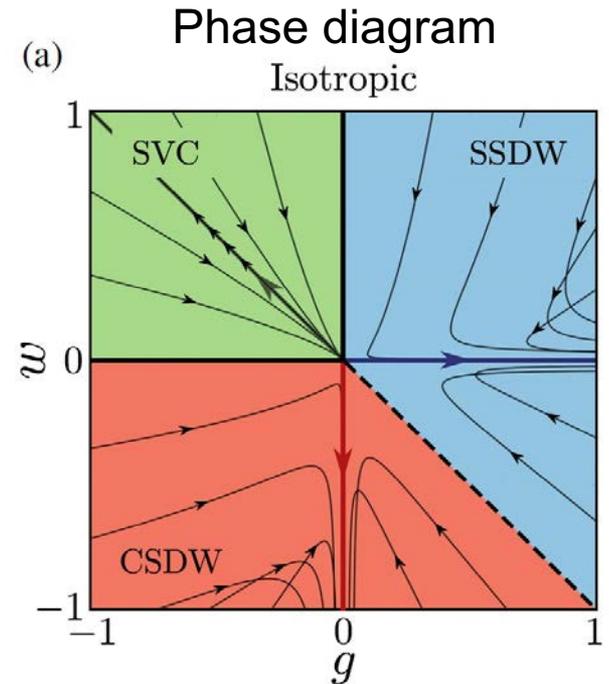
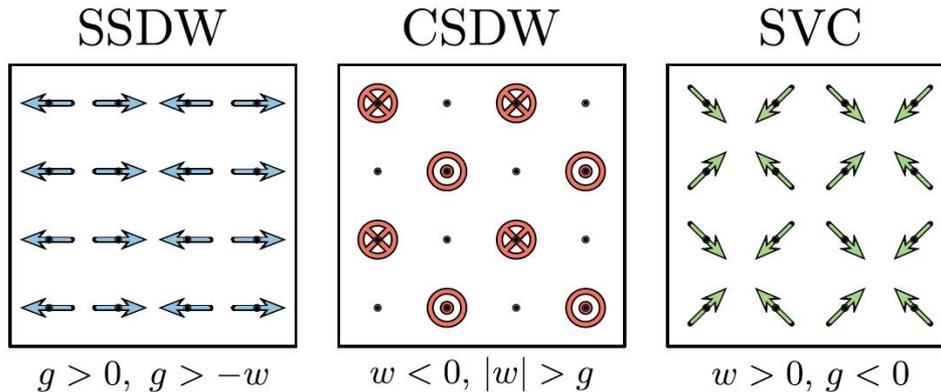
Universality + SOC leads to magnetic degeneracy



- RG flow continues on longer scales close to QCP
- Phases become more and more degenerate
- Basin of attraction of Gaussian fixed point increases with anisotropy

Vestigial orders from spin-density waves on the square lattice

- Three-types of **magnetic order** minimize free-energy



- All states break spatial symmetries in addition to $SO(3)$
- Construct **composite order** parameters

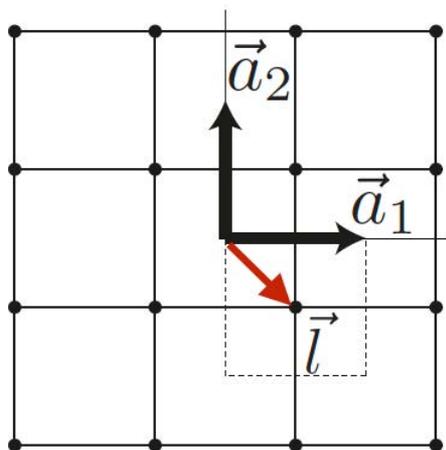
$$\phi_m = \sum_{\alpha, \beta=1}^{d_\Gamma} \eta_\alpha^* \Lambda_{\alpha\beta}^m \eta_\beta$$

- Symmetry group and irrep of primary order?
- Primary order breaks translational symmetry
 - Use extended point groups (treat as $q=0$ order)

[1] Lorenzana et al, PRL (2008); [2] Eremin et al, PRB (2010); [3] Brydon et al, PRB (2011); [4] Giovannetti et al, Nat. Commun. (2011); Wang et al., PRB (2015), M. H. Christensen, PPO, B. Andersen, R. M. Fernandes, PRL (2018).

Extended point group C_{4v}'''

- Extended point group: add translations $t_1=a_1$, $t_2=a_2$, a_1+a_2 to point group elements
- Spin-density wave with $Q_{1,2}$ then becomes $q = 0$ order
- Can analyze irreps of extended point group (instead of space group)



C_{4v} $h=8$	E	$2 C_4$	C_2	$2 \sigma_v$	$2 \sigma_d$
A_1	1	1	1	1	1
A_2	1	1	1	-1	-1
B_1	1	-1	1	1	-1
B_2	1	-1	1	-1	1
E	2	0	-2	0	0

$$\otimes \{t_1, t_2, t_1 + t_2\}$$

[1] Basko, PRB (2012); [2] Serbyn, Lee, PRB (2013); [3] Venderbos, PRB (2016).

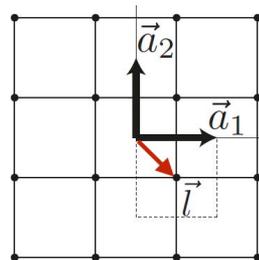
Vestigial order of $Q_{1,2}$ SDW on square lattice

TABLE VIII. Character table of the point group C_{4v}''' . Translations t_1 and t_2 correspond to $T(\vec{a}_1)$ and $T(\vec{a}_2)$, respectively, and $t_3 = T(\vec{a}_1 + \vec{a}_2)$. The conjugacy classes consist of the elements $C_1''' = \{I\}$, $C_2''' = \{t_1, t_2\}$, $C_3''' = \{t_3\}$, $C_4''' = \{C_2\}$, $C_5''' = \{t_1 C_2, t_2 C_2\}$, $C_6''' = \{t_3 C_2\}$, $C_7''' = \{C_4, C_4^{-1}, t_3 C_4, t_3 C_4^{-1}\}$, $C_8''' = \{t_1 C_4, t_1 C_4^{-1}, t_2 C_4, t_2 C_4^{-1}\}$, $C_9''' = \{\sigma_{v1}, \sigma_{v2}\}$, $C_{10}''' = \{t_1 \sigma_{v1}, t_2 \sigma_{v2}\}$, $C_{11}''' = \{t_2 \sigma_{v1}, t_1 \sigma_{v2}\}$, $C_{12}''' = \{t_3 \sigma_{v1}, t_3 \sigma_{v2}\}$, $C_{13}''' = \{\sigma_{d1}, \sigma_{d2}, t_3 \sigma_{d1}, t_3 \sigma_{d2}\}$, and $C_{14}''' = \{t_1 \sigma_{d1}, t_1 \sigma_{d2}, t_2 \sigma_{d1}, t_2 \sigma_{d2}\}$. The character table is taken from Ref. [21]. Notation is altered with respect to Ref. [21] to be consistent with the notation and definitions of this work.

Conjugacy class Point group C_{4v}'''	t_1, t_2		C_4				σ_v				σ_d			
	C_1'''	C_2'''	C_3'''	C_4'''	C_5'''	C_6'''	C_7'''	C_8'''	C_9'''	C_{10}'''	C_{11}'''	C_{12}'''	C_{13}'''	C_{14}'''
A_1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
A_2	1	1	1	1	1	1	1	1	-1	-1	-1	-1	-1	-1
B_1	1	1	1	1	1	1	-1	-1	1	1	1	1	-1	-1
B_2	1	1	1	1	1	1	-1	-1	-1	-1	-1	-1	1	1
E_1	2	2	2	-2	-2	-2	0	0	0	0	0	0	0	0
A_1'	1	-1	1	1	-1	1	1	-1	1	-1	-1	1	1	-1
A_2'	1	-1	1	1	-1	1	1	-1	-1	1	1	-1	-1	1
B_1'	1	-1	1	1	-1	1	-1	1	1	-1	-1	1	-1	1
B_2'	1	-1	1	1	-1	1	-1	1	-1	1	1	-1	1	-1
E_1'	2	-2	2	-2	2	-2	0	0	0	0	0	0	0	0
E_2	2	0	-2	2	0	-2	0	0	-2	0	0	2	0	0
E_3	2	0	-2	2	0	-2	0	0	2	0	0	-2	0	0
E_4	2	0	-2	-2	0	2	0	0	0	2	-2	0	0	0
E_5	2	0	-2	-2	0	2	0	0	0	-2	2	0	0	0

SDW order:

$$\mathbf{S}(\mathbf{r}) = \mathbf{m}_1 \sin(\mathbf{Q}_1 \cdot \mathbf{r}) + \mathbf{m}_2 \sin(\mathbf{Q}_2 \cdot \mathbf{r})$$

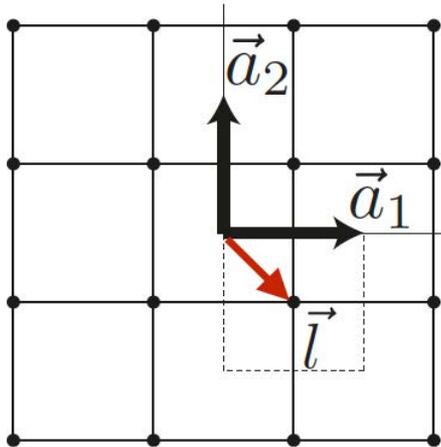


➤ Symmetry group: $\mathcal{G} = C_{4v}''' \otimes \text{SO}(3)$

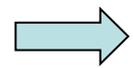
➤ Primary order $\eta_\alpha = (\mathbf{m}_1, \mathbf{m}_2)_\alpha$

➤ Transforms as $\Gamma = E_5 \otimes \Gamma^{S=1}$

Extended point group C_{4v}'''



- Symmetry group: $\mathcal{G} = C_{4v}''' \otimes \text{SO}(3)$
- Primary order $\eta_\alpha = (\mathbf{m}_1, \mathbf{m}_2)_\alpha$
- Transforms as $\Gamma = E_5 \otimes \Gamma^{S=1}$



$$\Gamma \otimes \Gamma = (E_5 \otimes E_5) \otimes (\Gamma^{S=1} \otimes \Gamma^{S=1})$$

Spatial irreps: $E_5 \otimes E_5 = A_1 \oplus B'_2 \oplus A'_2 \oplus B_1$

Spin irreps

$$\Gamma^{S*} \otimes \Gamma^S = \bigoplus_{j=0}^{2S} \Gamma^j$$

Construct all possible bilinears:

$$\phi_{m \equiv (r,j)}^\mu = \sum_{A,B} \eta_A \Lambda_{A,B}^{m,\mu} \eta_B$$

Pauli matrices τ^r (4x)

$$\Gamma \otimes \Gamma = (A_1 \oplus B'_2 \oplus A'_2 \oplus B_1) \otimes (\Gamma^0 \oplus \Gamma^1 \oplus \Gamma^2)$$

Gell-Mann matrices λ^j (9x)

$$\Lambda_{A,B}^{m \equiv (r,j),\mu} = \tau_{ab}^r \lambda_{\alpha\beta}^{j,\mu}$$

Singlet (scalar) vestigial orders

$$\Gamma \otimes \Gamma = (A_1 \oplus B'_2 \oplus A'_2 \oplus B_1) \otimes (\Gamma^0 \oplus \Gamma^1 \oplus \Gamma^2)$$

- S=0 singlet in spin space: **scalar vestigial orders**

$$\phi_{m \equiv (r,j)}^\mu = \sum_{A,B} \eta_A \Lambda_{A,B}^{m,\mu} \eta_B, \quad \text{with} \quad \lambda_{\alpha\beta}^{0,0} = \delta_{\alpha\beta}$$

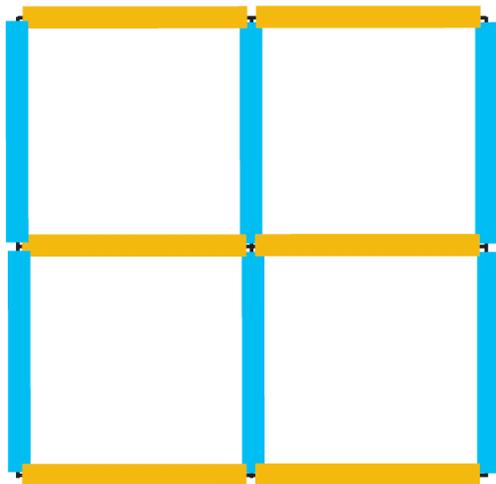
$$\phi_{(0,0)} = \mathbf{m}_1 \cdot \mathbf{m}_1 + \mathbf{m}_2 \cdot \mathbf{m}_2 \quad A_1 \text{ amplitude fluctuations (no broken symmetry)}$$

$$\phi_{(1,0)} = 2\mathbf{m}_1 \cdot \mathbf{m}_2 \quad \text{Composite order transforming as } B'_2 \text{ (CSDW)}$$

$$\phi_{(3,0)} = \mathbf{m}_1 \cdot \mathbf{m}_1 - \mathbf{m}_2 \cdot \mathbf{m}_2 \quad \text{Composite order transforming as } B_1 \text{ (nematic)}$$

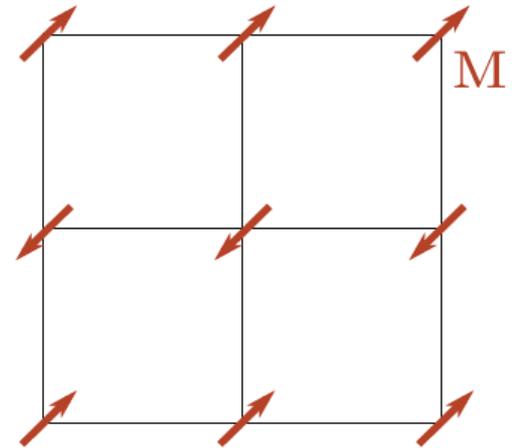
Nematic composite B_1 order

$\phi_{(3,0)} = \mathbf{m}_1 \cdot \mathbf{m}_1 - \mathbf{m}_2 \cdot \mathbf{m}_2$ Composite order transforming as B_1 (nematic)



Real-space: **bond order**

- Translations t_1, t_2 preserved
- C_4 and σ_d broken



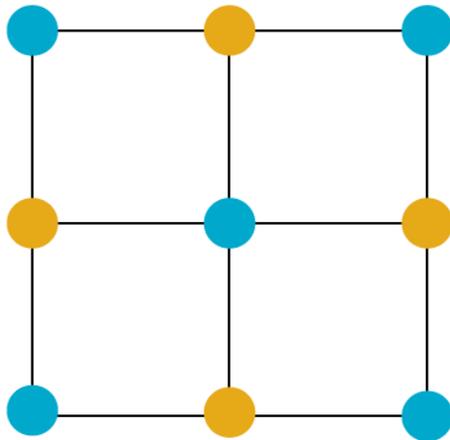
Primary order: **SSDW**

Conjugacy class Point group C_{4v}'''	t_1, t_2						C_4		σ_v			σ_d		
	c_1'''	c_2'''	c_3'''	c_4'''	c_5'''	c_6'''	c_7'''	c_8'''	c_9'''	c_{10}'''	c_{11}'''	c_{12}'''	c_{13}'''	c_{14}'''
B_1^-	1	1	1	1	1	1	-1	-1	1	1	1	1	-1	-1

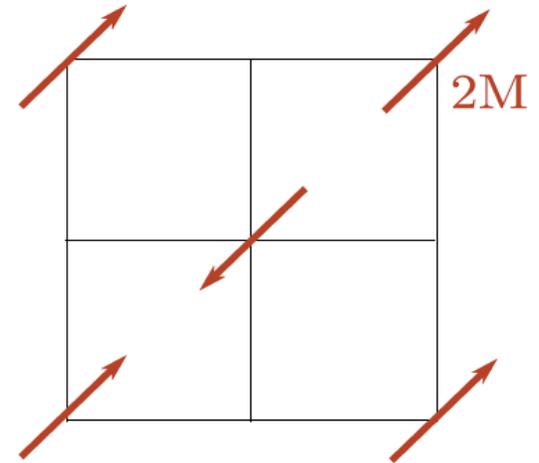
CDW (checkerboard) composite B'_2 order

$$\phi_{(1,0)} = 2\mathbf{m}_1 \cdot \mathbf{m}_2$$

Composite order transforming as B'_2
(SVDW)



- Translations t_1, t_2 broken
- C_4 and σ_v broken



Real-space: **site order**

Primary order: **CSDW**

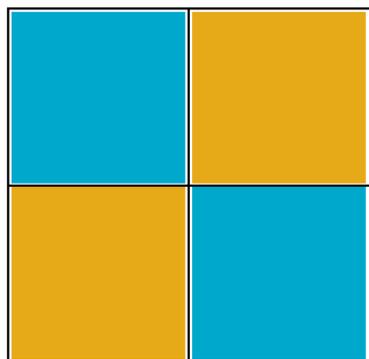
Conjugacy class Point group C_{4v}'''	t_1, t_2						C_4		σ_v		σ_d			
	c_1'''	c_2'''	c_3'''	c_4'''	c_5'''	c_6'''	c_7'''	c_8'''	c_9'''	c_{10}'''	c_{11}'''	c_{12}'''	c_{13}'''	c_{14}'''
B'_2	1	-1	1	1	-1	1	-1	1	-1	1	1	-1	1	-1
B_1	1	1	1	1	1	1	-1	-1	1	1	1	1	-1	-1

(Pseudo)-vector vestigial orders

$$\Gamma \otimes \Gamma = (A_1 \oplus B'_2 \oplus A'_2 \oplus B_1) \otimes (\Gamma^0 \oplus \Gamma^1 \oplus \Gamma^2)$$

- S=1 triplet in spin space: **vector vestigial orders**

$$\phi_{m \equiv (r,j)}^\mu = \sum_{A,B} \eta_A \Lambda_{A,B}^{m,\mu} \eta_B, \quad \text{with } \lambda_{\alpha\beta}^{1,\mu} = i\epsilon_{\alpha\beta\mu}$$

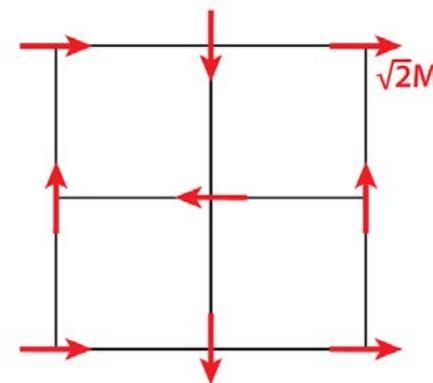


Real-space:
plaquette order

$$\phi_{(2,1)} = 2\mathbf{m}_1 \times \mathbf{m}_2$$

Composite order transforming as A'_2 :

- preserves C_4
- breaks mirrors
- breaks translation



Primary order:
spin-vortex crystal

Conjugacy class	t_1, t_2						C_4	σ_v	σ_d					
Point group C_{4v}'''	C_1'''	C_2'''	C_3'''	C_4'''	C_5'''	C_6'''	C_7'''	C_8'''	C_9'''	C_{10}'''	C_{11}'''	C_{12}'''	C_{13}'''	C_{14}'''
A'_2	1	-1	1	1	-1	1	1	-1	-1	1	1	-1	-1	1

Tensorial vestigial orders

$$\Gamma \otimes \Gamma = (A_1 \oplus B'_2 \oplus A'_2 \oplus B_1) \otimes (\Gamma^0 \oplus \Gamma^1 \oplus \Gamma^2)$$

- S=2 symmetric tensor in spin space

$$\phi_{m \equiv (r,j)}^{\mu} = \sum_{A,B} \eta_A \Lambda_{A,B}^{m,\mu} \eta_B, \quad \text{with } \lambda_{\alpha\beta}^{2,(\mu,\mu')} = \frac{1}{2} (\delta_{\alpha\mu} \delta_{\beta\mu'} + \delta_{\alpha\mu'} \delta_{\beta\mu}) - \frac{1}{3} \delta_{\alpha\beta} \delta_{\mu\mu'}.$$

$$\phi_{(0,2)}^{\mu\mu'} = m_1^\mu m_1^{\mu'} + m_2^\mu m_2^{\mu'} - \frac{1}{3} \delta_{\alpha\beta} (\mathbf{m}_1 \cdot \mathbf{m}_1 + \mathbf{m}_2 \cdot \mathbf{m}_2)$$

$$\phi_{(1,2)}^{\mu\mu'} = m_1^\mu m_2^{\mu'} + m_2^\mu m_1^{\mu'} - \frac{1}{3} \delta_{\mu\mu'} (\mathbf{m}_1 \cdot \mathbf{m}_2 + \mathbf{m}_2 \cdot \mathbf{m}_2)$$

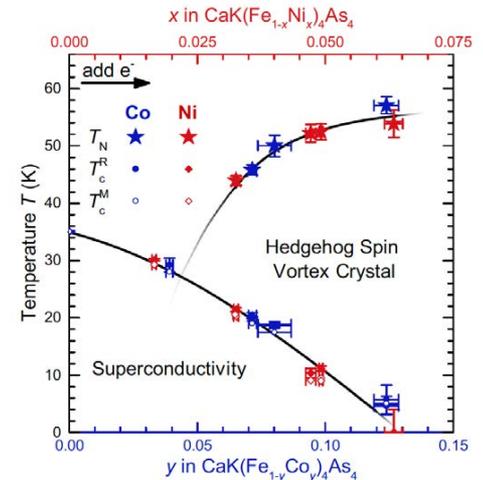
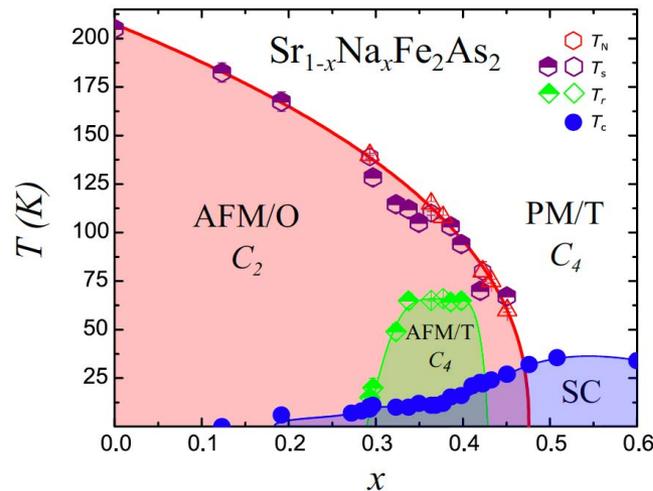
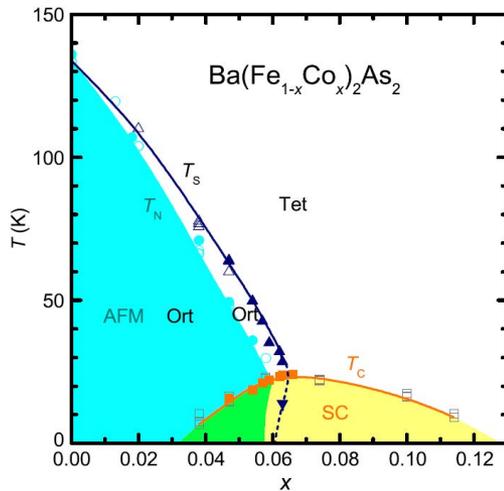
$$\phi_{(3,2)}^{\mu\mu'} = m_1^\mu m_1^{\mu'} - m_2^\mu m_2^{\mu'} - \frac{1}{3} \delta_{\mu\mu'} (\mathbf{m}_1 \cdot \mathbf{m}_1 - \mathbf{m}_2 \cdot \mathbf{m}_2)$$

Composite tensorial orders:

- $\phi_{(0,2)}$ transforms spatially as A_1 : **nematicity purely in spin space** (NiGa₂S₄)
- Presence of spin-orbit coupling would induce nematicity in real-space as well.

[1] Chandra, Coleman (1991), [2] Nakatsuji, Science (2005).

Materials: vestigial orders in iron-based superconductors



- Size of vestigial phase depends on microscopics, size of fluctuations
 - Vestigial orders (often) found on hole-doped side
 - Not found on electron-doped side: joint first-order transition
- Vestigial order can be induced by breaking corresponding symmetry (1144)
 - Path to control magnetic order

[1] S. Nandi *et al.*, PRL **104**, 057006 (2010); [2] Taddei *et al.*, PRB (2016); [3] W. R. Meier *et al.*, npj Quantum Materials (2018).

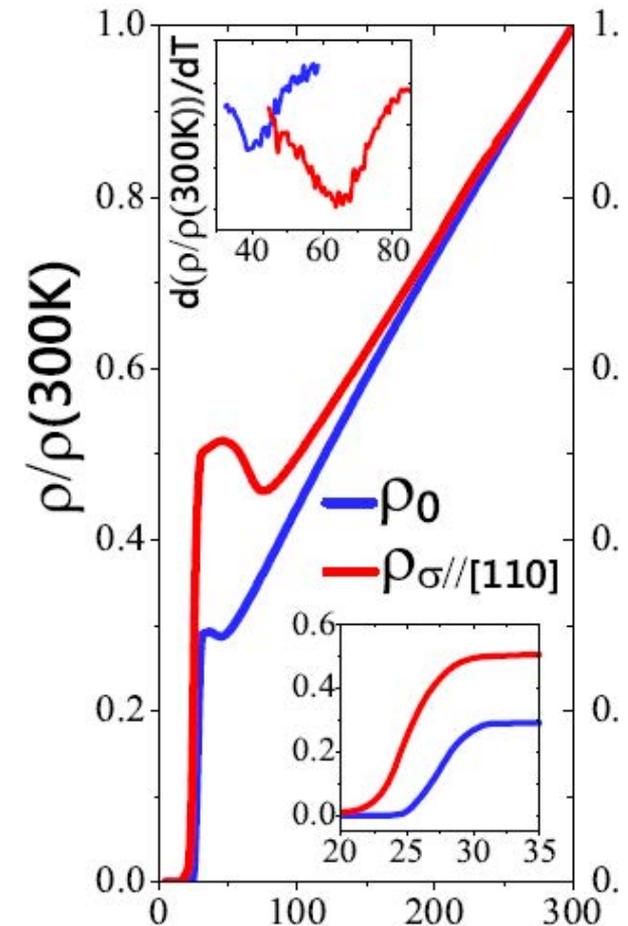
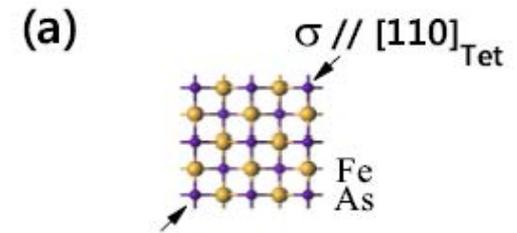
Controlling magnetic order

- **How can we control phases?**
 - Doping, pressure, magnetic field
 - Other possibilities

Coupling to vestigial order parameter

Simplest case: SSDW

- Apply **external strain** σ to cause orthorhombic distortion
- Acts as “conjugate field” for emergent order parameter $\phi_{nematic}$
- $\Delta F = \sigma \phi_{nematic}$
- **Transition temperature T_N to stripe order increases** (27K in example)

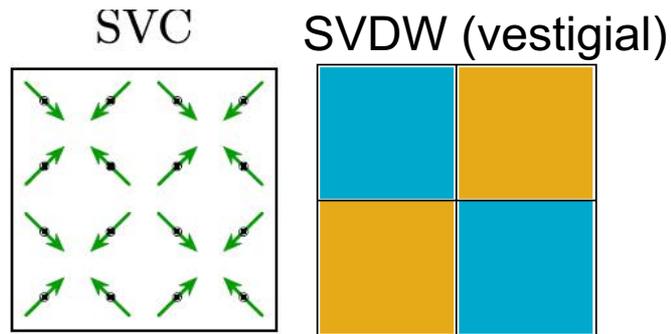


[1] Kuo et al., PRB 86, 134507 (2012)

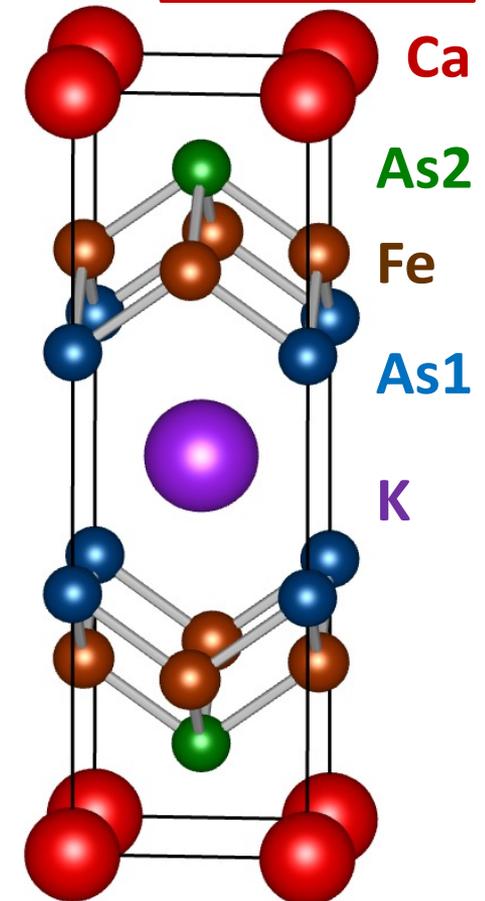
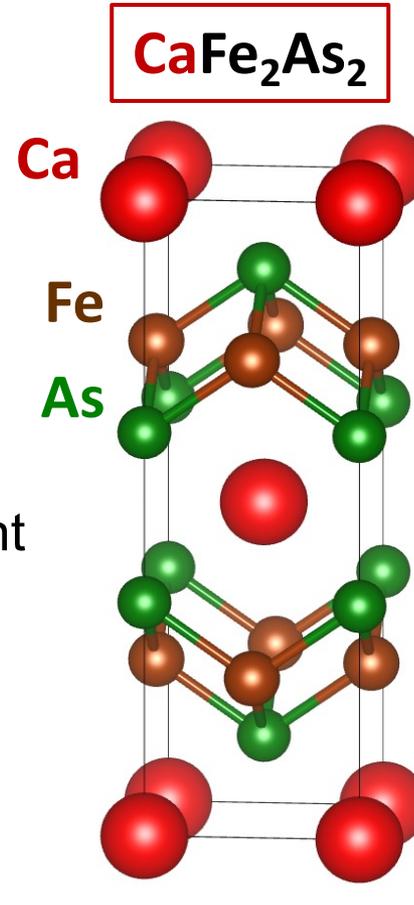
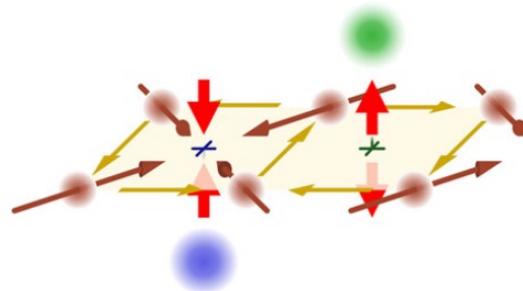
CaKFe₄As₄: coupling to SVDW emergent order

CaKFe₄As₄

How to generate Spin Vortex
Crystal magnetic order?



- Realize conjugate field to emergent SVDW order
- Two inequivalent As sites
- Breaks glide plane (-4) symmetry
- Lowers SVC magnetic state to be ground state

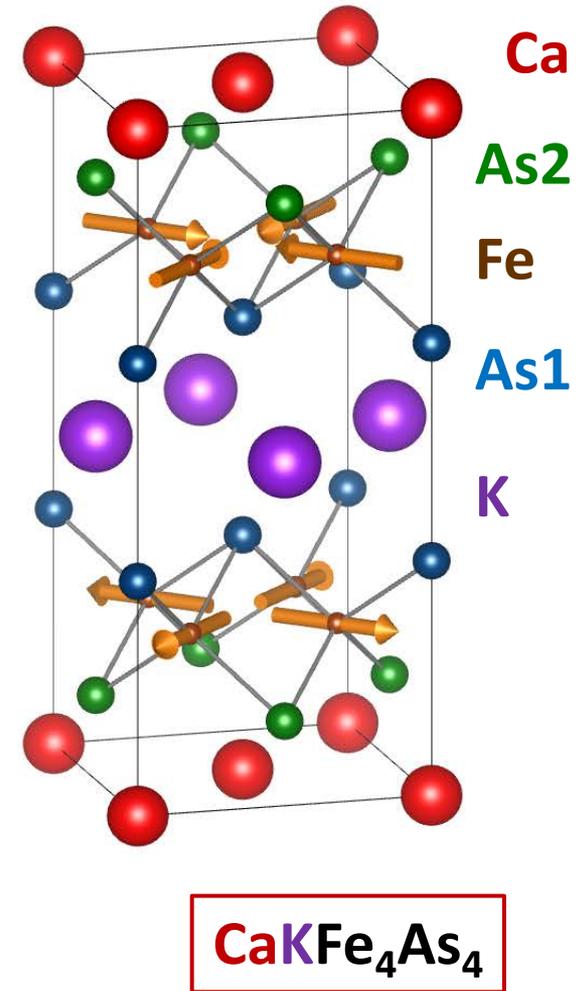
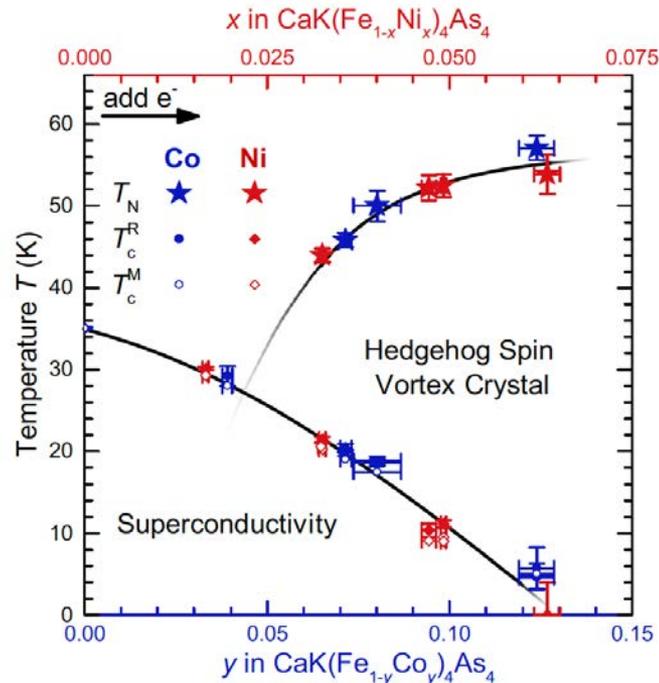


$$F_{\eta} = -\frac{1}{2}\eta \cdot (M_1 \times M_2).$$

CaKFe₄As₄: coupling to SVDW emergent order

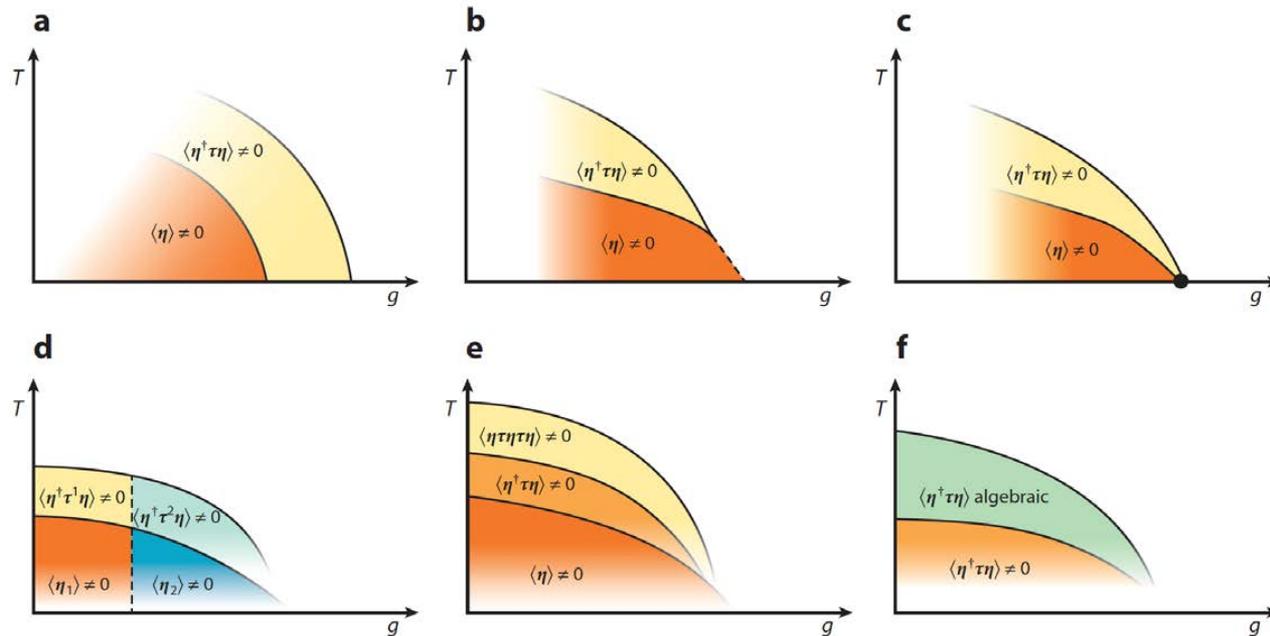
- Crystal structure generates conjugate field for emergent SVDW
- Lowers **SVC magnetic state** $\frac{\eta_c}{2|a|} = \sqrt{\frac{E_{GS}}{E_{SVC}(0)}} - 1$
- First time SVC phase is experimentally realized!**

$$F_\eta = -\frac{1}{2}\eta \cdot (M_1 \times M_2).$$



W. R. Meier, ..., PPO, ..., P. C. Canfield, npj Quantum Materials (2018).

Summary



- Vestigial orders naturally leads to complex phase diagrams with multiple phases having comparable transition temperatures
- Powerful concept to explain complexity of quantum materials beyond competing orders
- Vestigial order can be used to control phase diagram, including the associated primary “mother” phase

[1] R. M. Fernandes, PPO, J. Schmalian, Annu. Rev. Cond. Mat., in press (2019).