3D HONEYCOMB IRIDATES: THE PURSUIT OF KITAEV

Eric Lee | University of Toronto

KITP: Novel states in Spin-Orbit Coupled Quantum Matter: from Models to Materials

July 28 2015

COLLABORATORS

HEUNG-SIK KIM (TORONTO)
ROBERT SCHAFFER (TORONTO)
JEFFREY RAU (WATERLOO)
YUAN-MING LU (OHIO)
SUBHRO BHATTACHARJEE (BANGALORE)
HAE-YOUNG KEE (TORONTO)
YONG BAEK KIM (TORONTO)

β-Li_2IrO_3	H0	HYPERHONEYCOMB
γ-Li_2IrO_3	H1	STRIPYHONEYCOMB
		A_2IrO_3
α-$(Li/Na)_2IrO_3$	H∞	2D HONEYCOMB


TRI-COORDINATED
EDGED-SHARED
IrO6 OCTAHEDRA
LARGE
SPIN-ORBIT + CORRELATIONS
SMALL
DISTORTIONS
HYPERHONEYCOMB
STRIPYHONEYCOMB
2D HONEYCOMB
CANDIDATE
KITAEV
SPIN LIQUID

MAGNETIC ORDER

Li_2IrO_3: SPIRAL

HYPERHONEYCOMB

STRIPYHONEYCOMB

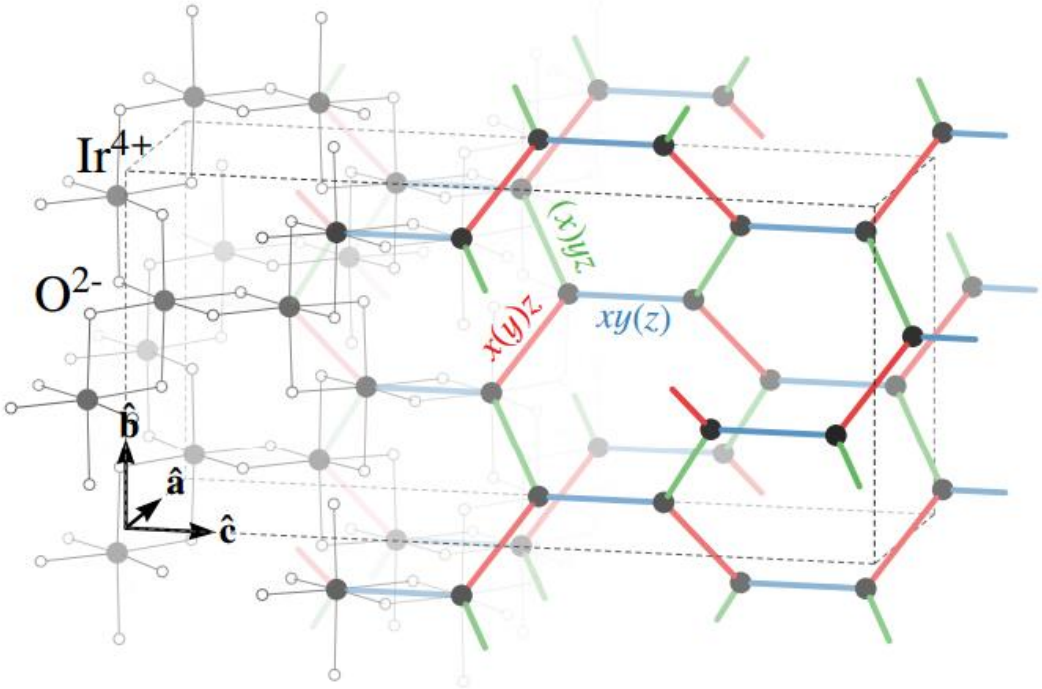
2D HONEYCOMB

CANDIDATE KITAEV SPIN LIQUID

HYPERHONEYCOMB
STRIPYHONEYCOMB
2D HONEYCOMB

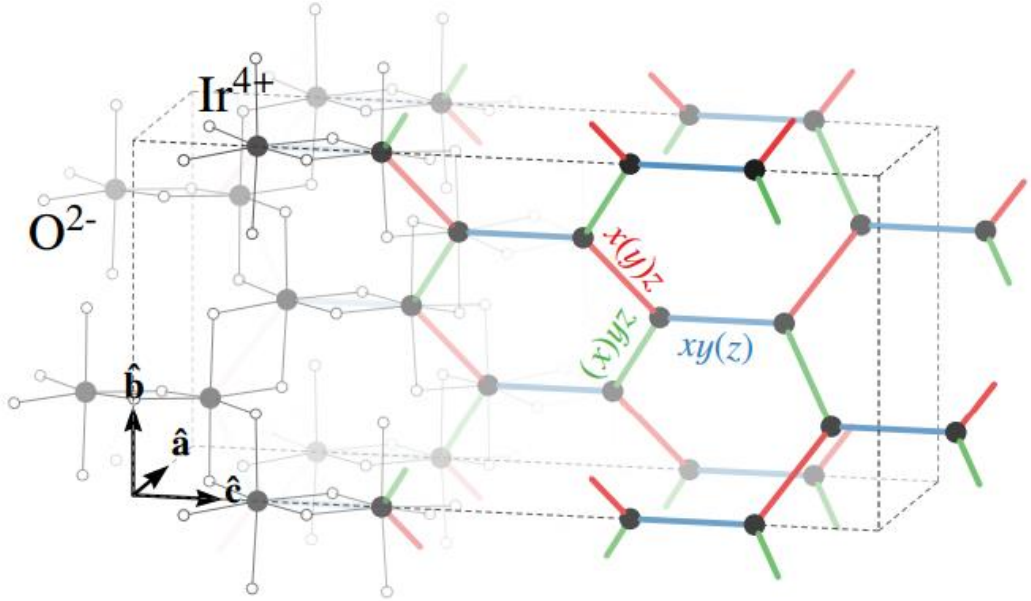
WHERE DID THE
KITAEV
PHYSICS GO?

CRYSTAL STRUCTURE



HYPERHONEYCOMB

T TAKAYAMA ET AL.
PRL 114 077202 (2015)



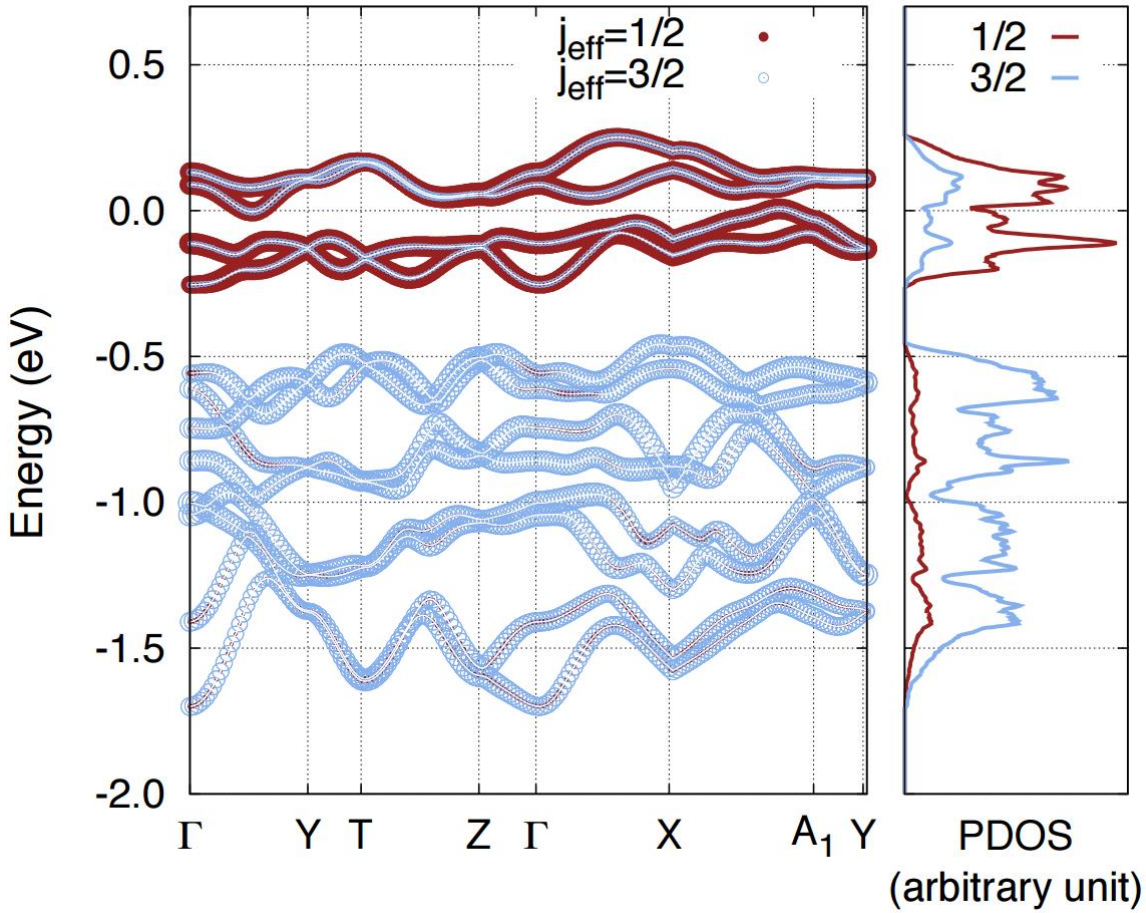
STRIPYHONEYCOMB

K MODIC ET AL.
NAT COMM 5 4203 (2014)

CRYSTAL STRUCTURE

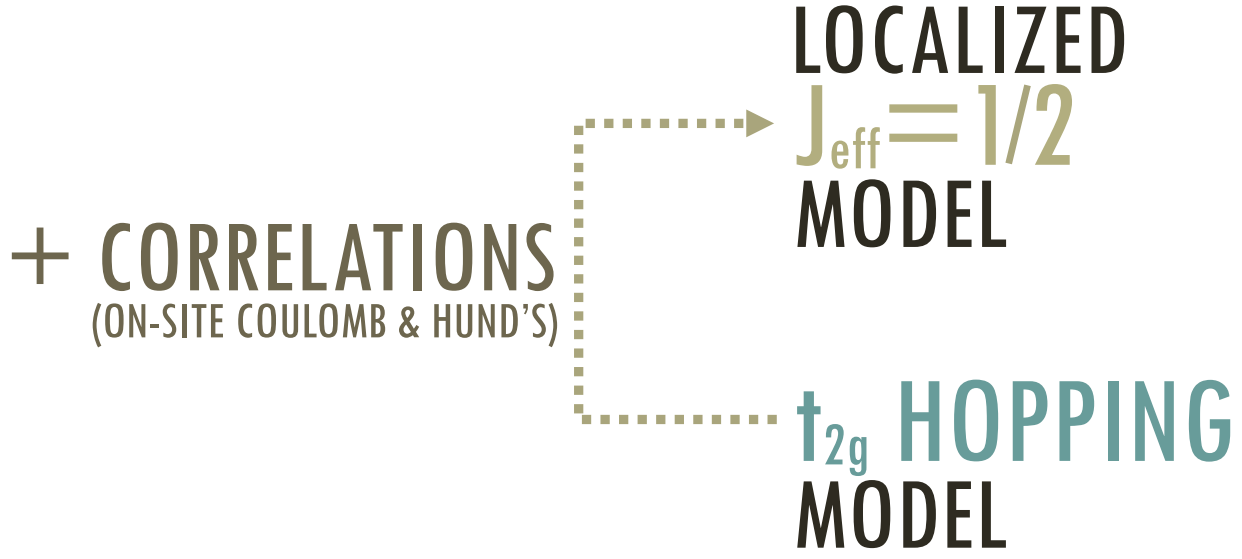
	Ir-Ir DISTANCE (Å)	Ir-Ir-Ir ANGLE (°)	Ir-O-Ir ANGLE (°)
HYPERHONEYCOMB	2.974±0.003	120.0±0.3	94.5±0.1
STRIPYHONEYCOMB	2.962±0.022	120.0±0.1	93.5±3.1
2D-Na_2IrO_3	3.132±0.004	120.1±0.2	98.5±0.8

GGA with SOC



HYPERHONEYCOMB
VALIDITY OF
$J_{eff}=1/2$
PICTURE

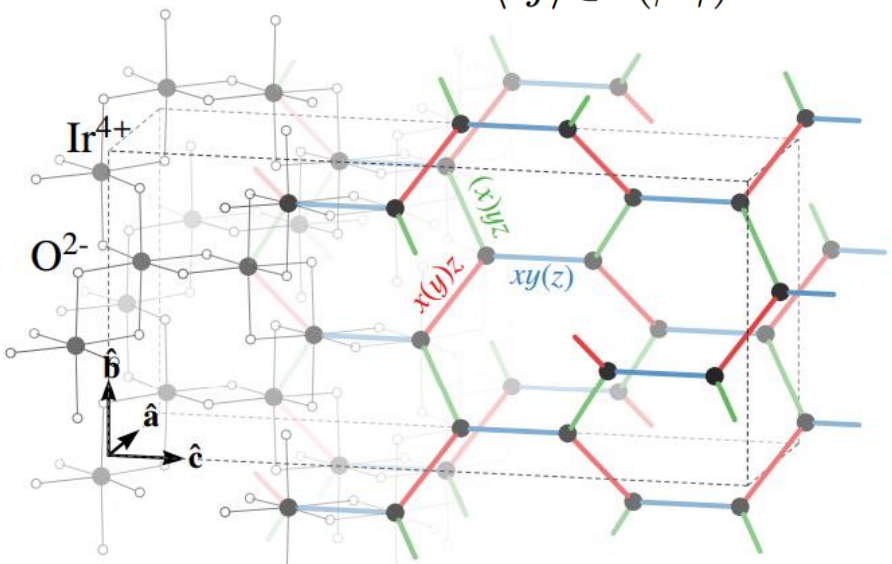
HS KIM, EKH LEE, YB KIM
arXiv:1502.00006 (2015)


+ CORRELATIONS
(ON-SITE COULOMB & HUND'S)
LOCALIZED
$J_{eff}=1/2$
MODEL
t_{2g} HOPPING
MODEL

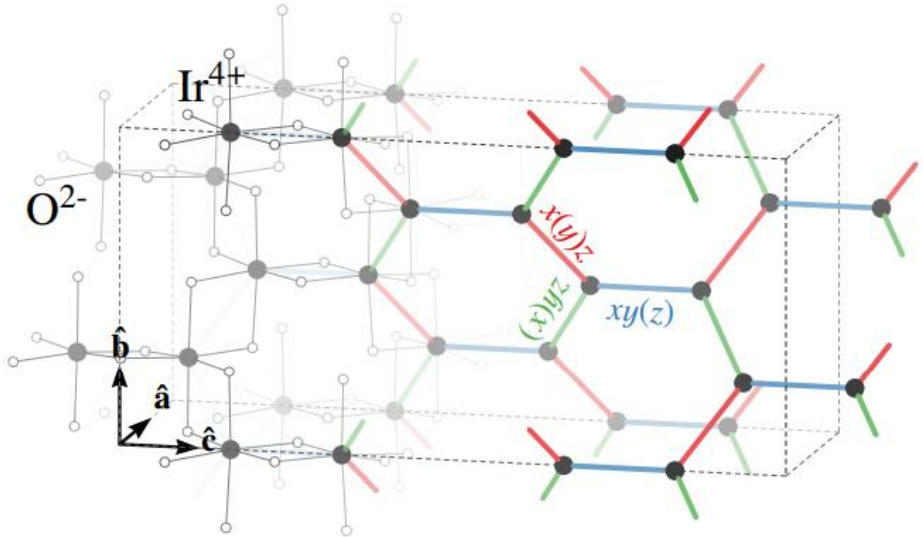
GENERICALLY EDGED-SHARED IrO_6 OCTAHEDRA

LOCALIZED $J_{eff}=1/2$ MODEL

$$H = \sum_{\langle ij \rangle \in \alpha(\beta\gamma)} JS_i \cdot S_j + KS_i^\alpha S_j^\alpha + \Gamma^\alpha (S_i^\beta S_j^\gamma + S_i^\gamma S_j^\beta)$$



HYPERHONEYCOMB



STRIPYHONEYCOMB

JG RAU, EKH LEE, HY KEE
PRL 112, 077204 (2014)

KITAEV MODEL

$$H = \sum_{\langle ij \rangle \in \alpha(\beta\gamma)} J S_i \cdot S_j + K S_i^\alpha S_j^\alpha + \Gamma^\alpha (S_i^\beta S_j^\gamma + S_i^\gamma S_j^\beta)$$

$$b_i^x, b_i^y, b_i^z, c$$

$$S_i^\alpha = \frac{1}{2} i b_i^\alpha c$$

$$H = \frac{i}{2} \sum_{\langle ij \rangle \in \alpha} u_{ij}^\alpha c_i c_j \qquad \text{WHERE} \quad u_{ij}^\alpha = i b_i^\alpha b_j^\alpha$$

A KITAEV
ANNALS OF PHYSICS 321, 2 (2006)

KITAEV MODEL

$$H = \frac{i}{2} \sum_{\langle ij \rangle \in \alpha} u_{ij}^{\alpha} c_i c_j$$

$$[u_{ij}^{\alpha}, H] = 0 \qquad \mathcal{W}_P = \prod_{\text{loop}} u_{ij}^{\alpha}$$

HYPERHONEYCOMB
0-FLUX SECTOR

STRIPYHONEYCOMB
π-FLUX SECTOR

R SCHAFFER, EKH LEE, YM LU, YB KIM
PRL 114, 116803 (2015)

KITAEV MODEL

$$\mathbf{H}_n^{\Phi} = \sum_k \vec{c}^{\,T}_{n,-k} H^{\Phi}_{n,k} \vec{c}_{n,k} \quad \text{WHERE} \quad H^{\Phi}_{n,k} = \begin{bmatrix} 0 & -iD^{\Phi}_{n,k} \\ i\left(D^{\Phi}_{n,k}\right)^{\dagger} & 0 \end{bmatrix}$$

GAPLESS MODES DETERMINED BY TWO EQUATIONS

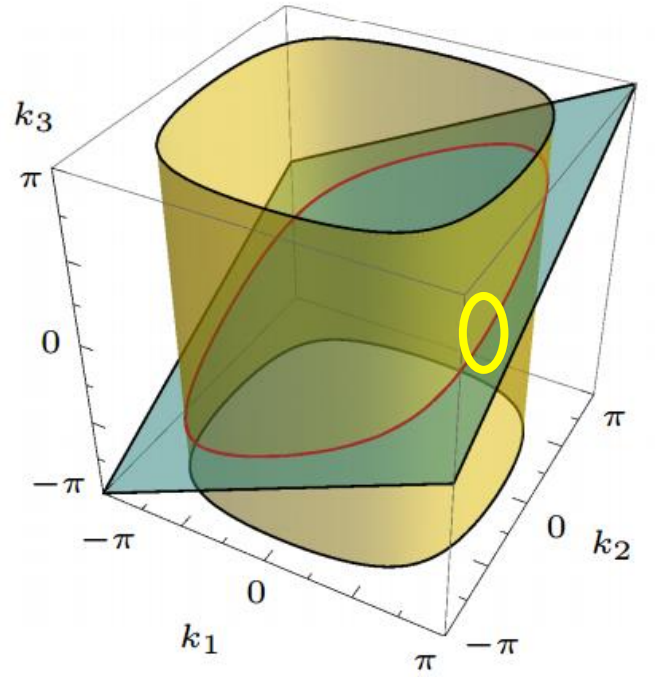
$$\mathrm{Re}\left[\det(D_k)\right] = 0$$
$$\mathrm{Im}\left[\det(D_k)\right] = 0$$

& 3 UNKNOWNS

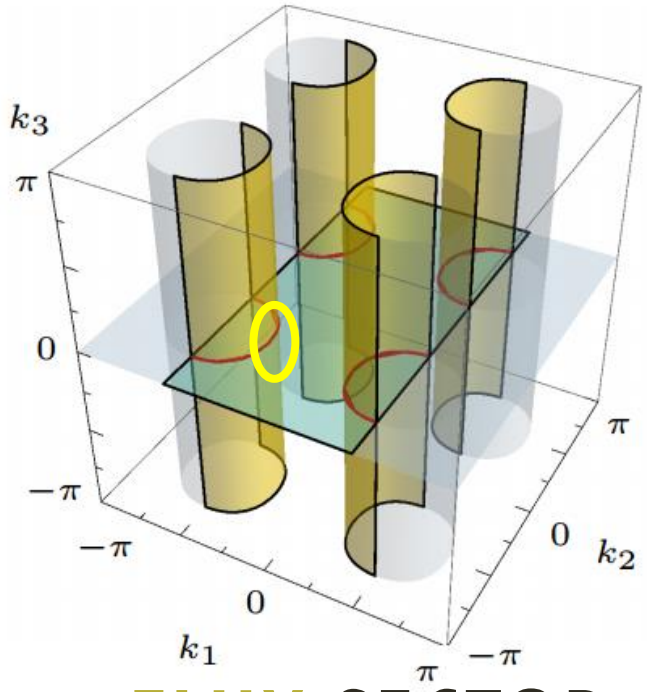
NODAL RINGS

R SCHAFFER, EKH LEE, YM LU, YB KIM
PRL 114, 116803 (2015)

NODAL RING SPECTRA



BDI CLASS

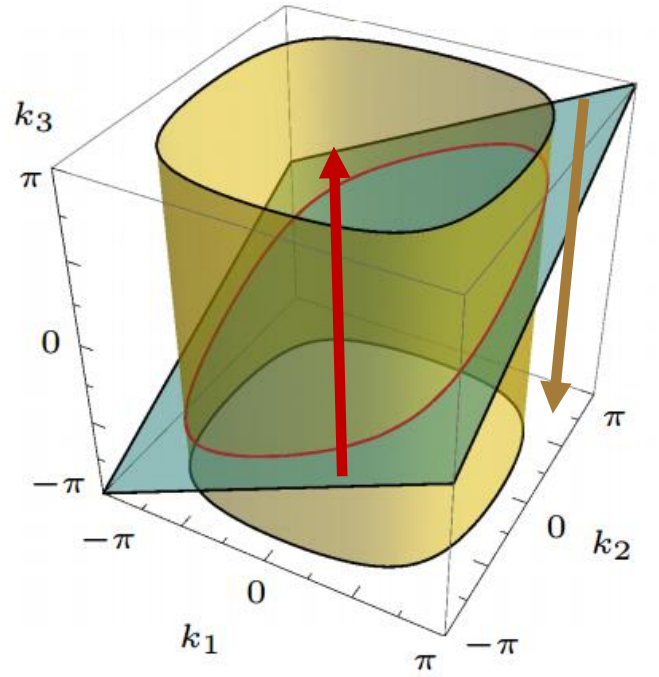


0-FLUX SECTOR
HYPERHONEYCOMB

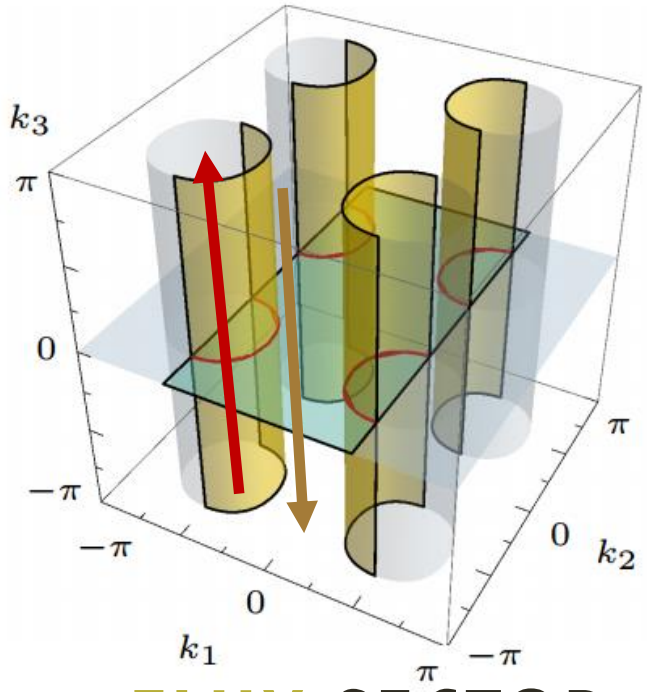
π-FLUX SECTOR
STRIPYHONEYCOMB

TOPOLOGICAL INVARIANT $$\nu = \frac{1}{4\pi i} \oint \mathrm{d}k \mathrm{Tr}[D_{\mathbf{k}}^{-1} \partial_k D_{\mathbf{k}} - (D^\dagger)_{\mathbf{k}}^{-1} \partial_k D_{\mathbf{k}}^\dagger]$$

NODAL RING SPECTRA



BDI CLASS

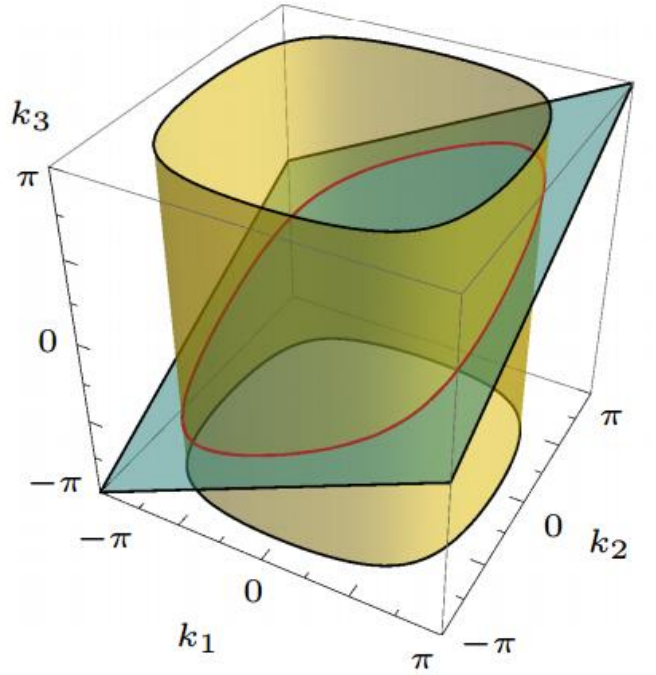


0-FLUX SECTOR
HYPERHONEYCOMB

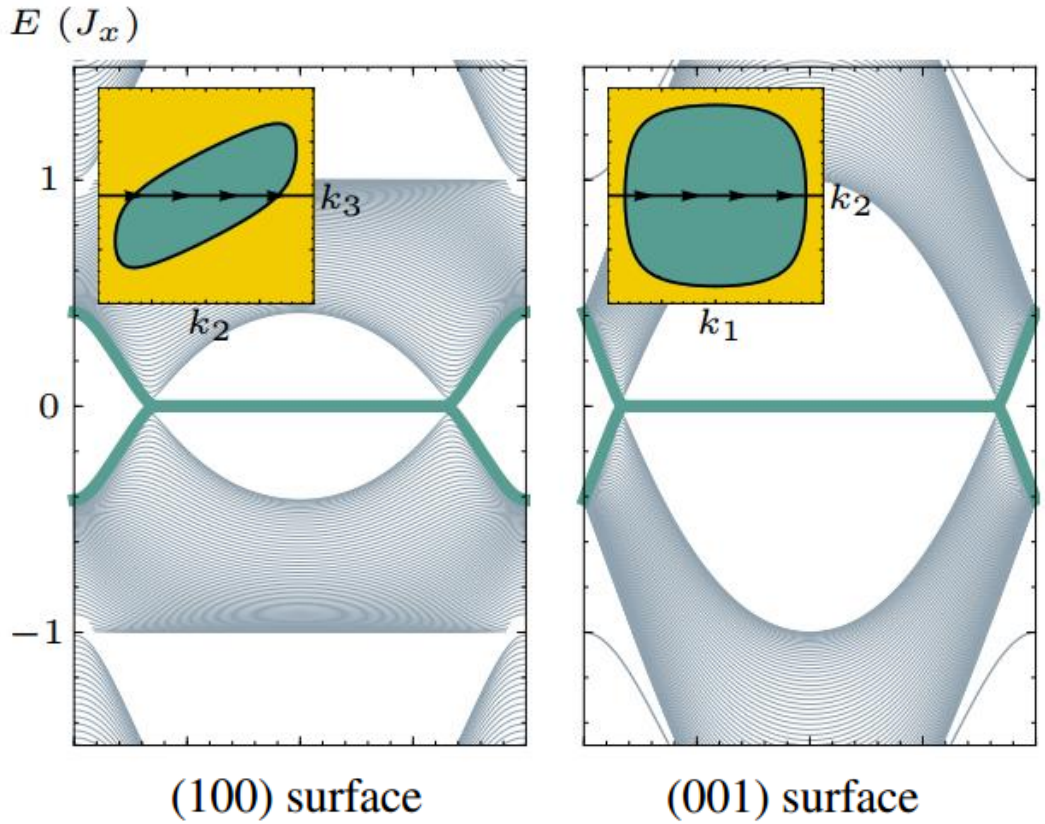
π-FLUX SECTOR
STRIPYHONEYCOMB

TOPOLOGICAL INVARIANT $$\nu = \frac{1}{4\pi i} \oint \mathrm{d}k \mathrm{Tr}[D_{\mathbf{k}}^{-1} \partial_k D_{\mathbf{k}} - (D^\dagger)_{\mathbf{k}}^{-1} \partial_k D_{\mathbf{k}}^\dagger]$$

NODAL RING SPECTRA



0-FLUX SECTOR
HYPERHONEYCOMB

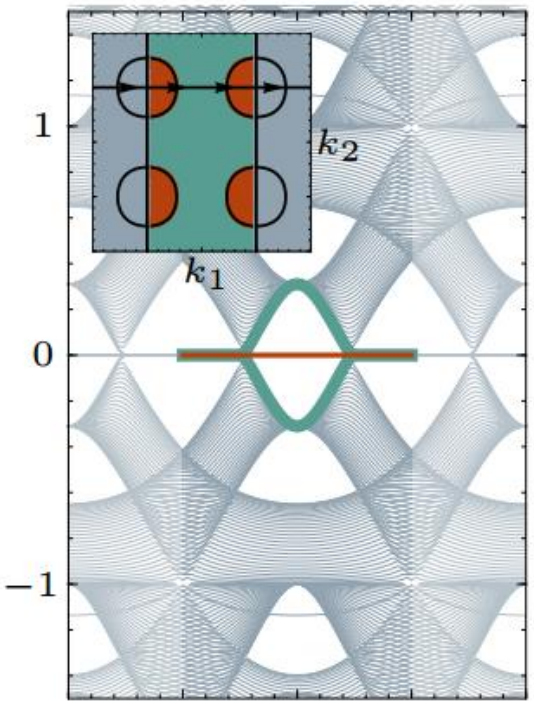


(100) surface (001) surface

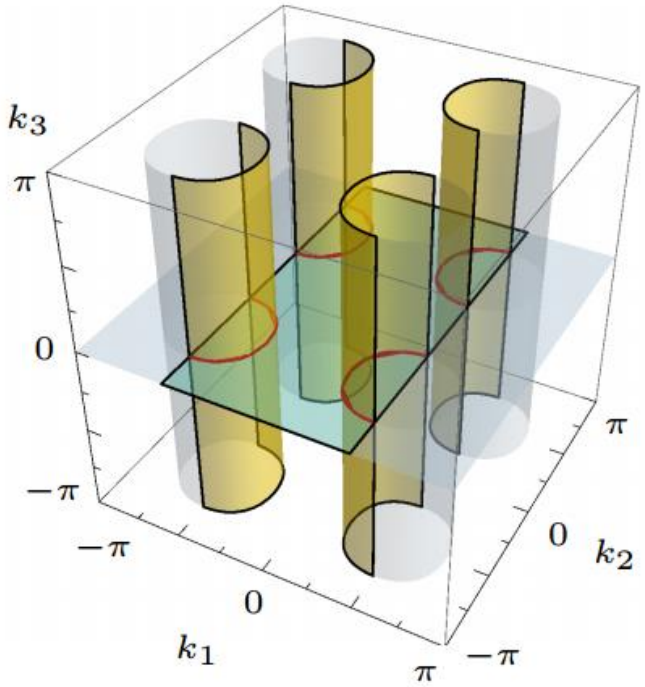
$$\nu = 0\ 1\ 2$$

R SCHAFFER, EKH LEE, YM LU, YB KIM
PRL 114, 116803 (2015)

NODAL RING SPECTRA



(001) surface

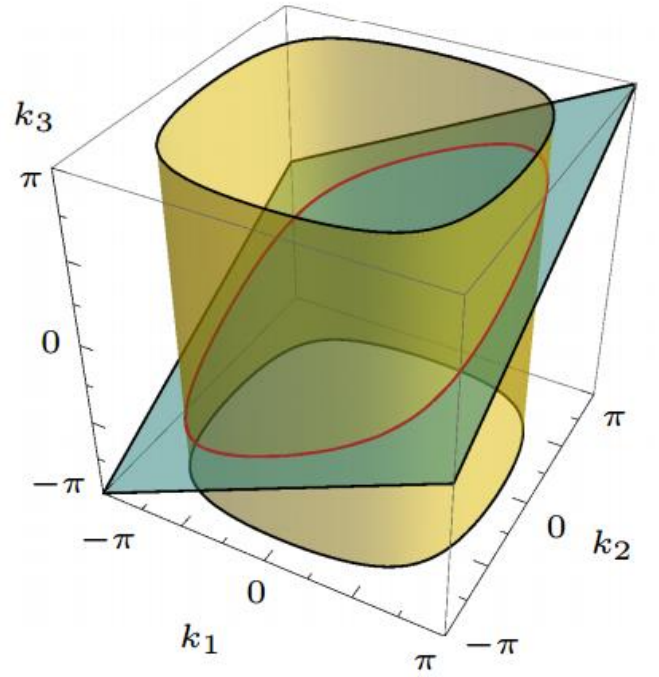


π-FLUX SECTOR
STRIPYHONEYCOMB

$$\nu = 0\ 1\ 2$$

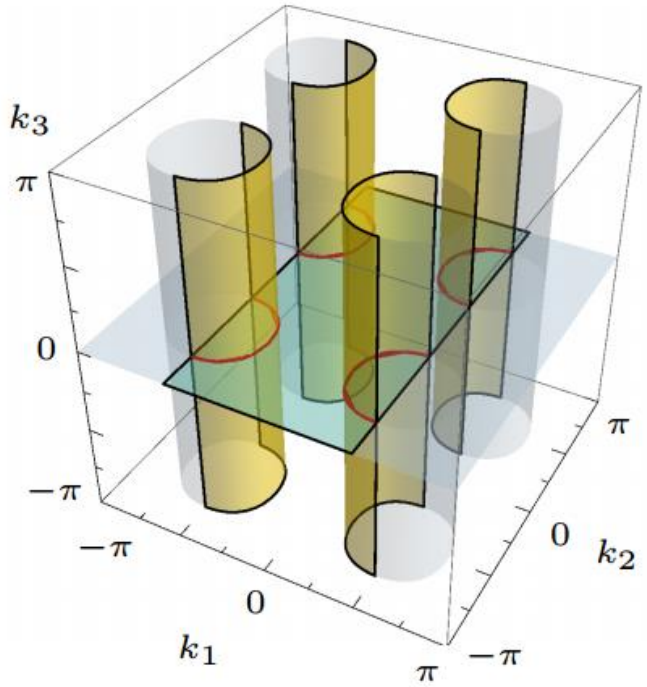
R SCHAFFER, EKH LEE, YM LU, YB KIM
PRL 114, 116803 (2015)

NODAL RING SPECTRA



0-FLUX SECTOR
HYPERHONEYCOMB

TOPOLOGICAL
SPINON
SEMIMETAL



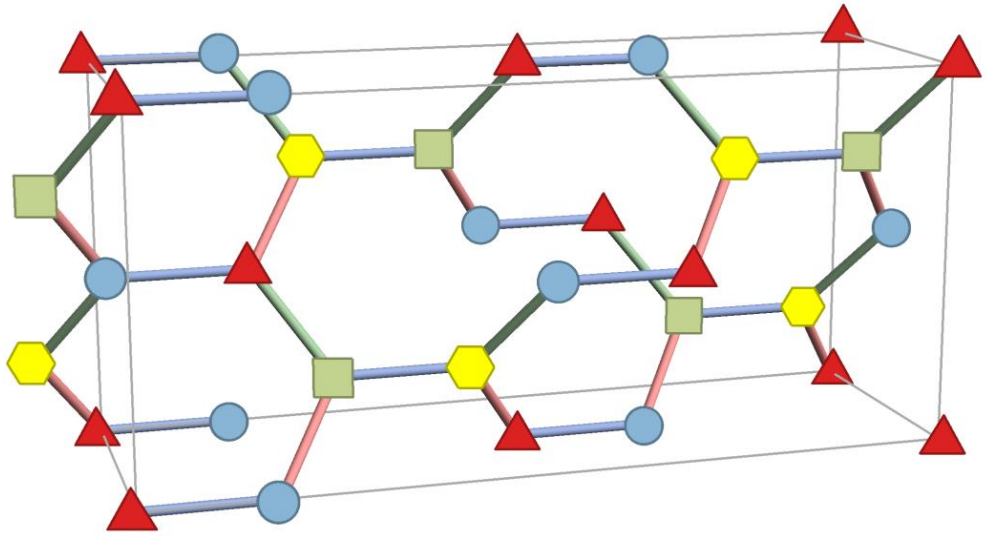
π-FLUX SECTOR
STRIPYHONEYCOMB

R SCHAFFER, EKH LEE, YM LU, YB KIM
PRL 114, 116803 (2015)

HEISENBERG-KITAEV MODEL

FOUR-SUBLATTICE TRANSFORMATION

$$H = \sum_{\langle ij \rangle \in \alpha(\beta\gamma)} JS_i \cdot S_j + KS_i^\alpha S_j^\alpha + \Gamma^\alpha (S_i^\beta S_j^\gamma + S_i^\gamma S_j^\beta)$$



$$(J, K) \longrightarrow (-J, K - 2J)$$

G KHALIULLIN
PROG TH. PHYS 160, 155 (2005)

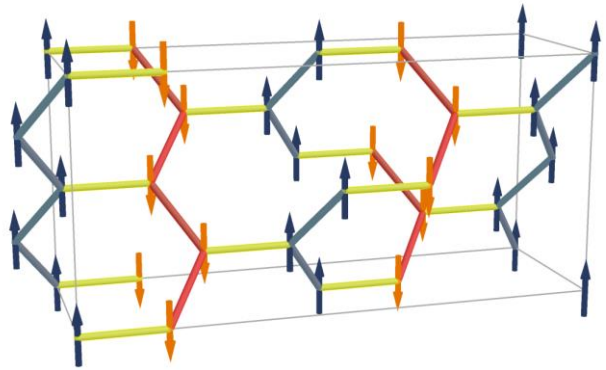
J CHALOUPKA, G JACKELI, G KHALIULLIN
PRL 105, 027204 (2010)

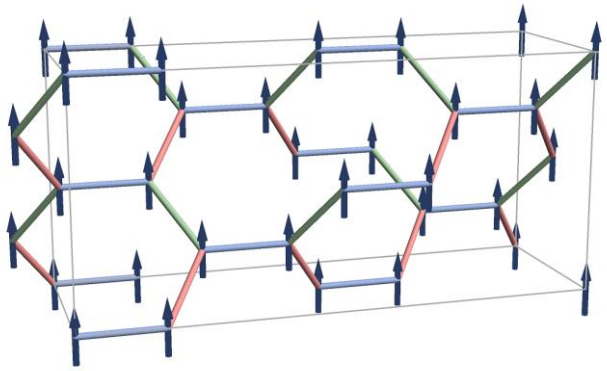
I KIMCHI, A VISHWANATH
PRB 89, 014414 (2014)

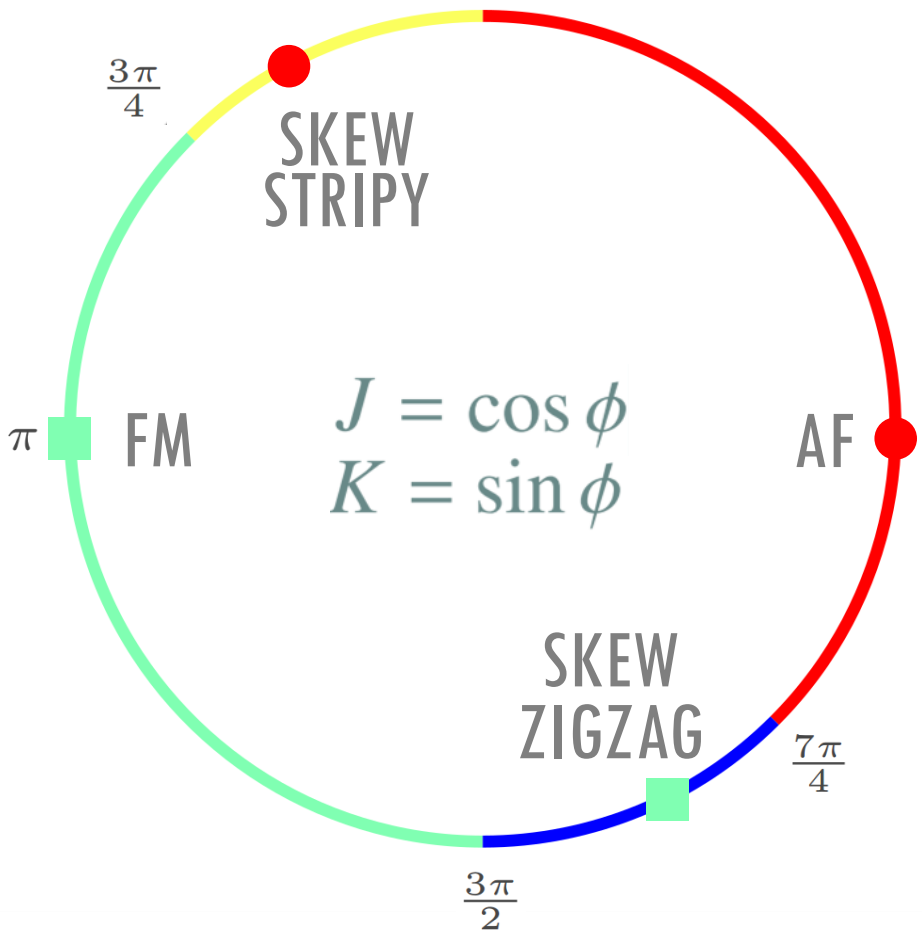
EKH LEE, R SCHAFFER, S BHATTACHAREE, YB KIM
PRB 89, 045117 (2014)

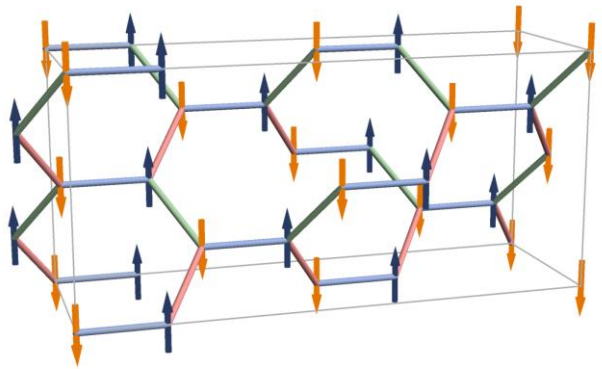
HEISENBERG-KITAEV MODEL

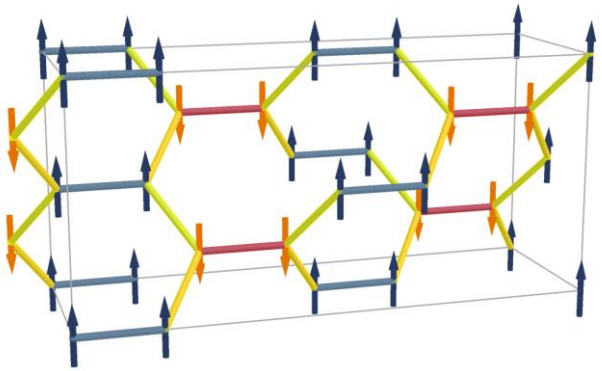
FOUR-SUBLATTICE TRANSFORMATION











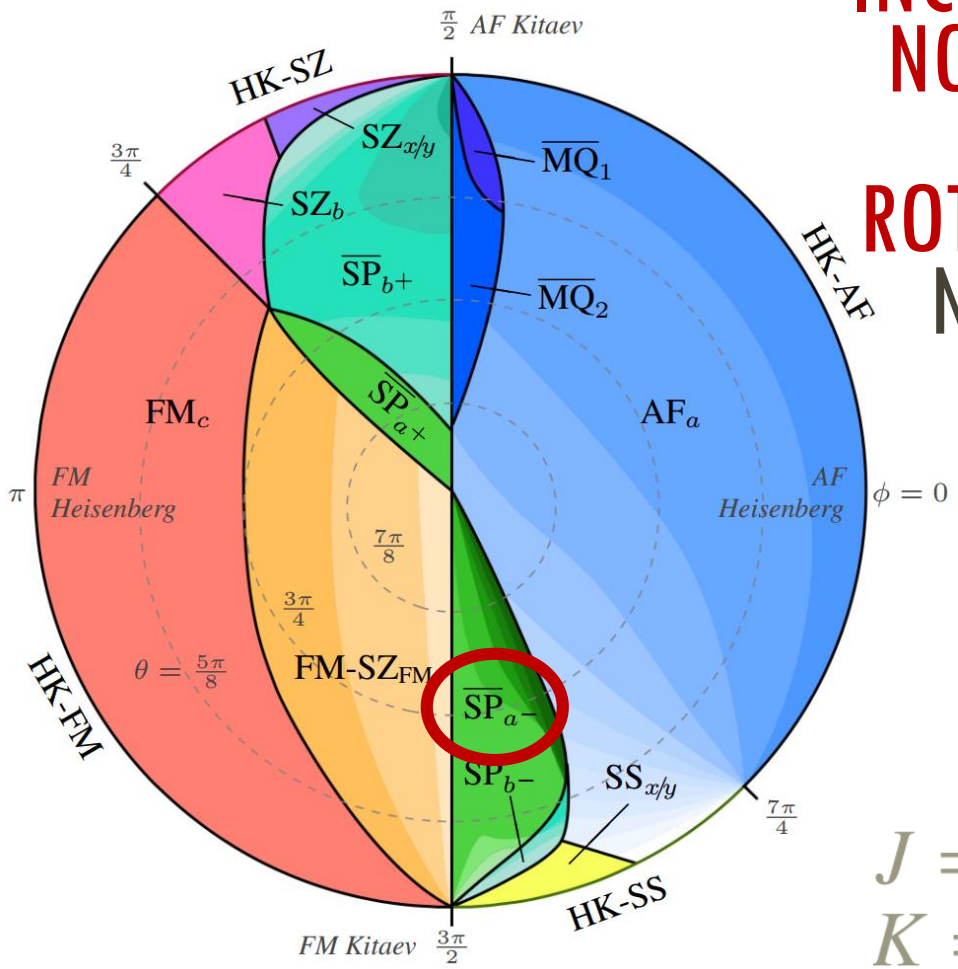
EKH LEE, R SCHAFFER, S BHATTACHAREE, YB KIM
PRB 89, 045117 (2014)

JKΓ MODEL

$$H = \sum_{\langle ij \rangle \in \alpha(\beta\gamma)} J S_i \cdot S_j + K S_i^\alpha S_j^\alpha + \Gamma^\alpha (S_i^\beta S_j^\gamma + S_i^\gamma S_j^\beta)$$

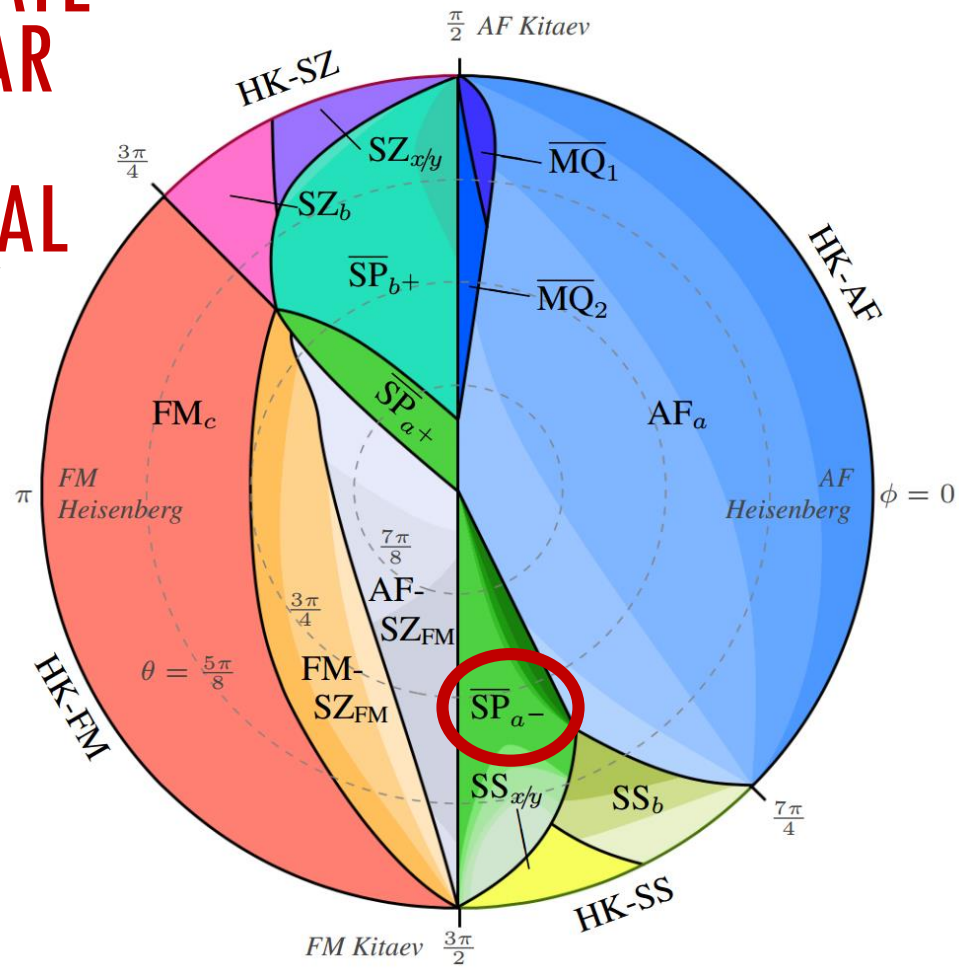
EKH LEE, YB KIM
PRB 91, 064407 (2014)

INCOMMENSURATE NON-COPLANAR COUNTER-ROTATING SPIRAL NEAR KITAEV LIMIT



HYPERHONEYCOMB

$$J = \sin\theta\cos\phi$$
$$K = \sin\theta\sin\phi$$
$$\Gamma = \cos\theta$$

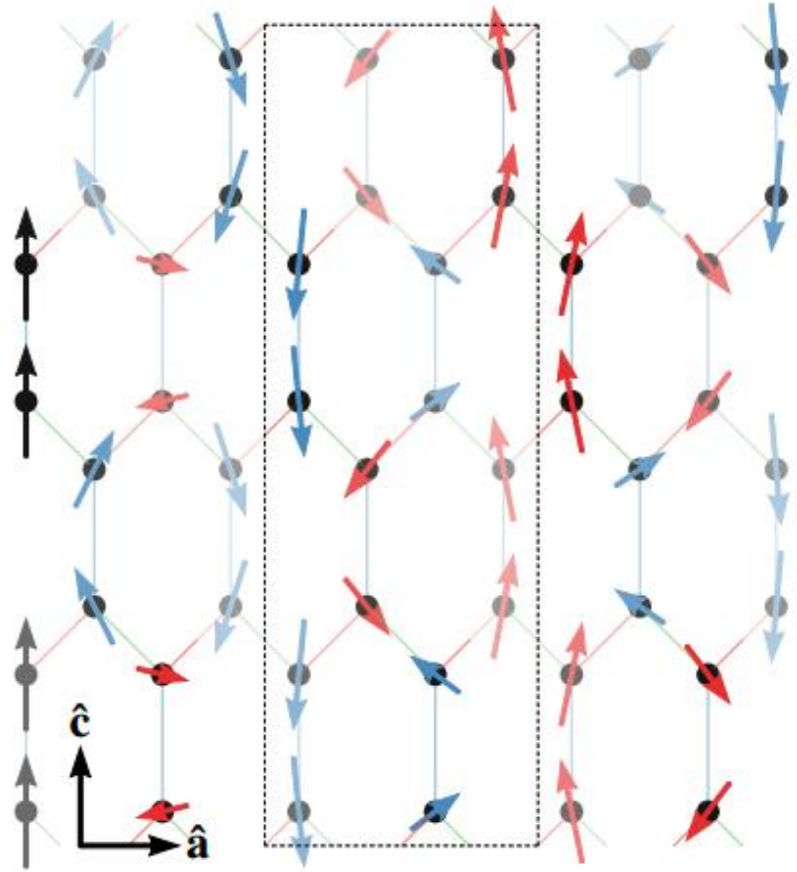


STRIPYHONEYCOMB

EKH LEE, YB KIM
PRB 91, 064407 (2014)

HYPERHONEYCOMB

EXPERIMENT

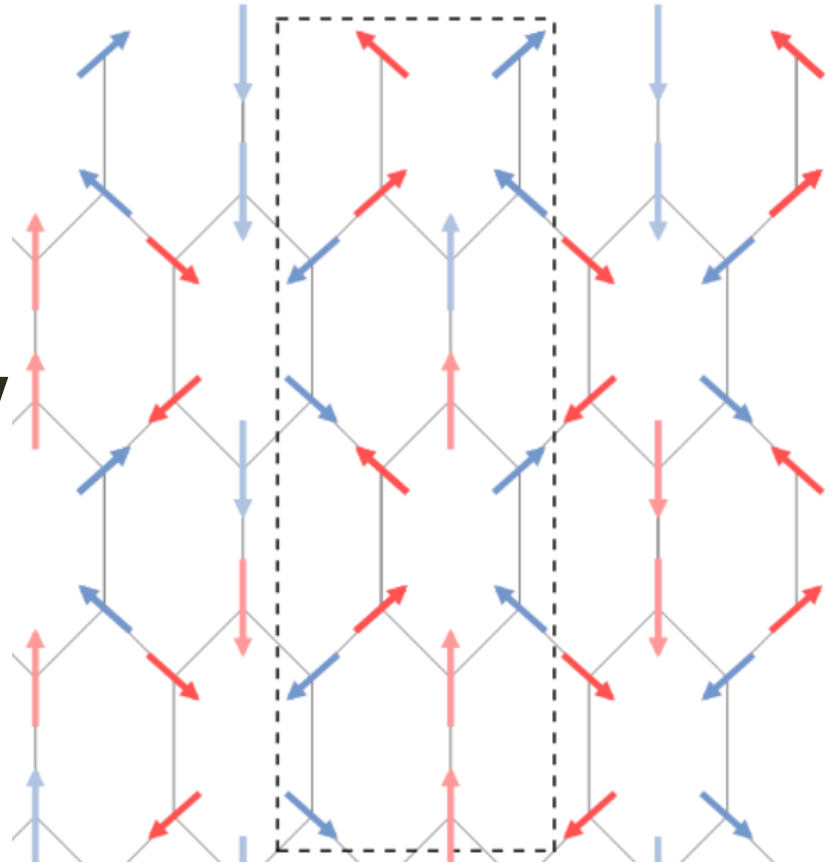


(iA_a, iC_b, F_c)

SYMMETRY AGREES

MAGNETIC BASIS VECTOR

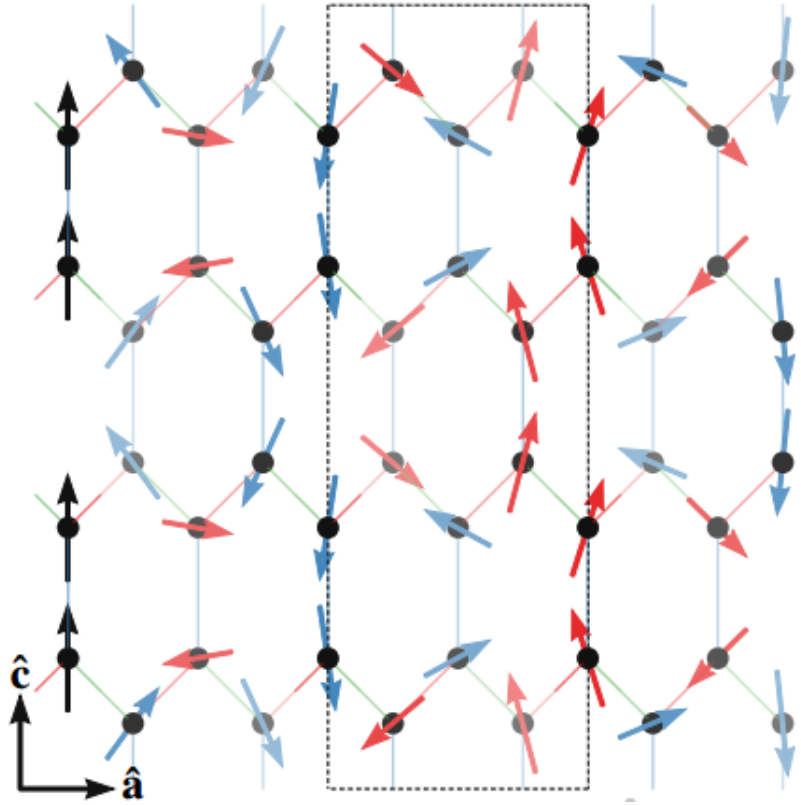
THEORY



(iA_a, iC_b, F_c)

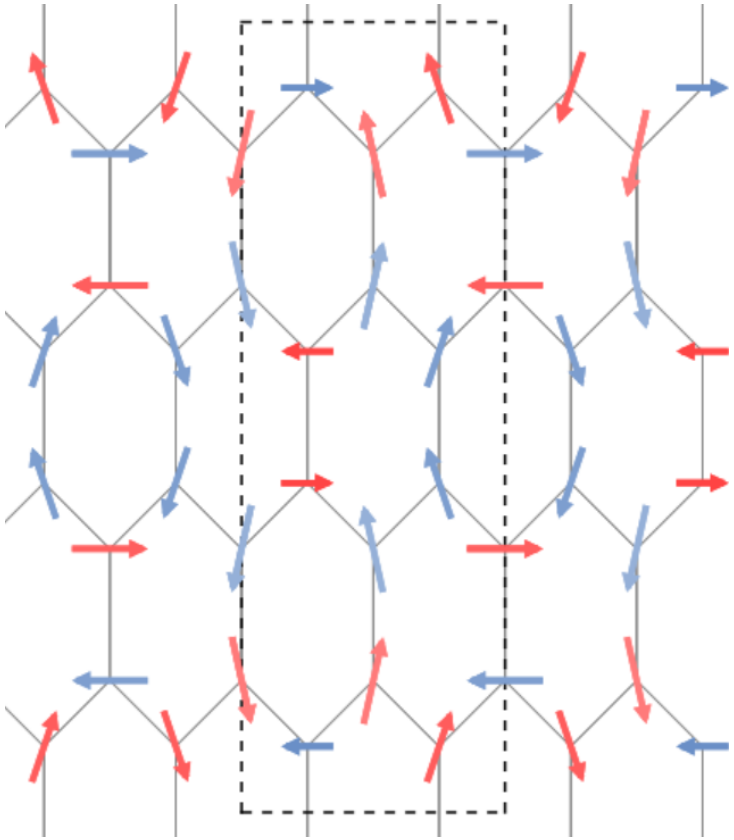
STRIPYHONEYCOMB

EXPERIMENT



$$[i(A,-A)_a, \boxed{(-1)^m i(F,-F)_b}, (F,F)_c]$$

THEORY



$$[i(A,-A)_a, \boxed{-i(C,-C)_b}, (F,F)_c]$$

SYMMETRY DISAGREES IN *b* COMP

MAGNETIC BASIS VECTOR

CRYSTAL STRUCTURE

	Ir-Ir DISTANCE (Å)	Ir-Ir-Ir ANGLE (°)	Ir-O-Ir ANGLE (°)
HYPERHONEYCOMB	2.974±0.003	120.0±0.3	94.5±0.1
STRIPYHONEYCOMB	2.962±0.022	120.0±0.1	93.5±3.1
2D-Na_2IrO_3	3.132±0.004	120.1±0.2	98.5±0.8

COUPLED ZIGZAG CHAIN MODEL

FM KITAEV, HIGHLY BOND ANISOTROPIC

$$H = \sum_{\langle ij \rangle \in \gamma} [J \vec{S}_i \cdot \vec{S}_j + K S_i^\gamma S_j^\gamma] + \sum_{\langle ij \rangle \in Z} I_c (\hat{r}_{ij} \cdot \vec{S}_i)(\hat{r}_{ij} \cdot \vec{S}_j)$$

$$J_Z = J + \frac{1}{2} I_c \qquad K_Z = K - \frac{1}{2} I_c$$

$$J_{X/Y} = J \qquad K_{X/Y} = K$$

$$\Gamma_Z = \frac{1}{2} I_c$$

$$\Gamma_{X/Y} = 0$$

I KIMCHI, R COLDEA, A VISHWANATH
PRB 91, 245134 (2015)

COMPARISON STUDY

MODELS

JKΓ CZC

TORONTO BERKELEY

METHODS

CLASSICAL (SIM ANNEALING) SOFT-SPIN (MIX BY HAND)

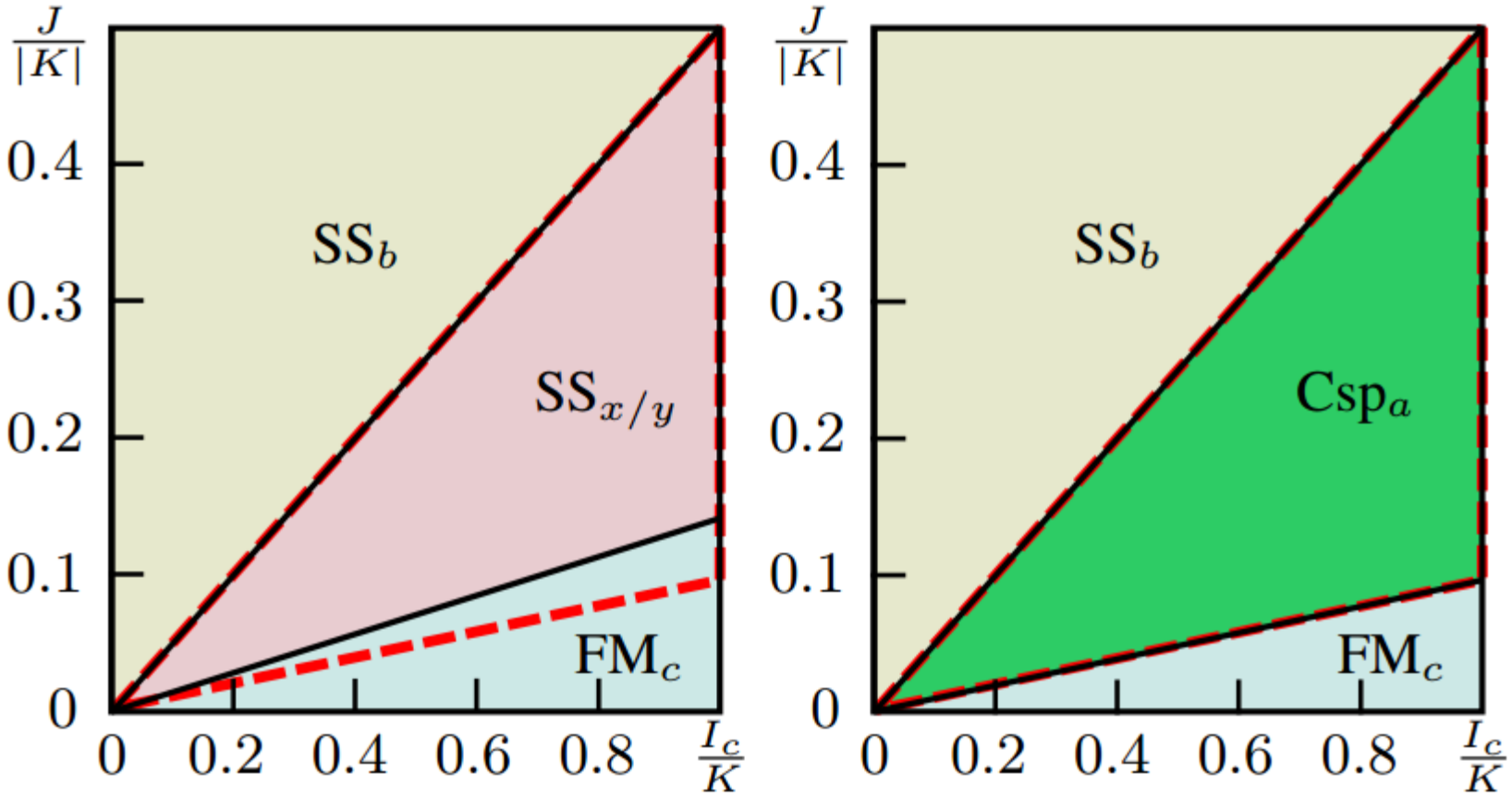
MATERIALS

HYPERHONEYCOMB STRIPYHONEYCOMB

EKH LEE, J RAU, YB KIM
arXiv:150606746 (2015)

COMPARISON STUDY

METHODS-CZC BERKELEY



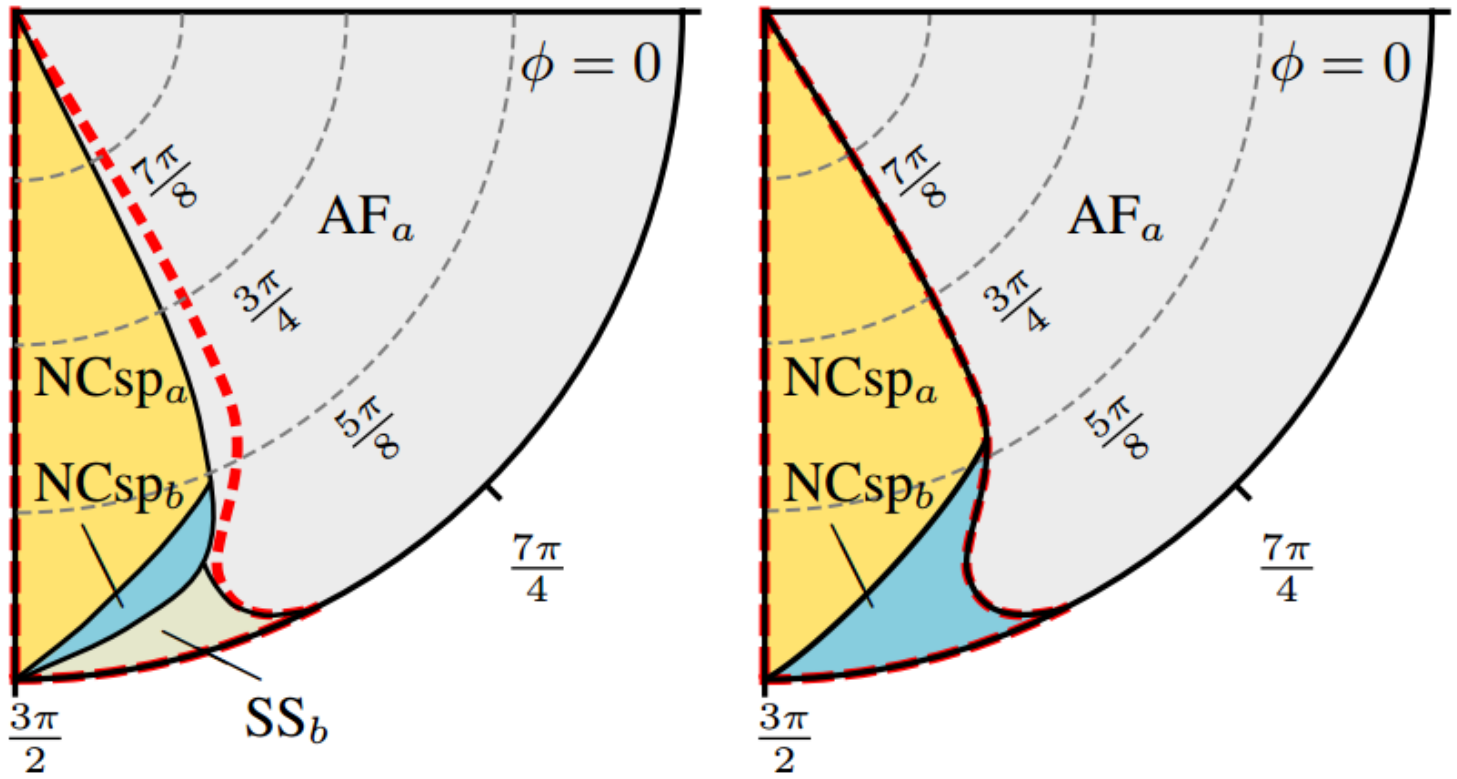
CLASSICAL SOFT-SPIN

BOTH MATERIALS

EKH LEE, J RAU, YB KIM
arXiv:150606746 (2015)

COMPARISON STUDY

METHODS-JKΓ TORONTO



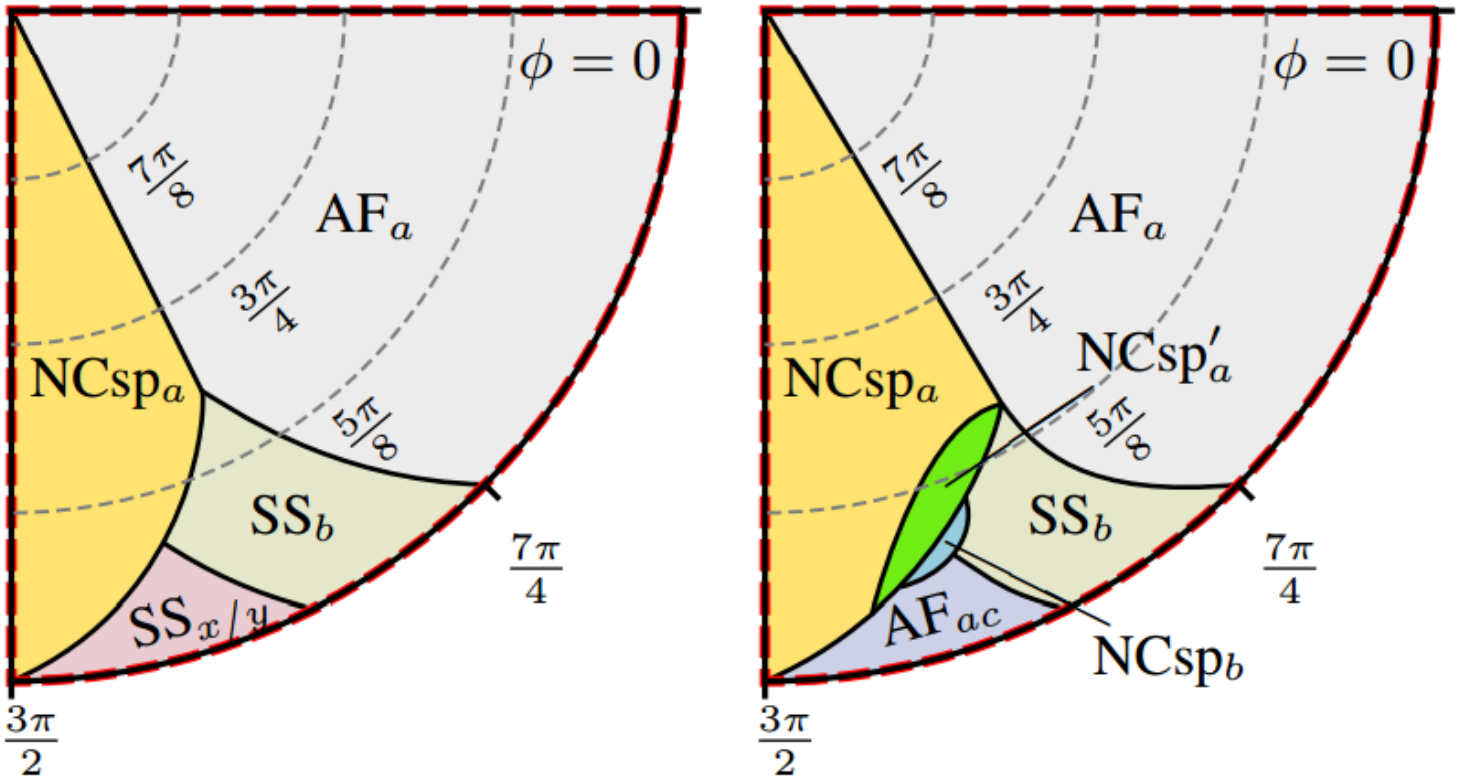
CLASSICAL SOFT-SPIN

HYPERHONEYCOMB

EKH LEE, J RAU, YB KIM
arXiv:150606746 (2015)

COMPARISON STUDY

METHODS-JKΓ TORONTO



CLASSICAL SOFT-SPIN

STRIPYHONEYCOMB

EKH LEE, J RAU, YB KIM
arXiv:150606746 (2015)

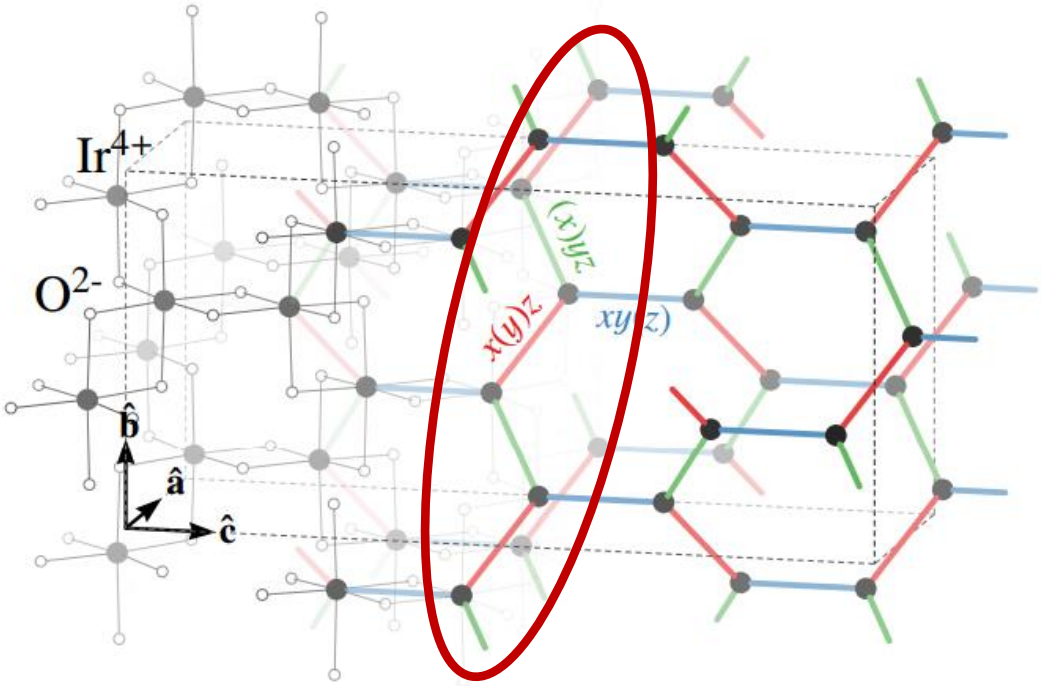
COMPARISON STUDY

RESULTS

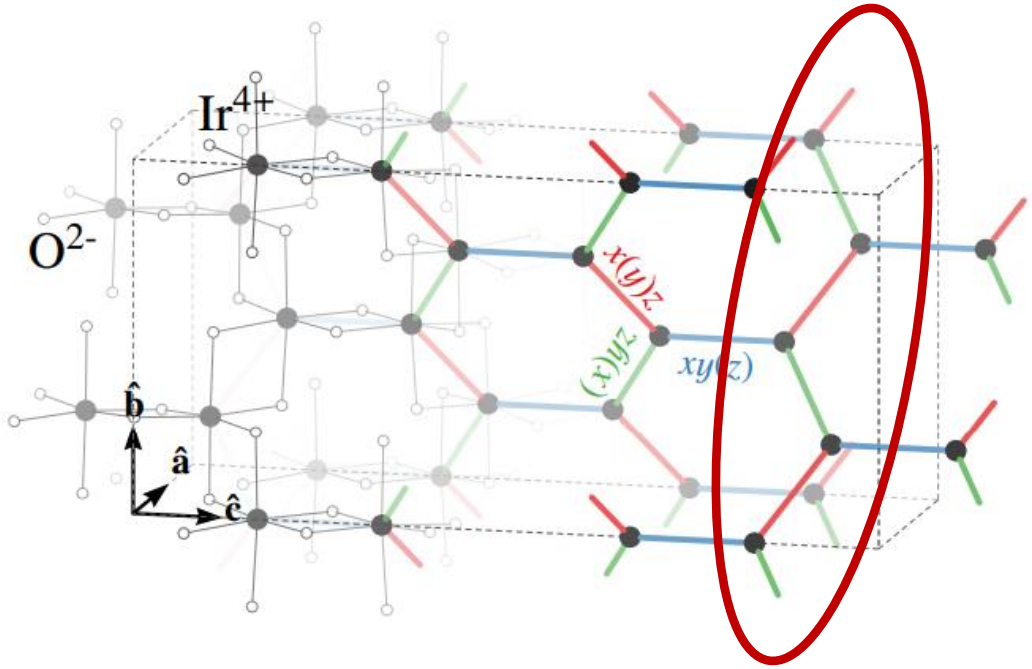
	CLASSICAL (SIM ANN)	SOFT-SPIN (MIX BY HAND)
JKΓ TORONTO	H0: SAME AS EXP H1: DIFF FROM EXP	H0: SAME AS EXP (NO MIX) H1: SAME AS EXP (W MIX)
CZC BERKELEY	COMMENSURATE	H0: SAME AS EXP (W MIX) H1: SAME AS EXP (W MIX)

EKH LEE, J RAU, YB KIM
arXiv:150606746 (2015)

DECOUPLED CHAIN LIMIT

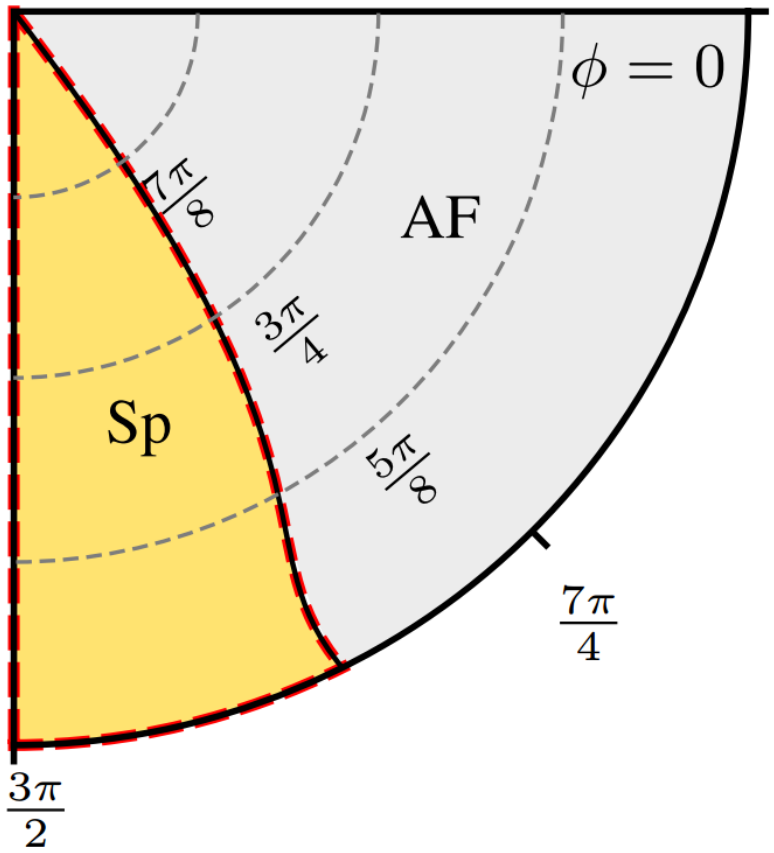


HYPERHONEYCOMB

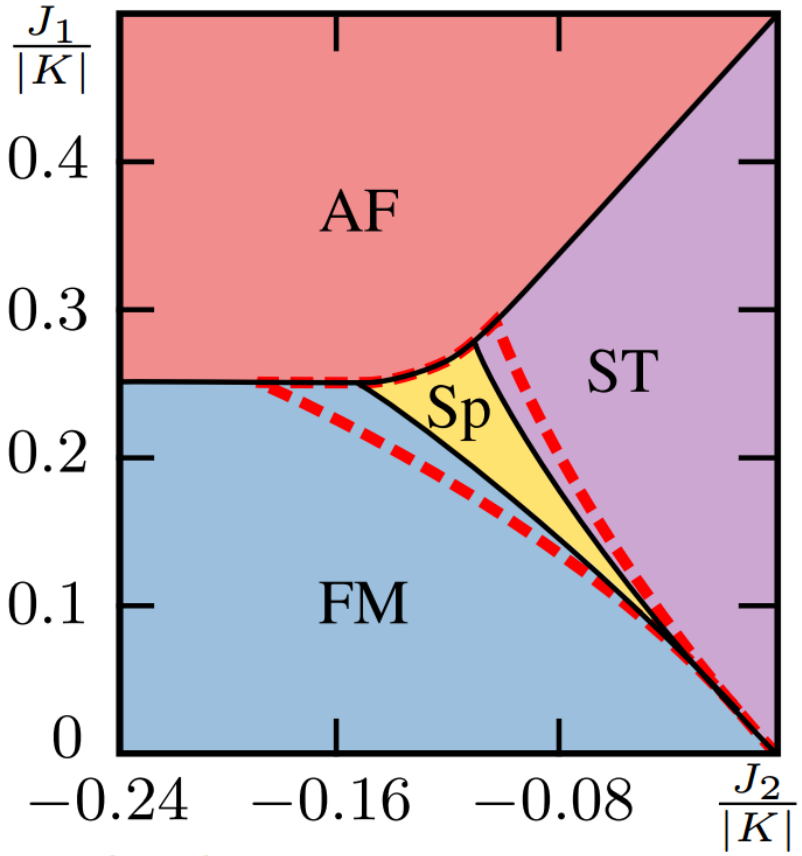


STRIPYHONEYCOMB

DECOUPLED CHAIN LIMIT - CLASSICAL



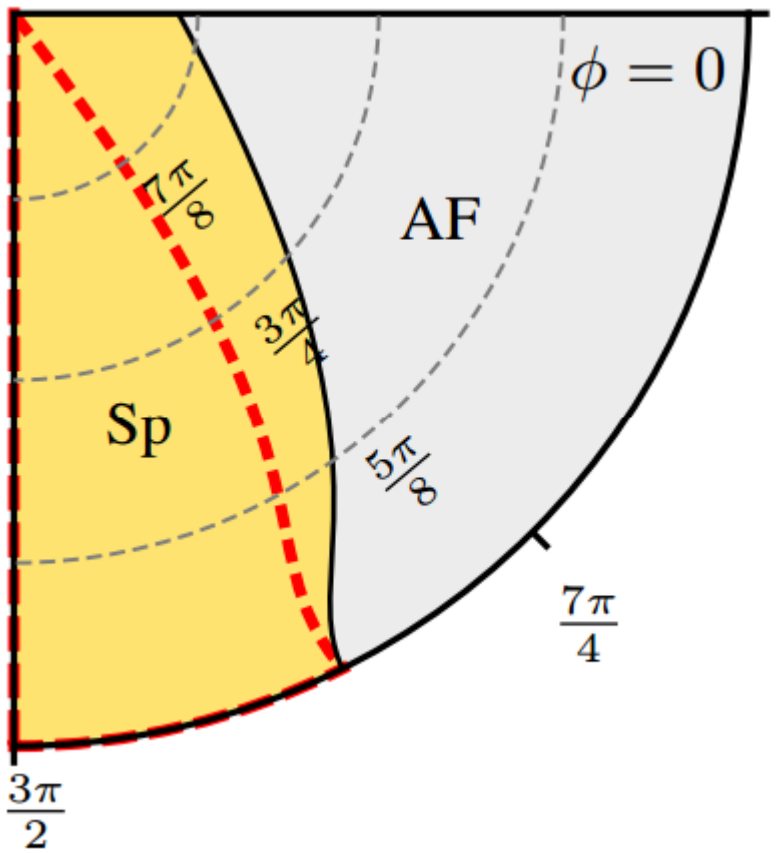
JKΓ TORONTO



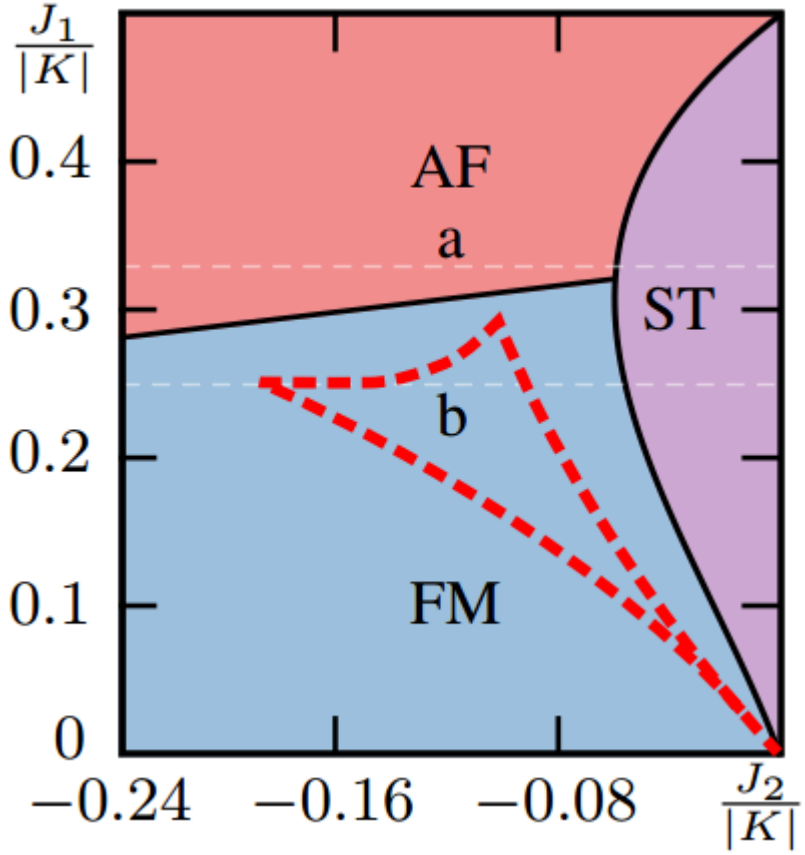
CZC+J2 BERKELEY

EKH LEE, J RAU, YB KIM
arXiv:150606746 (2015)

DECOUPLED CHAIN LIMIT - DMRG



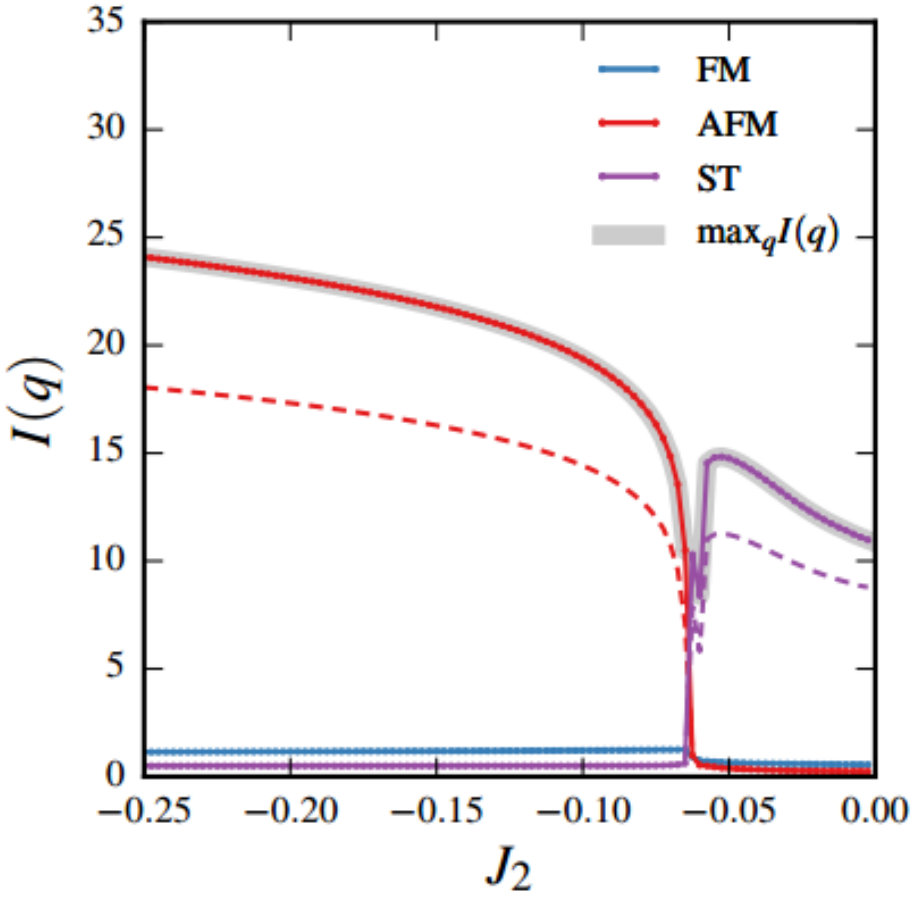
JKΓ TORONTO



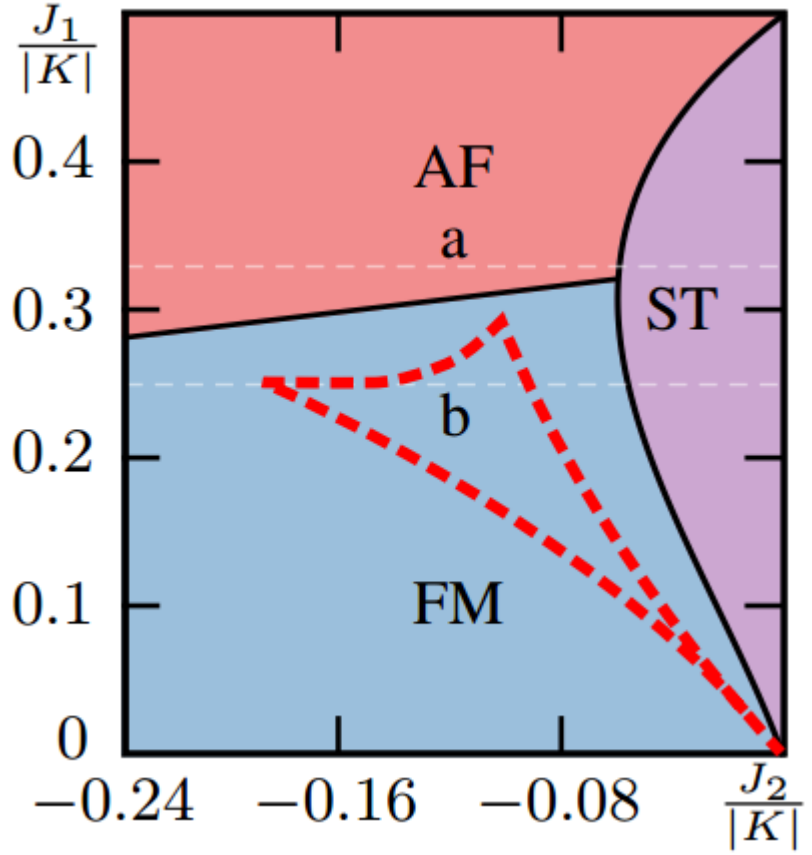
CZC+J2 BERKELEY

EKH LEE, J RAU, YB KIM
arXiv:150606746 (2015)

DECOUPLED CHAIN LIMIT - DMRG



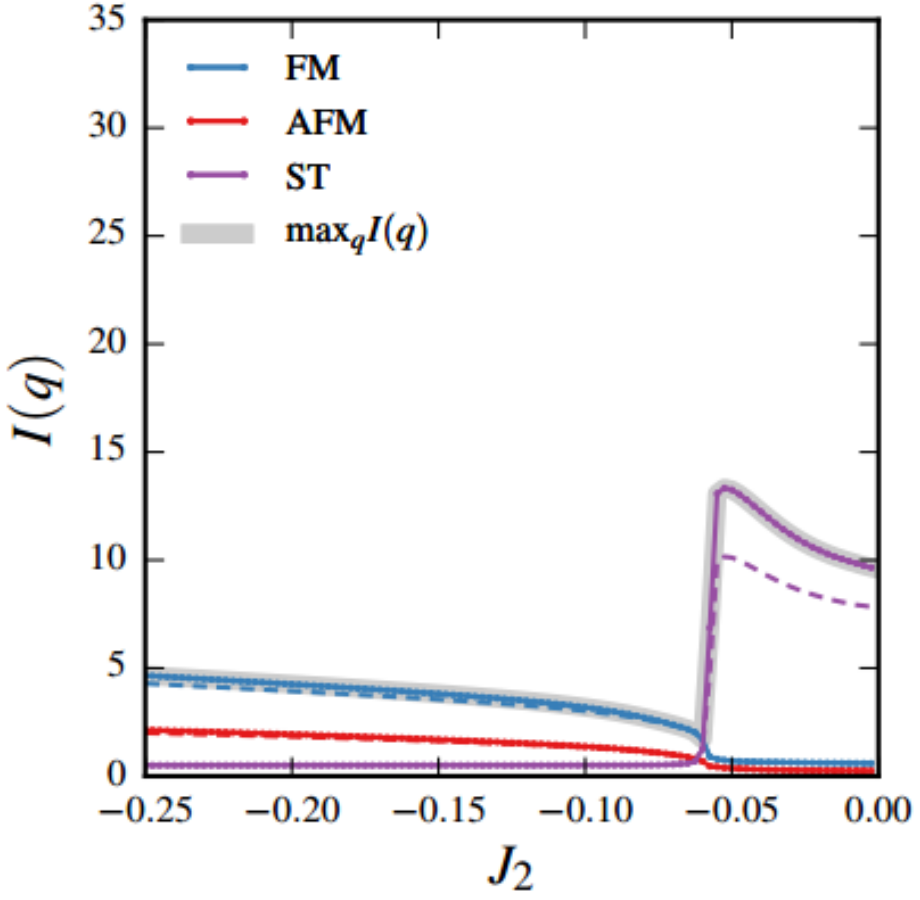
(a) $J_1 = 0.33$



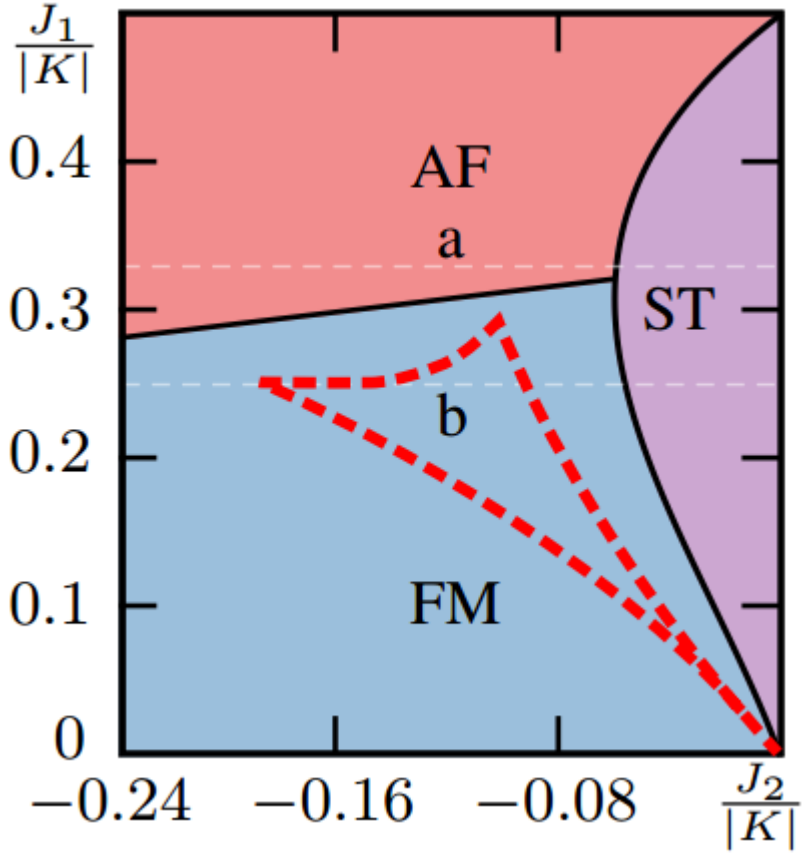
CZC+J2 BERKELEY

EKH LEE, J RAU, YB KIM
arXiv:150606746 (2015)

DECOUPLED CHAIN LIMIT - DMRG



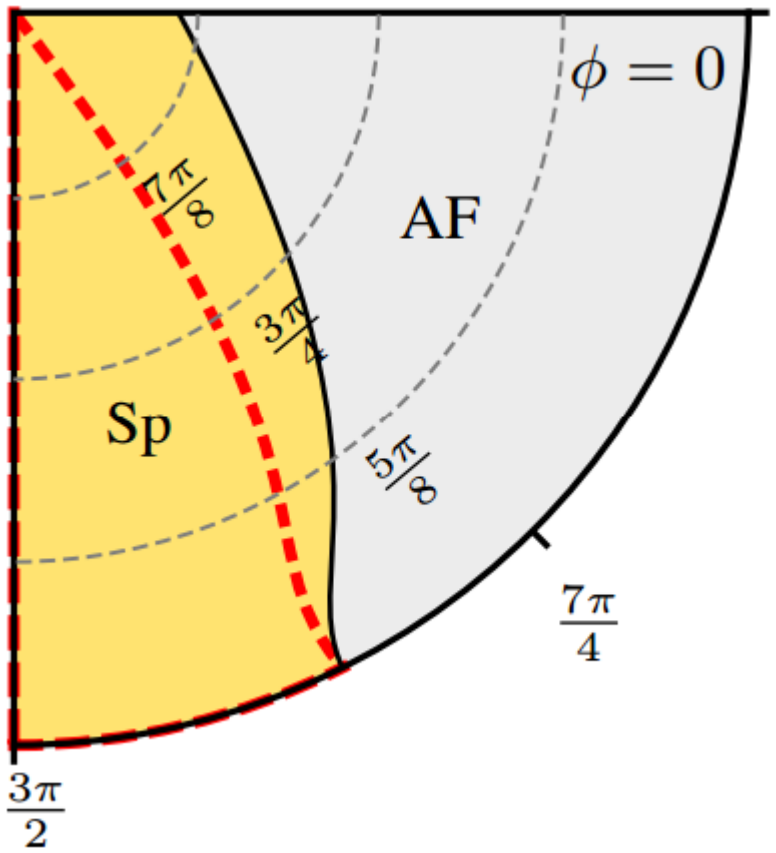
(b) $J_1 = 0.25$



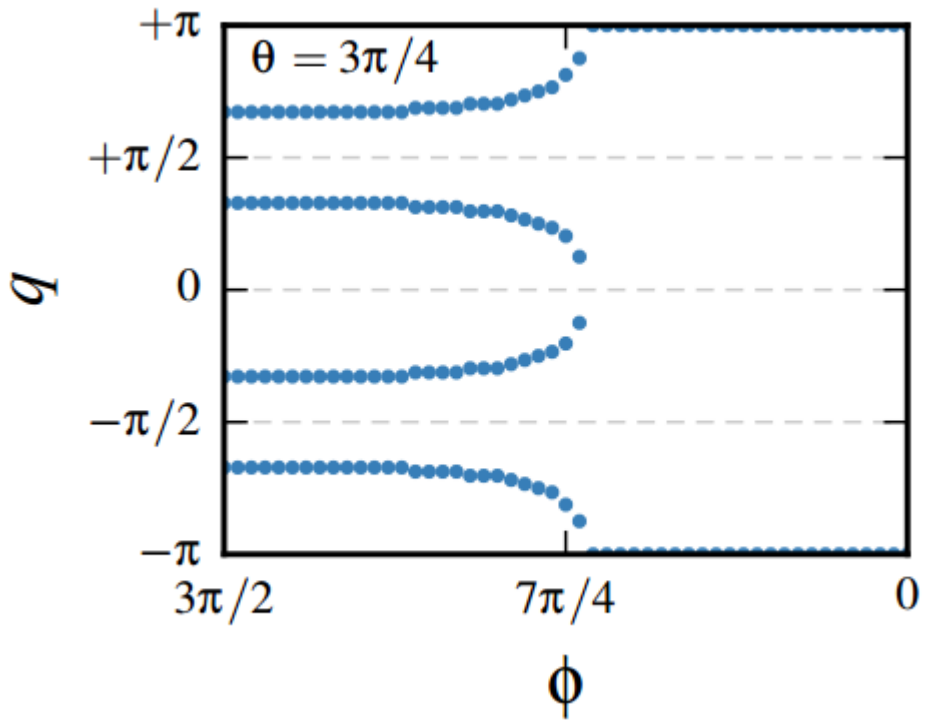
CZC+J2 BERKELEY

EKH LEE, J RAU, YB KIM
arXiv:150606746 (2015)

DECOUPLED CHAIN LIMIT - DMRG



JKΓ TORONTO



LOCATION OF MAX PEAK

EKH LEE, J RAU, YB KIM
arXiv:150606746 (2015)

SUMMARY

HYPERHONEYCOMB

STRIPYHONEYCOMB

TOPOLOGICAL SPINON “SEMIMETAL”
ISOTROPIC REGION OF KITAEV SPIN LIQUID

$J_{eff} = 1/2$
PICTURE IS VALID

NEAR FM KITAEV
LIMIT

BOND
ISOTROPIC

BOND
ANISOTROPIC

Γ ALONG X/Y STABLIZES SPIRAL