Understanding Spin-1 Kagomé Antiferromagnet Through Hida Model

Brijesh Kumar
(JNU, New Delhi)

05 December 2018 @ *ICTS* Bengaluru
(2nd Asia-Pacific Workshop on Quantum Magnetism)

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[work done *with* ***Pratyay Ghosh***]
PRB **97**, 014413 (2018)
PRB **93**, 014427 (2016)

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Acknowledgement

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UGC (through UPE-II project)

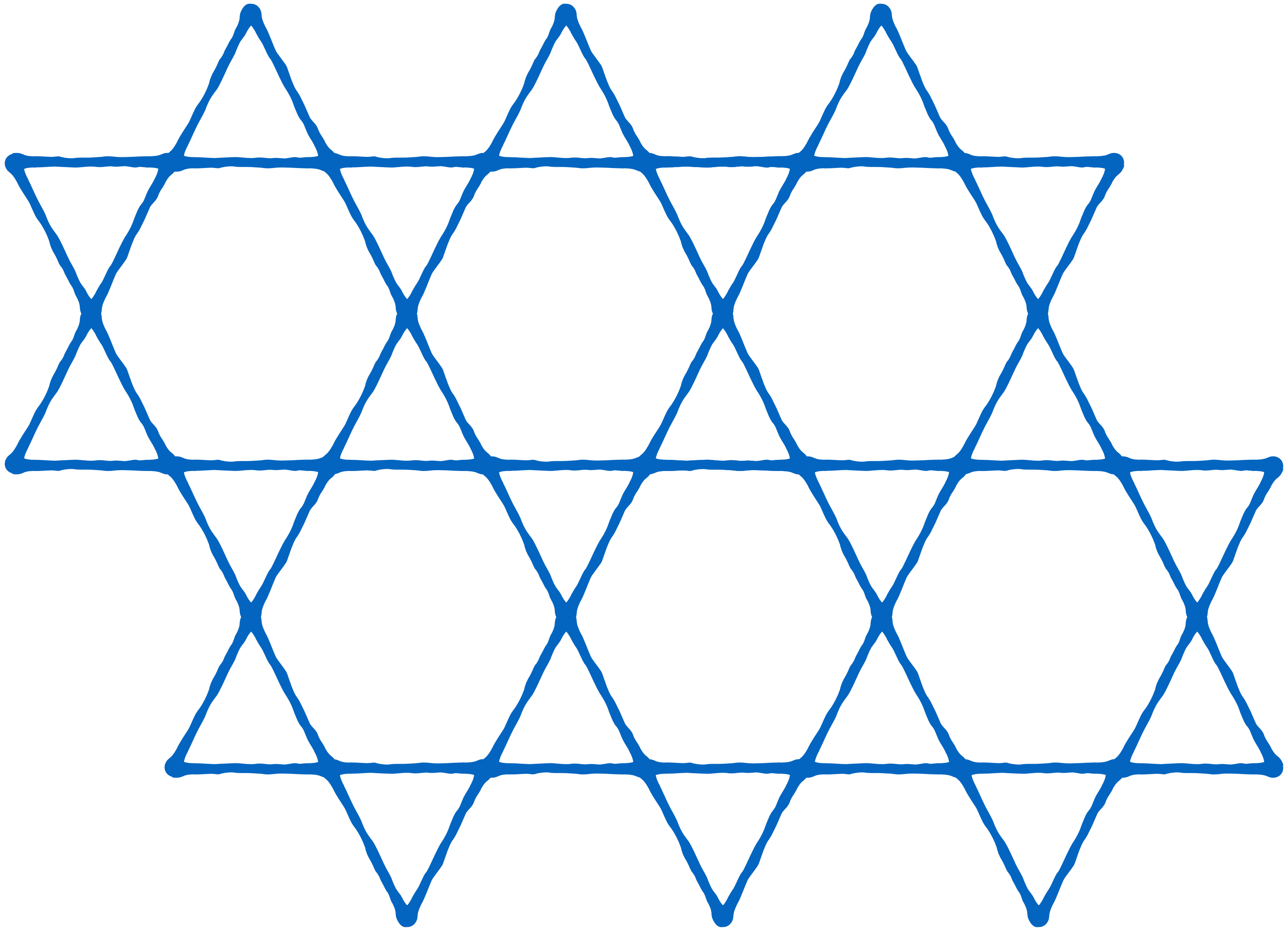
DST (through PURSE and FIST programs)

CSIR (for students' fellowships)

Computing facility:

IUAC (New Delhi), and **SPS** (JNU)

Kagome Lattice



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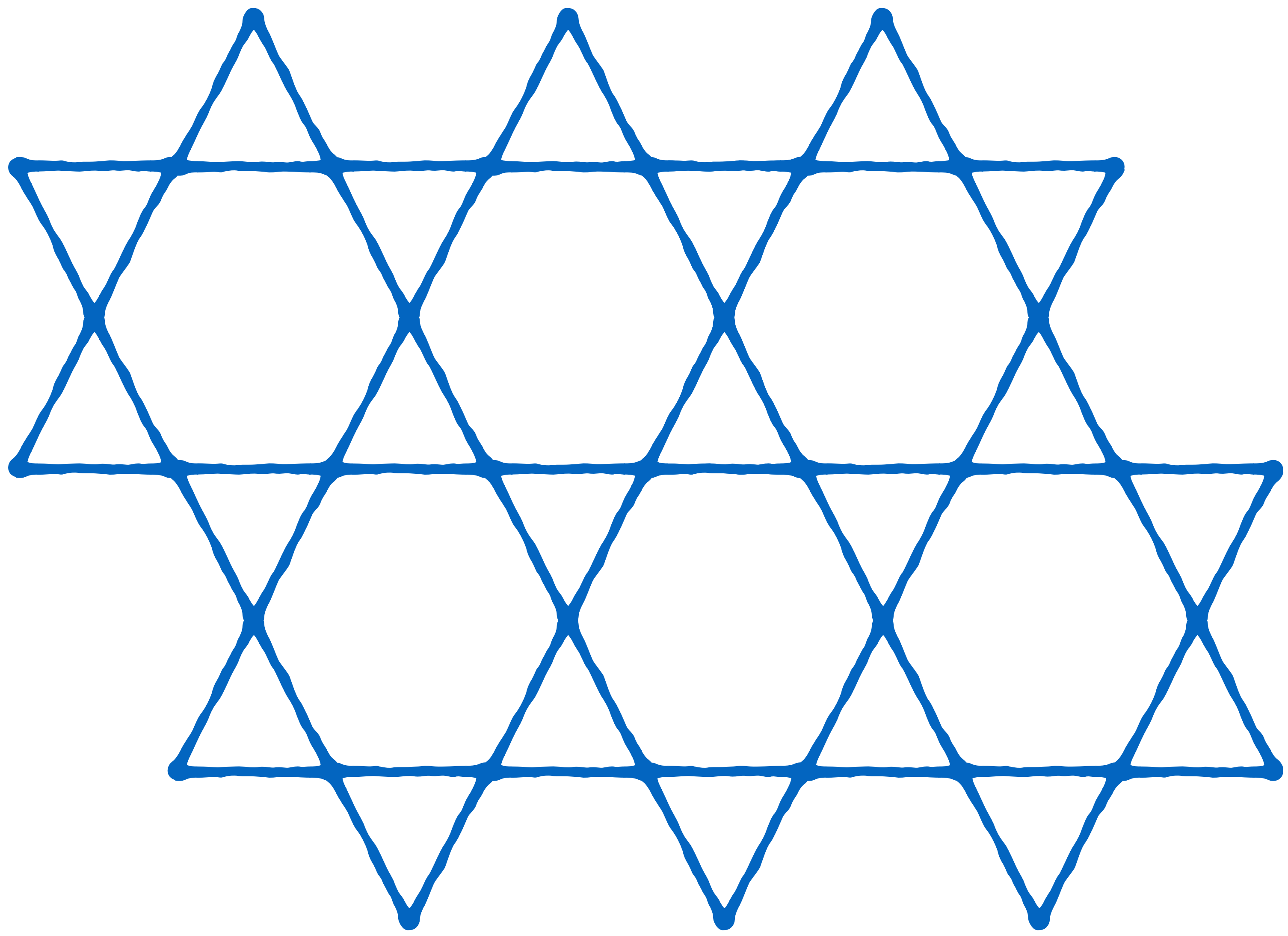

Heisenberg Antiferromagnet

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

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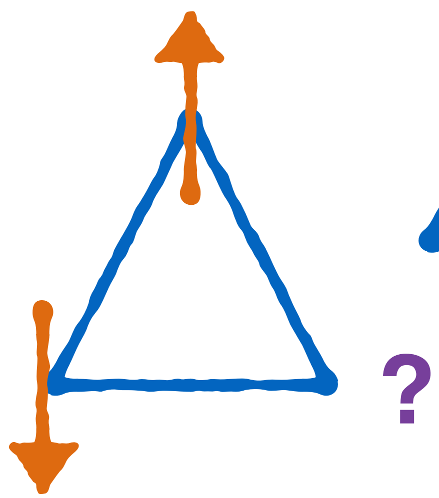
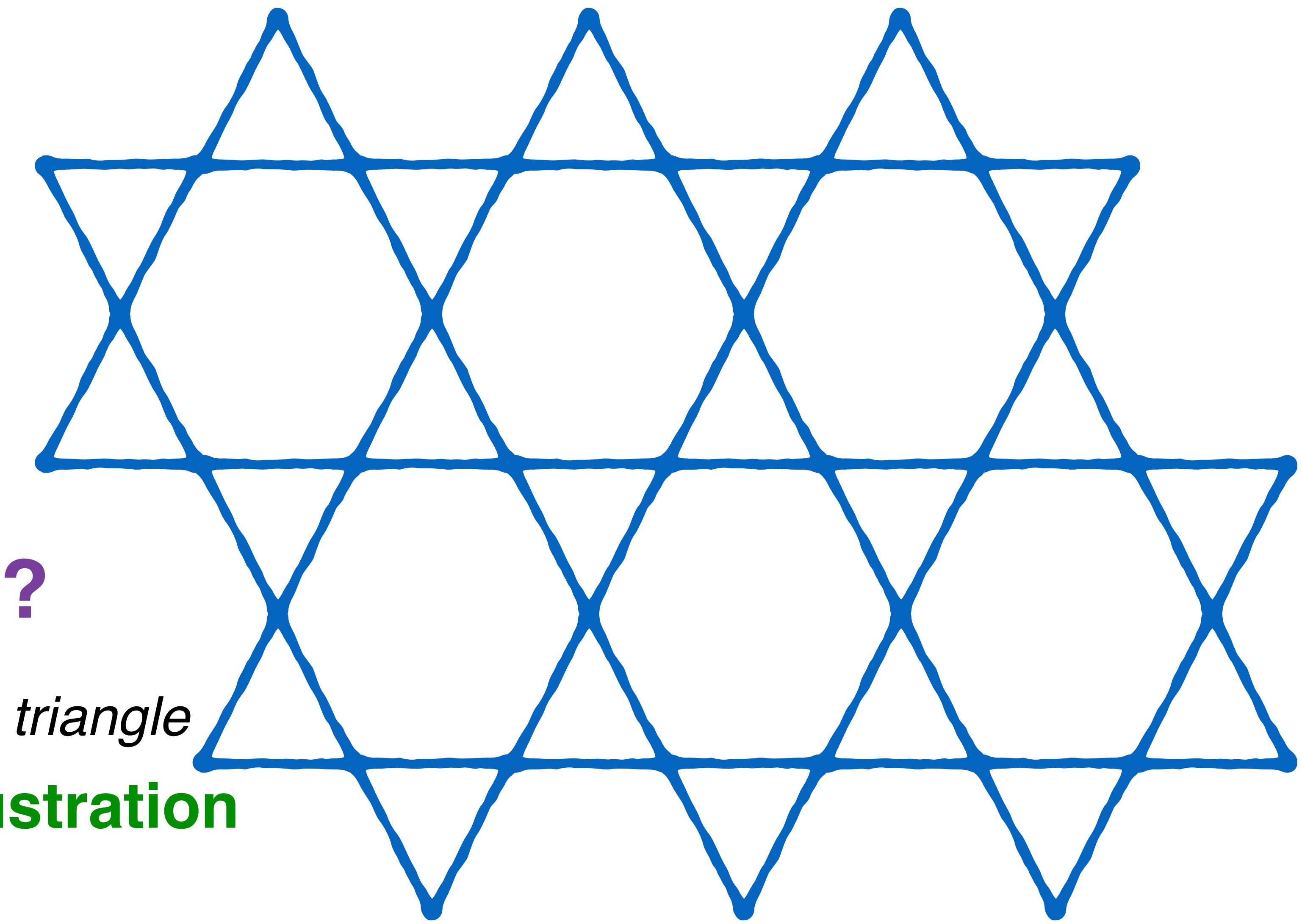


antiferromagnetic triangle

“Geometric” Frustration



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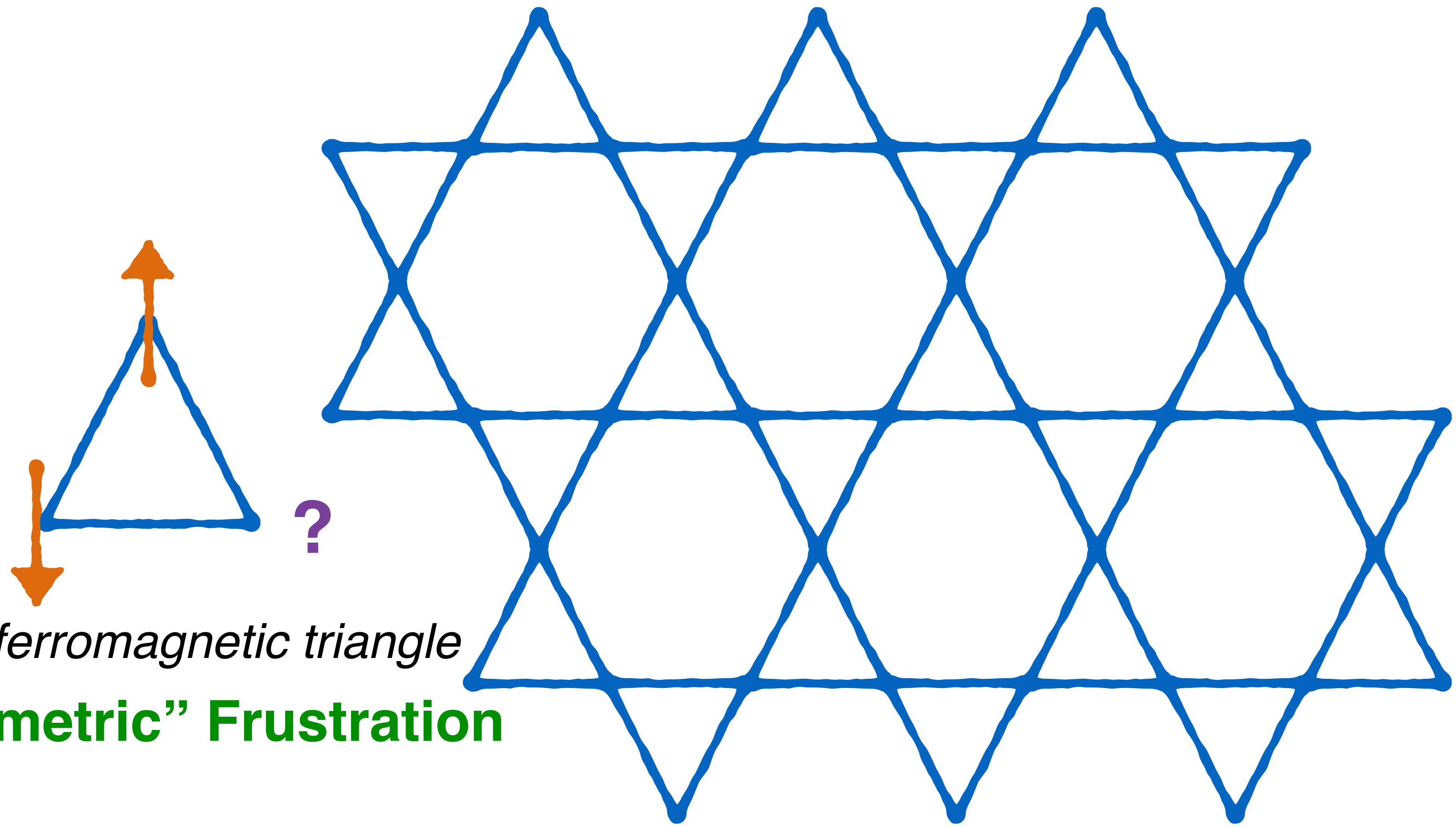


"Geometric" Frustration

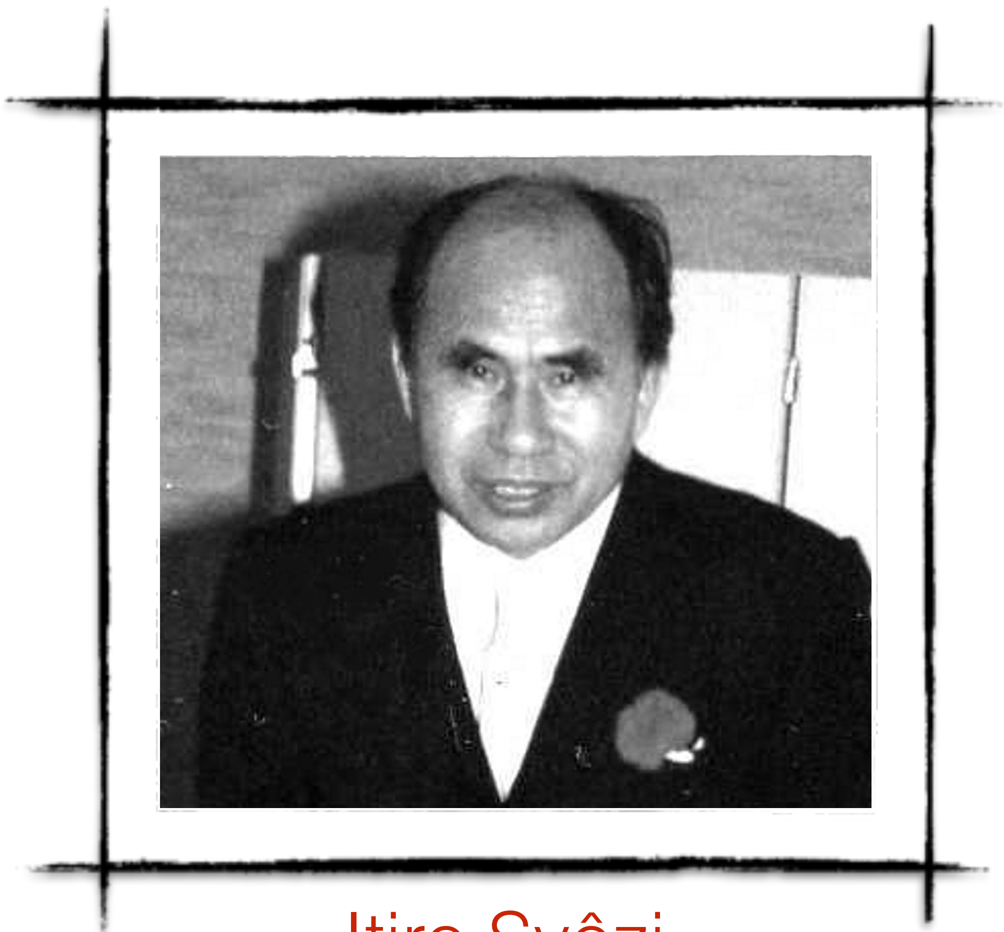
Heisenberg Antiferromagnet

"Highly" Frustrated Spin Model

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

Kagome Lattice

Appears first, through star-triangle relation, in the study of the Ising model on a “decorated” honeycomb lattice



Itiro Syôzi

Prog. Theor. Phys. **6**, 306 (1951)

***“… But** in the antiferromagnetic case, there is no phase change.”*

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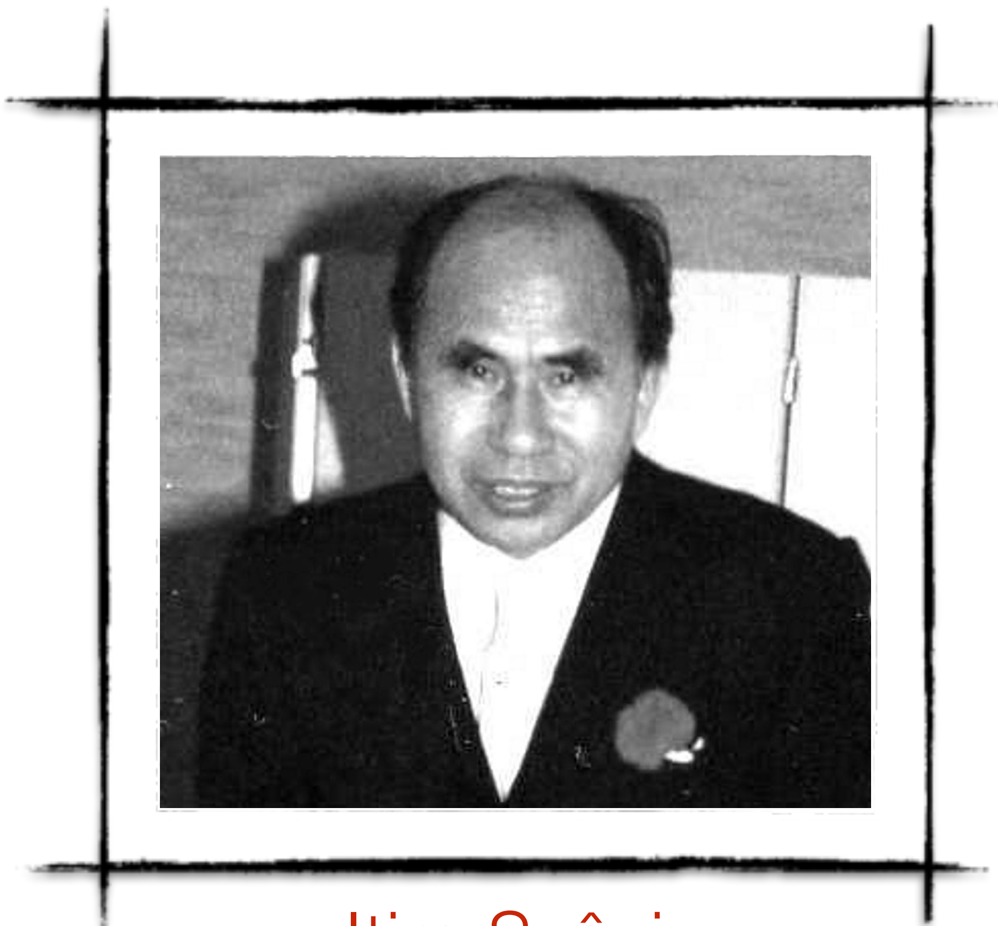

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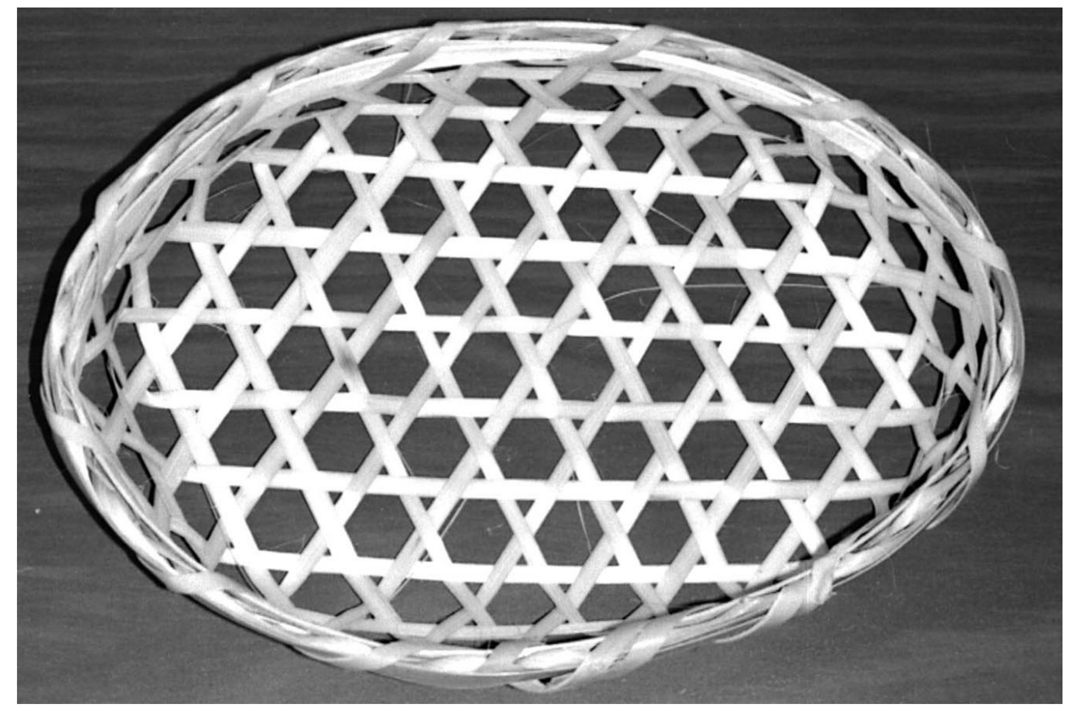
so named by Kodi Husimi…



Kagome = basket with holes

Kagome: The story of the basketweave lattice
M. Mekata, Physics Today 56, 12 (2003)

"… But *in the antiferromagnetic case, there is no phase change.*"

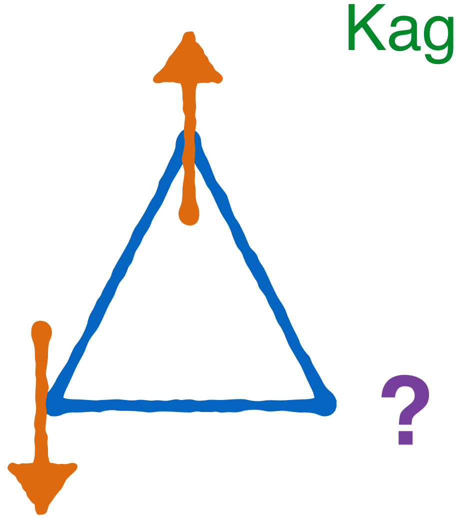
Kagome Antiferromagnets

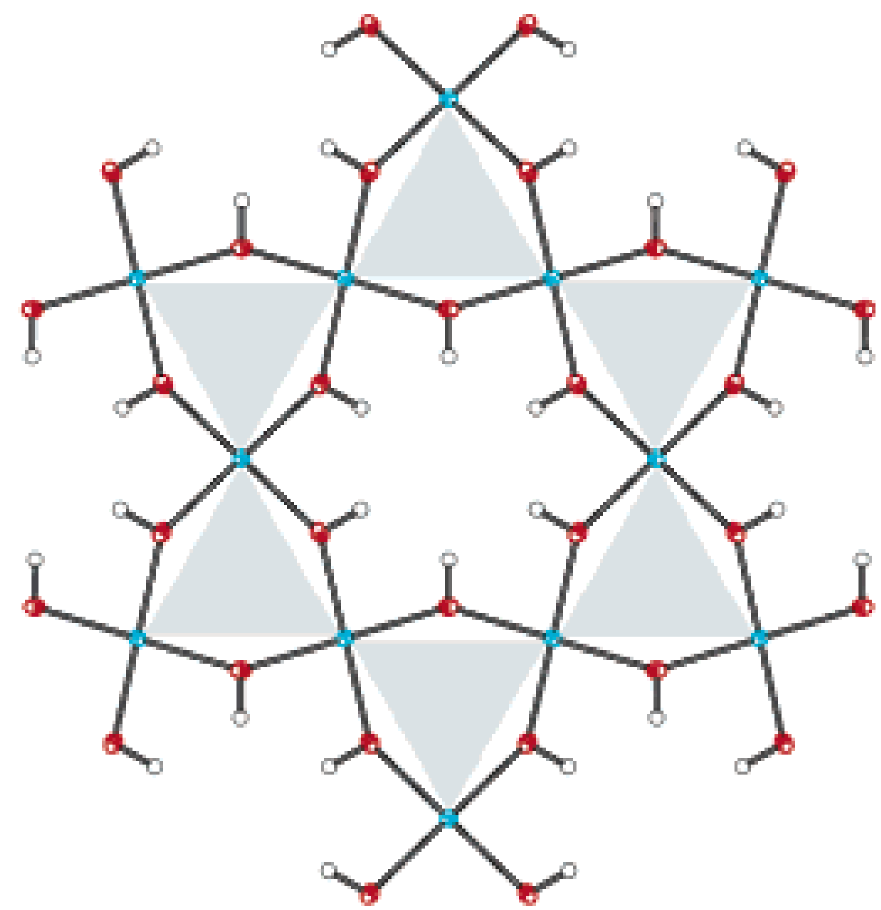
Herbertsmithite

$$ZnCu_3(OH)_6Cl_2$$

nearly perfect quantum spin-1/2
Kagome Heisenberg Antiferromagnet

Shores et al, JACS (2005)





$Cu_3(OH)_6$ *Kagome layer*

Absence of magnetic order in the ground state…

KHA: Spin-1/2 case

(KHA = Kagome Heisenberg Antiferromagnet)

Most, extensively studied.

And, heatedly debated…

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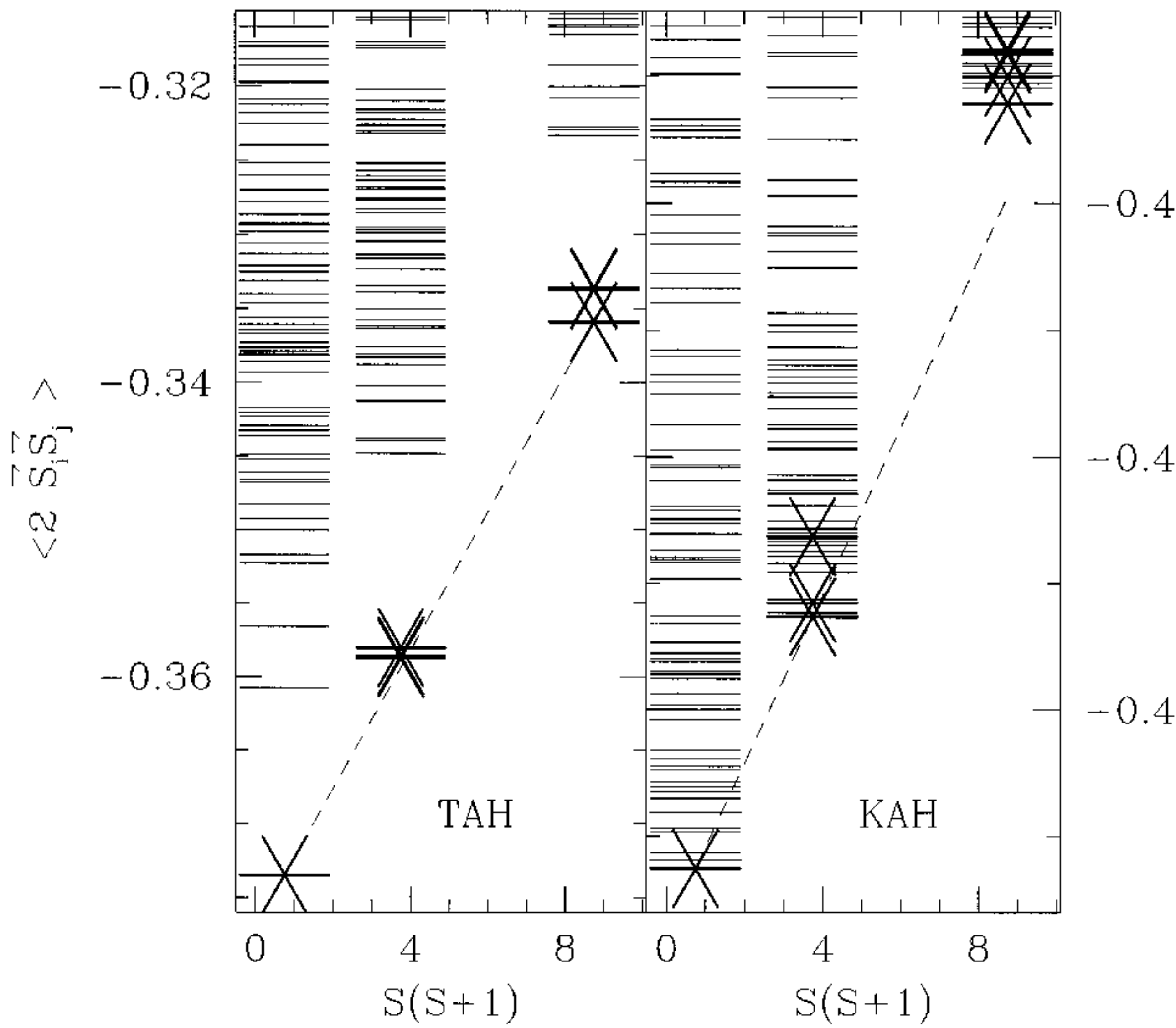

Lecheminant el al, PRB (1997)

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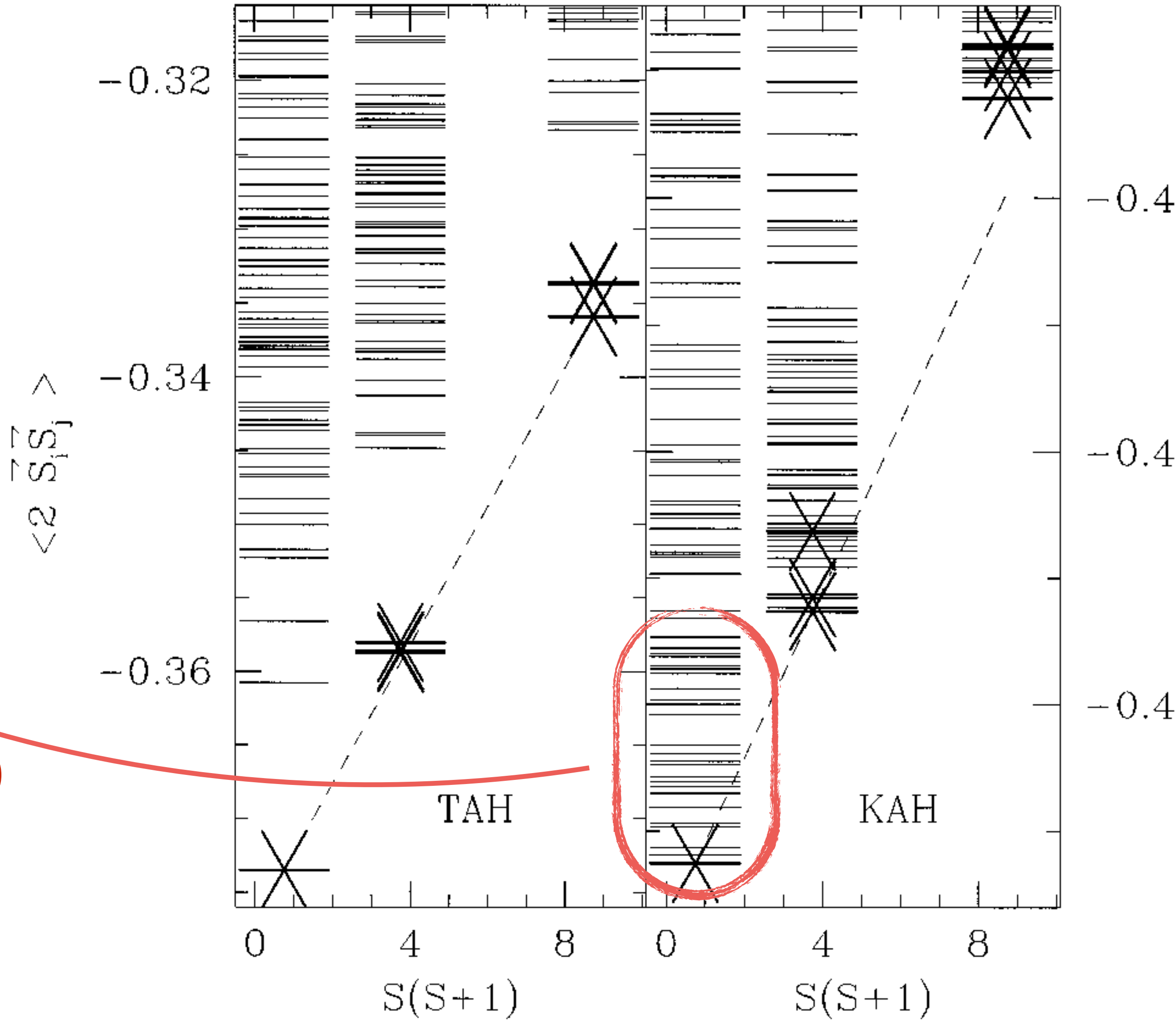
1.15^L

Mila, PRL (1998)



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Quantum spin liquid state

$$\langle \mathbf{S}_i \rangle = 0$$

do all correlations decay exponentially?

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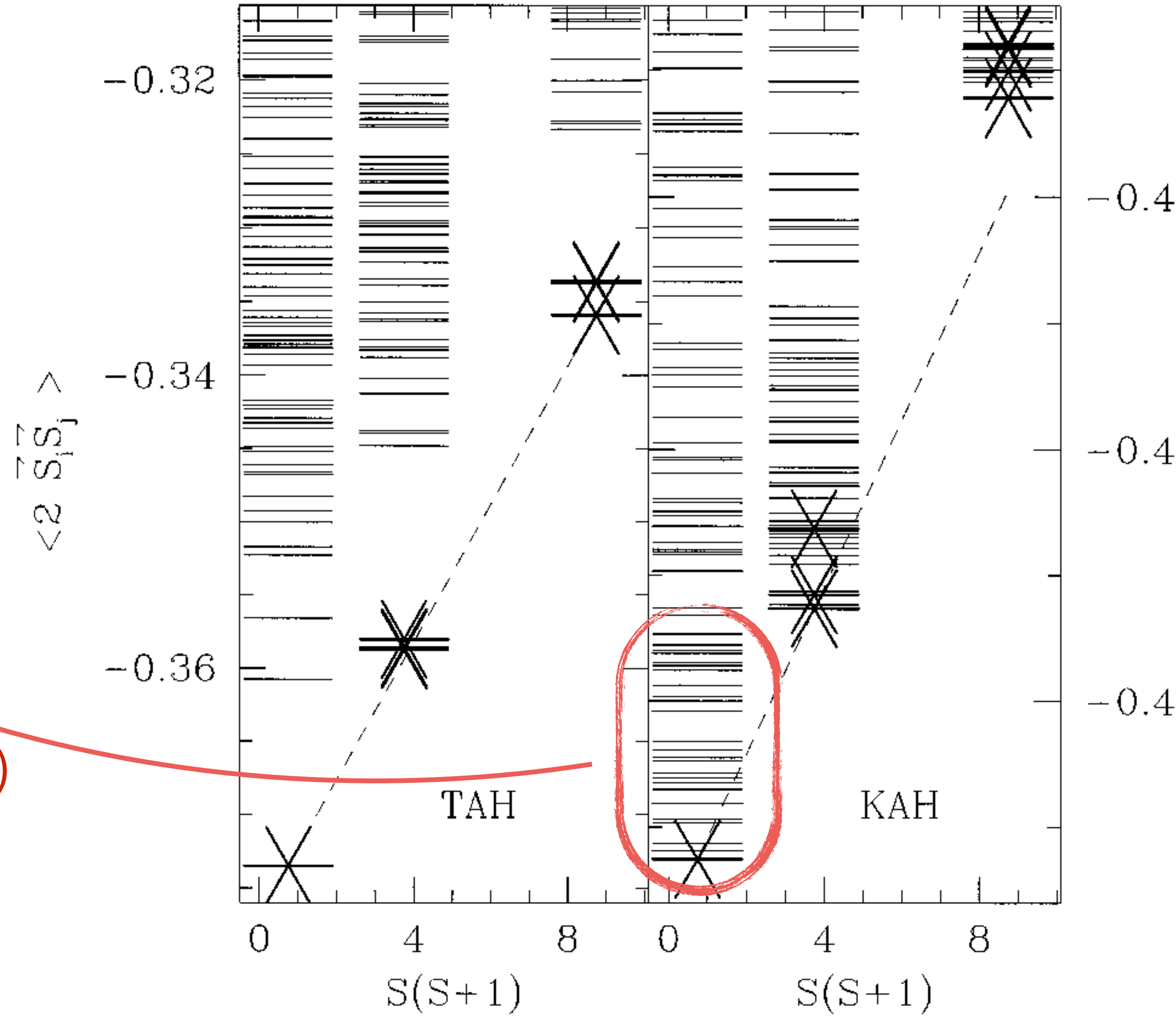

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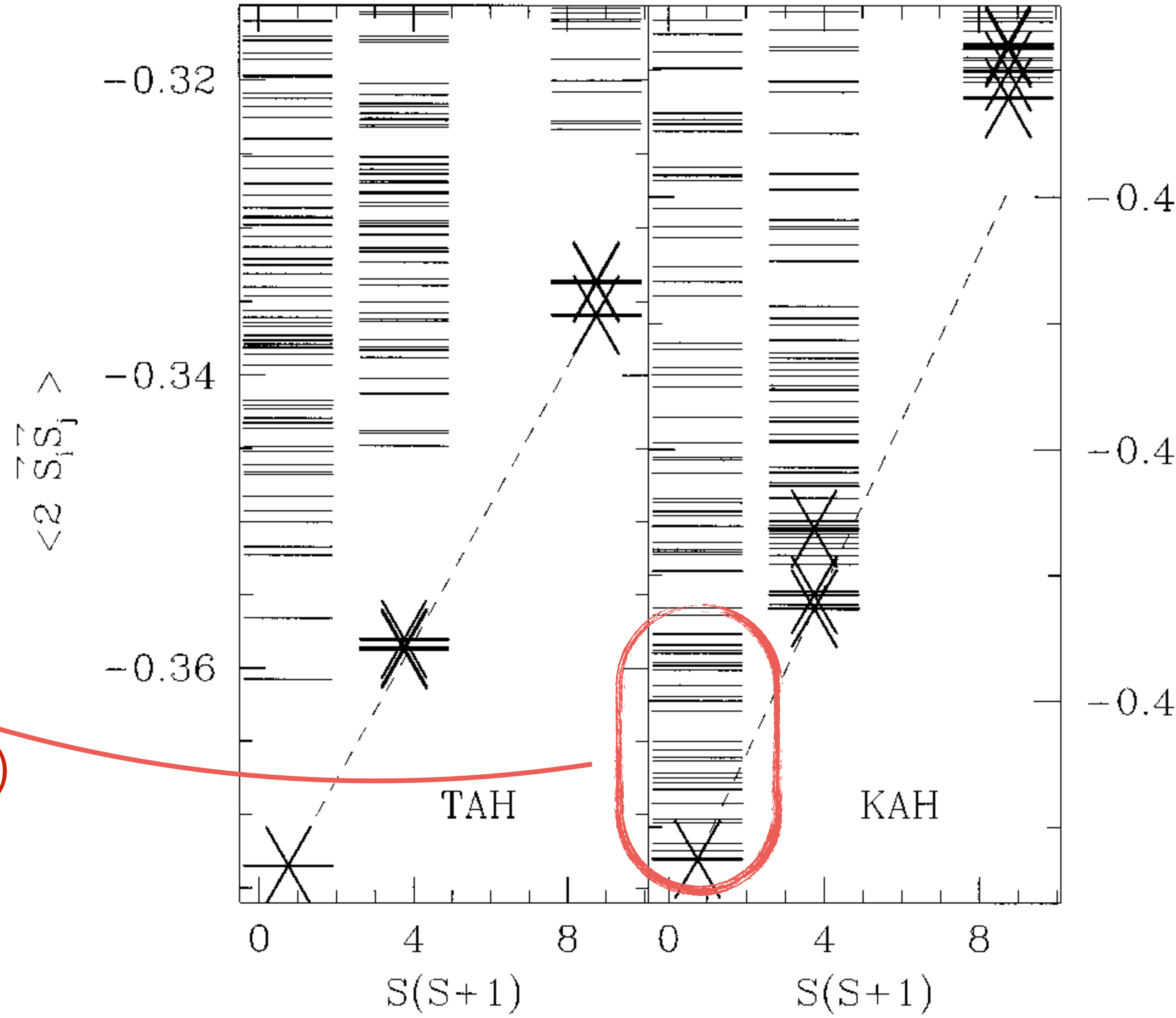


Lecheminant el al, PRB (1997)

Gapped RVB ? S. Yan et al (2011)

Gapless Algebraic? Y. Iqbal el al (2013)

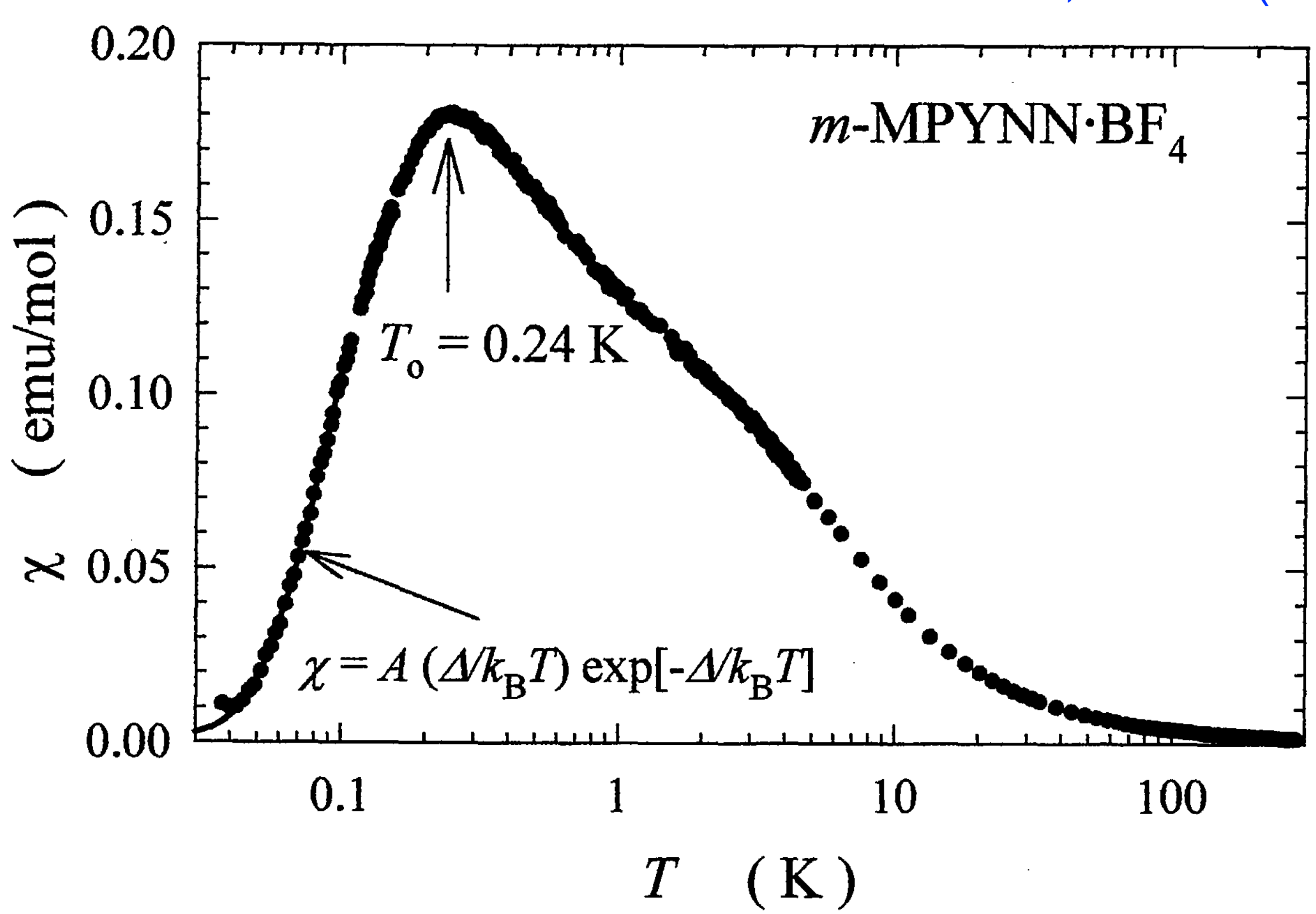
Valence bond crystal? A. Ralko el al (2018)

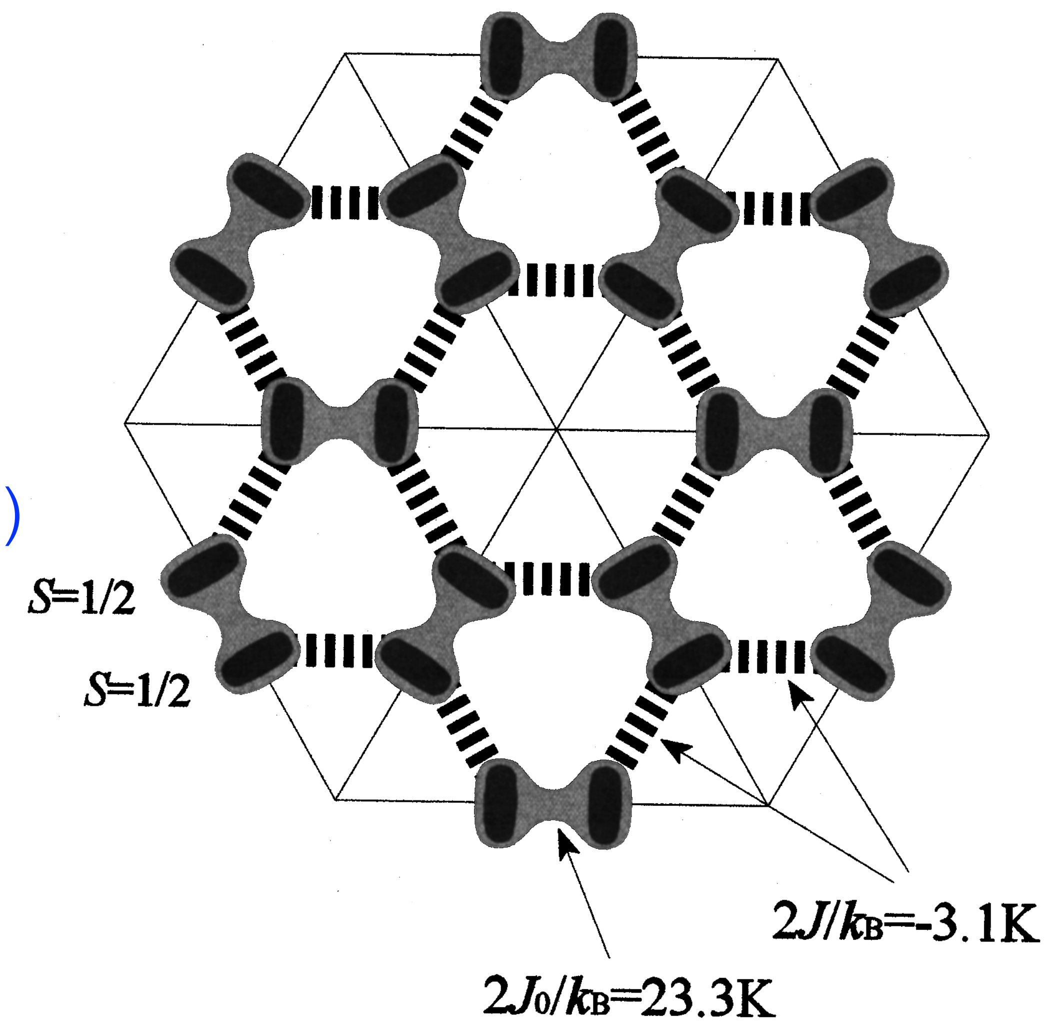
Spin-1 KHA

$$m - MPYNN.BF_4$$

(m-N-methylperidium-α-nitronyl-nitroxide)

Wada et al, JPSJ (1997)





Watanabe et al, PRB (1998)

Spin-1 KHA

exhibit spin gap behaviour

NaV_6O_{11}

Kato et al, JPSJ (2001)

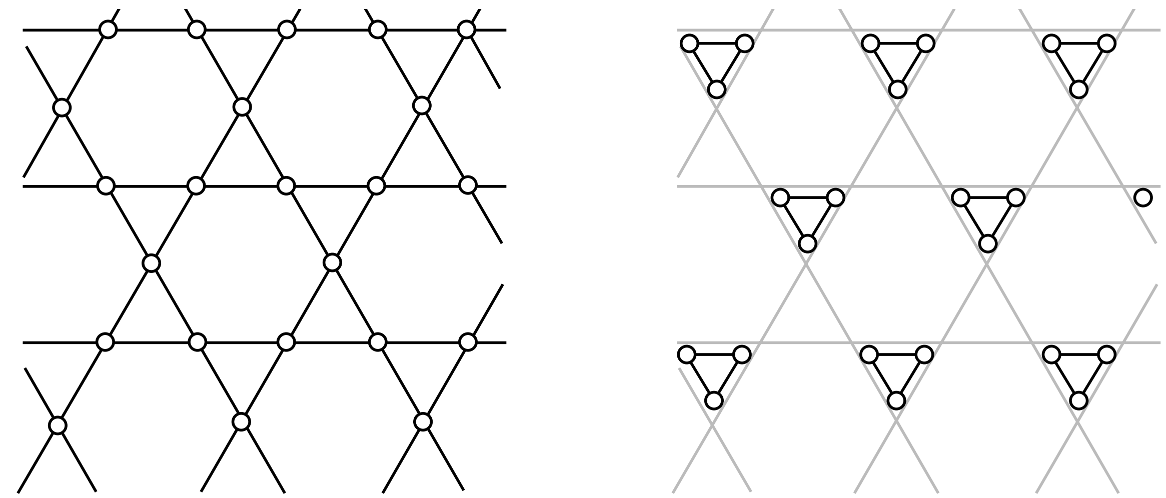
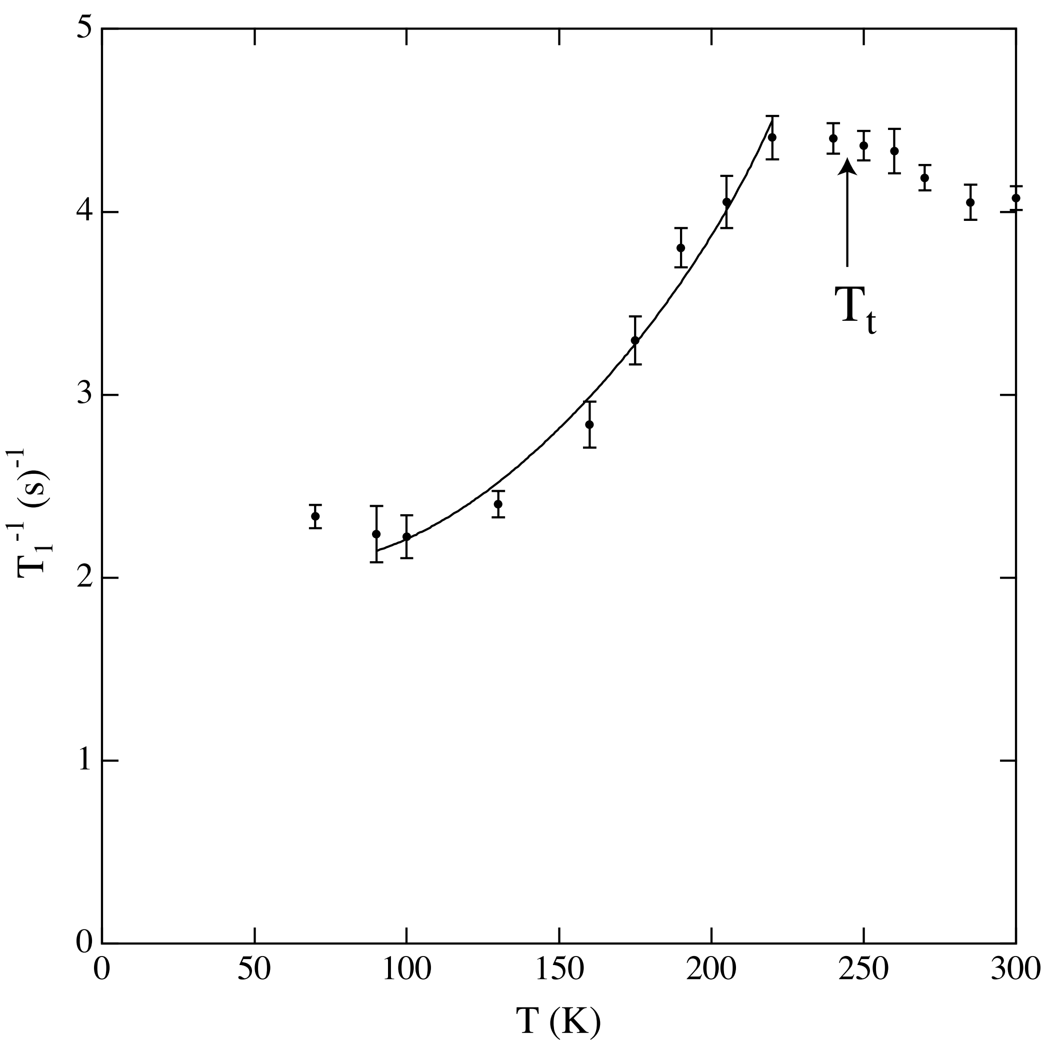


Fig. 1. (a) Crystal structure of NaV_6O_{11} at room temperature. Dashed lines express a unit cell. (b) V(1) kagomé lattice at $T > T_t$. (c) Distorted V(1) kagome lattice at $T < T_t$.



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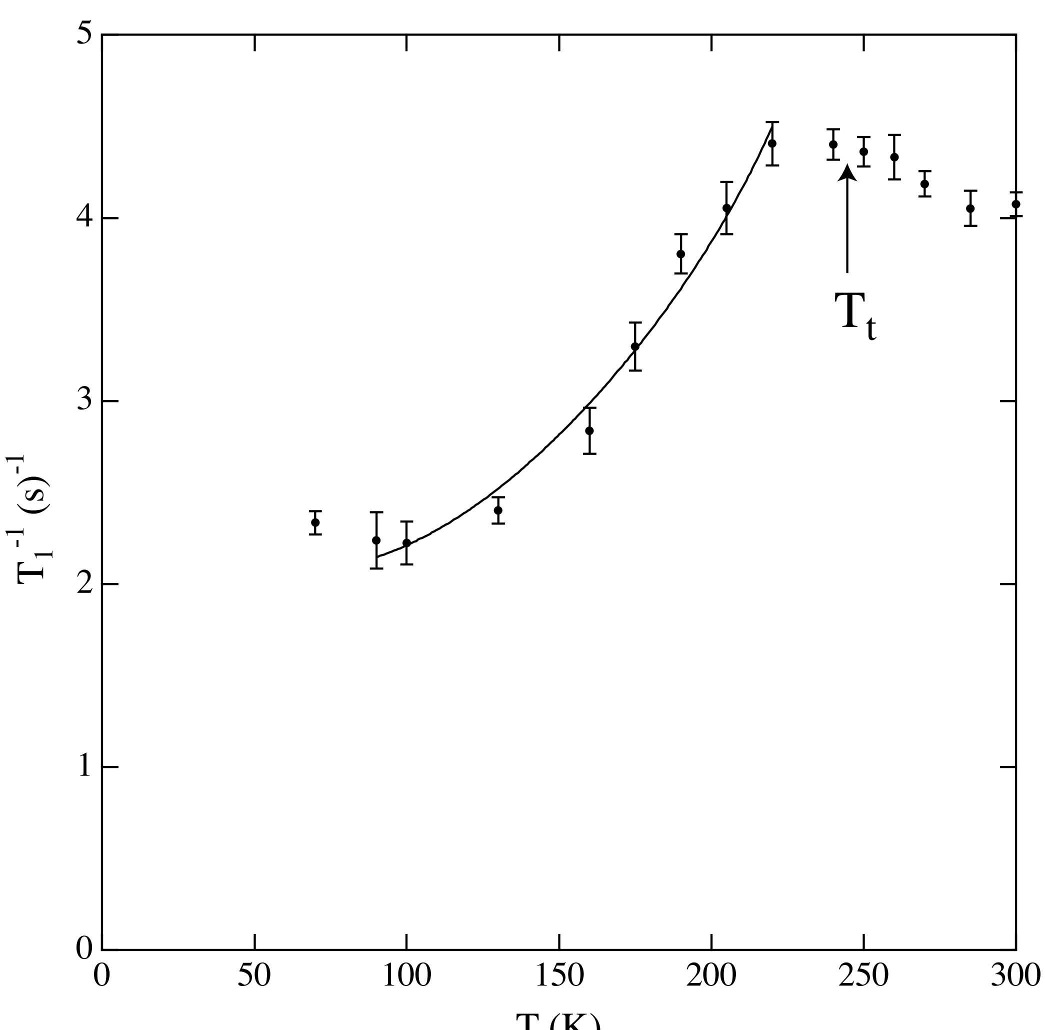

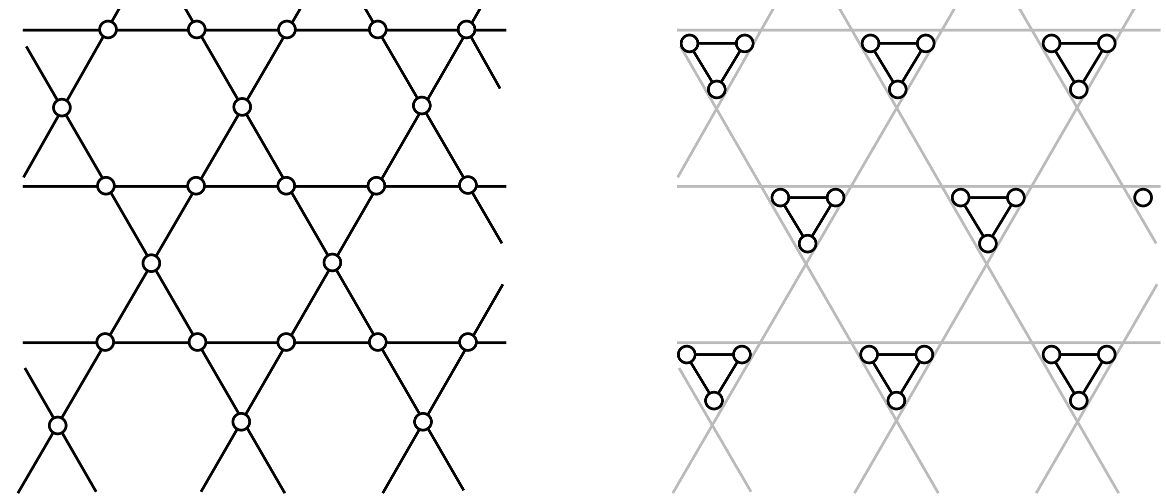

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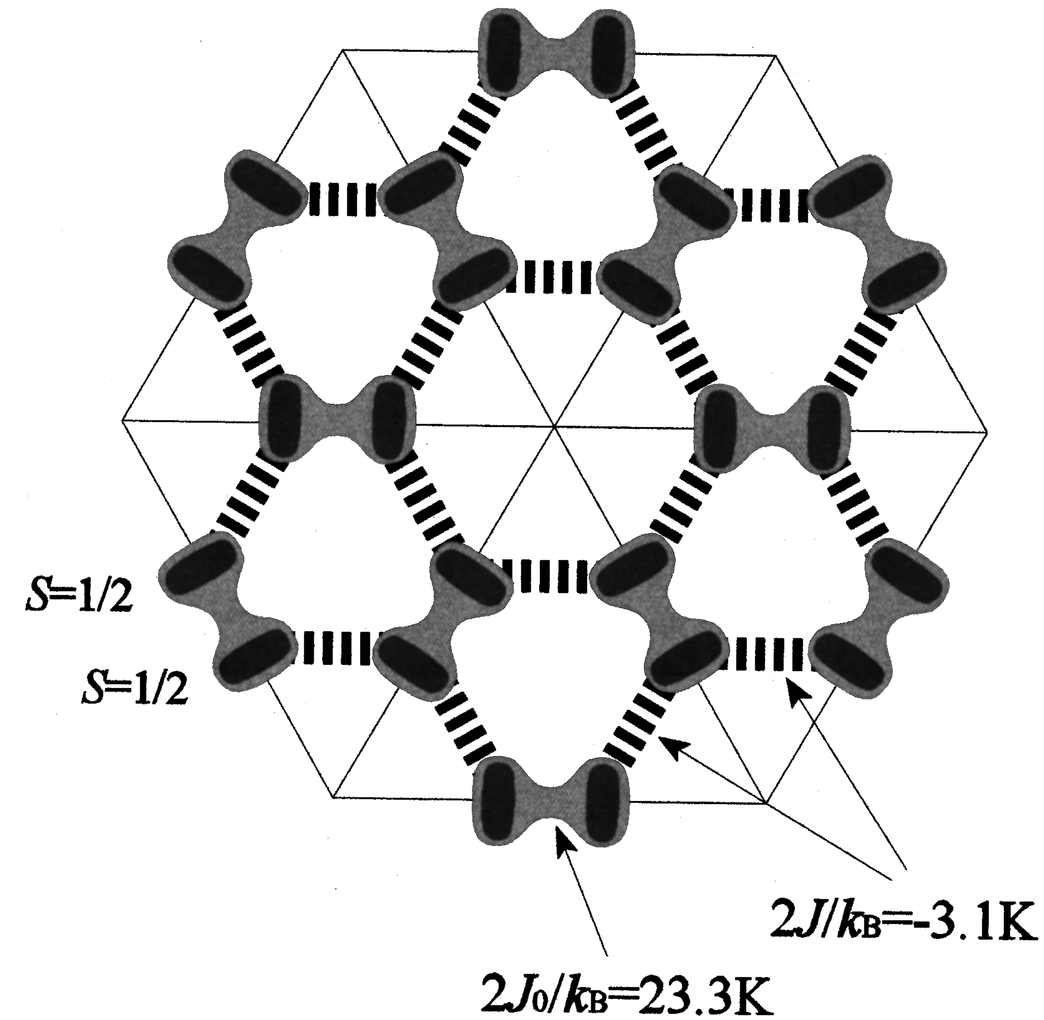
Another spin-1 Kagome compound

$KV_3Ge_2O_9$

Hara et al, JPSJ (2012)

Spin-1 KHA

[Kazuo Hida, JPSJ (2000)]

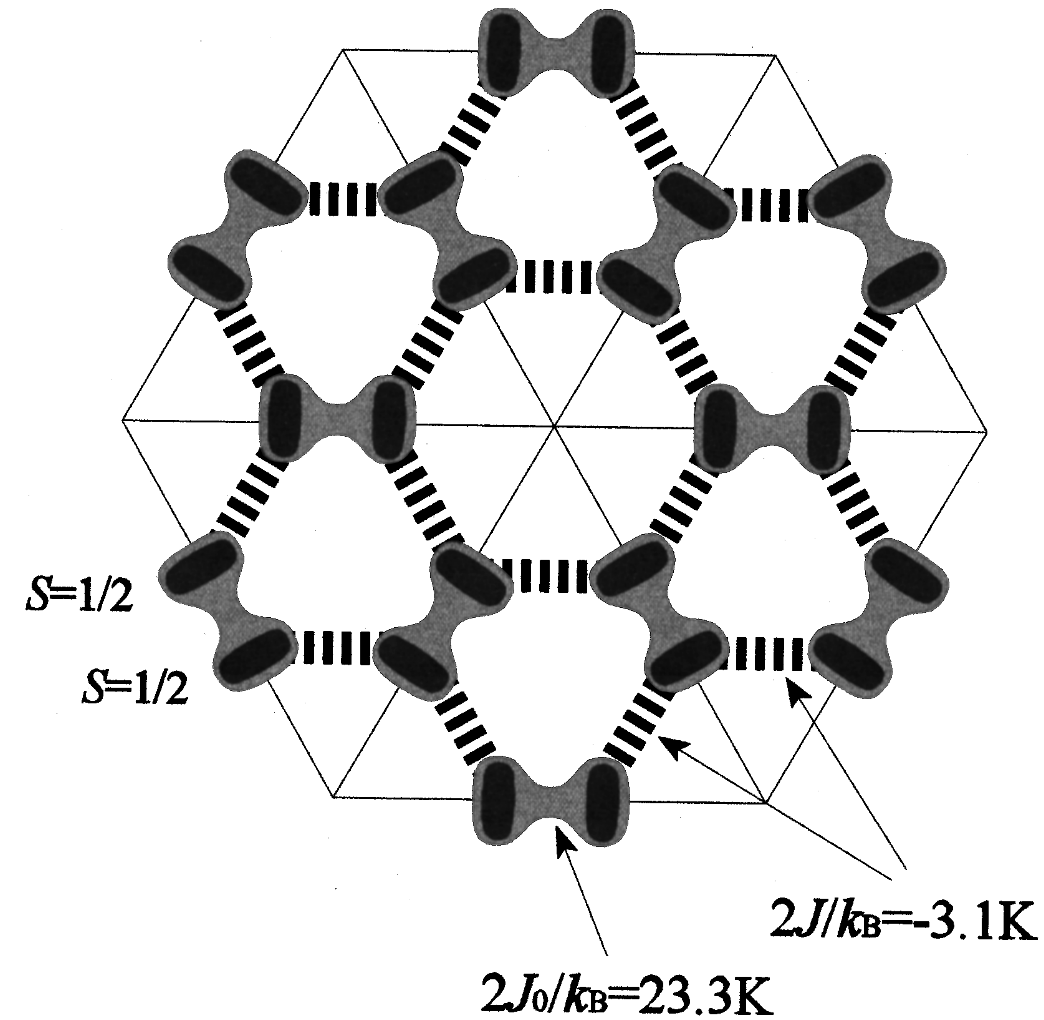


$$m - MPYNN.BF_4$$

Spin-1 KHA

[Kazuo Hida, JPSJ (2000)]

Minimal Model
(quantum spin-1/2 on honeycomb lattice)



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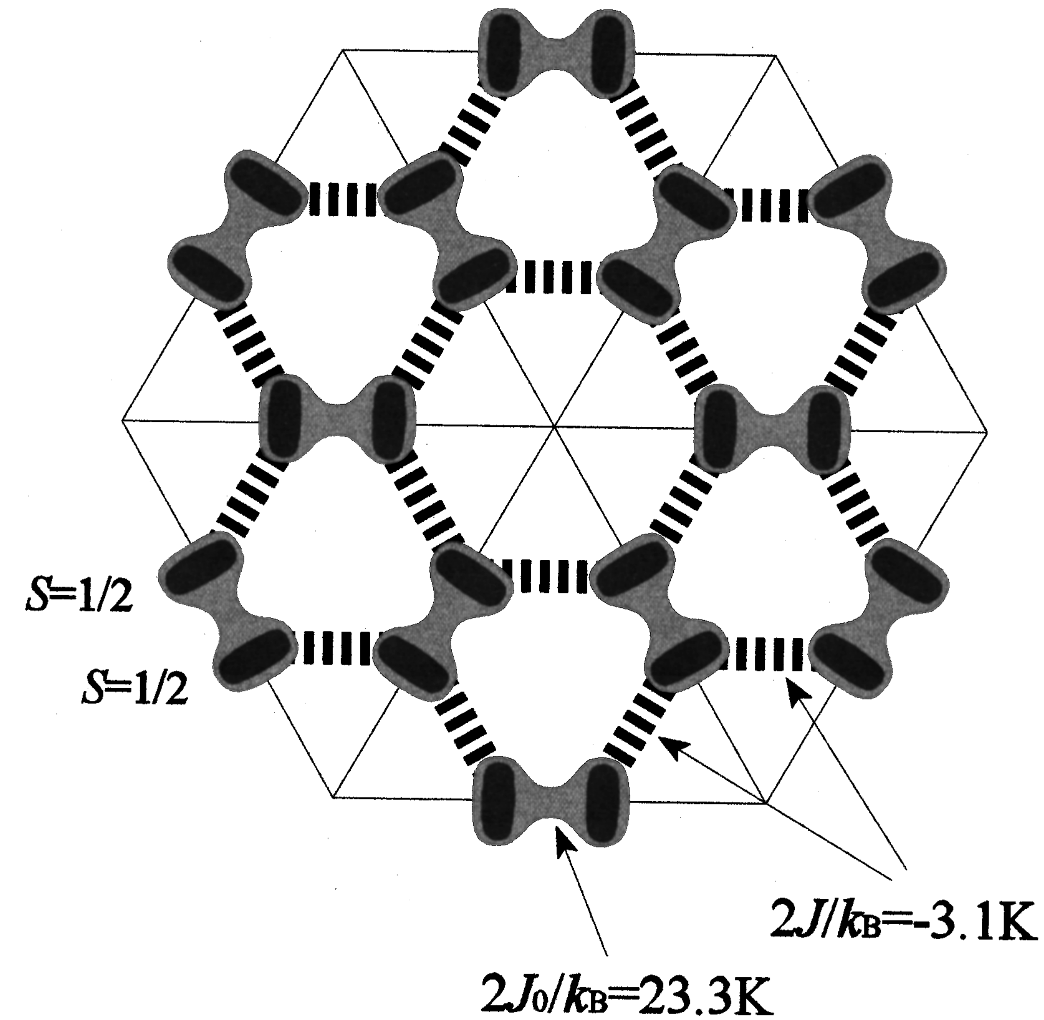

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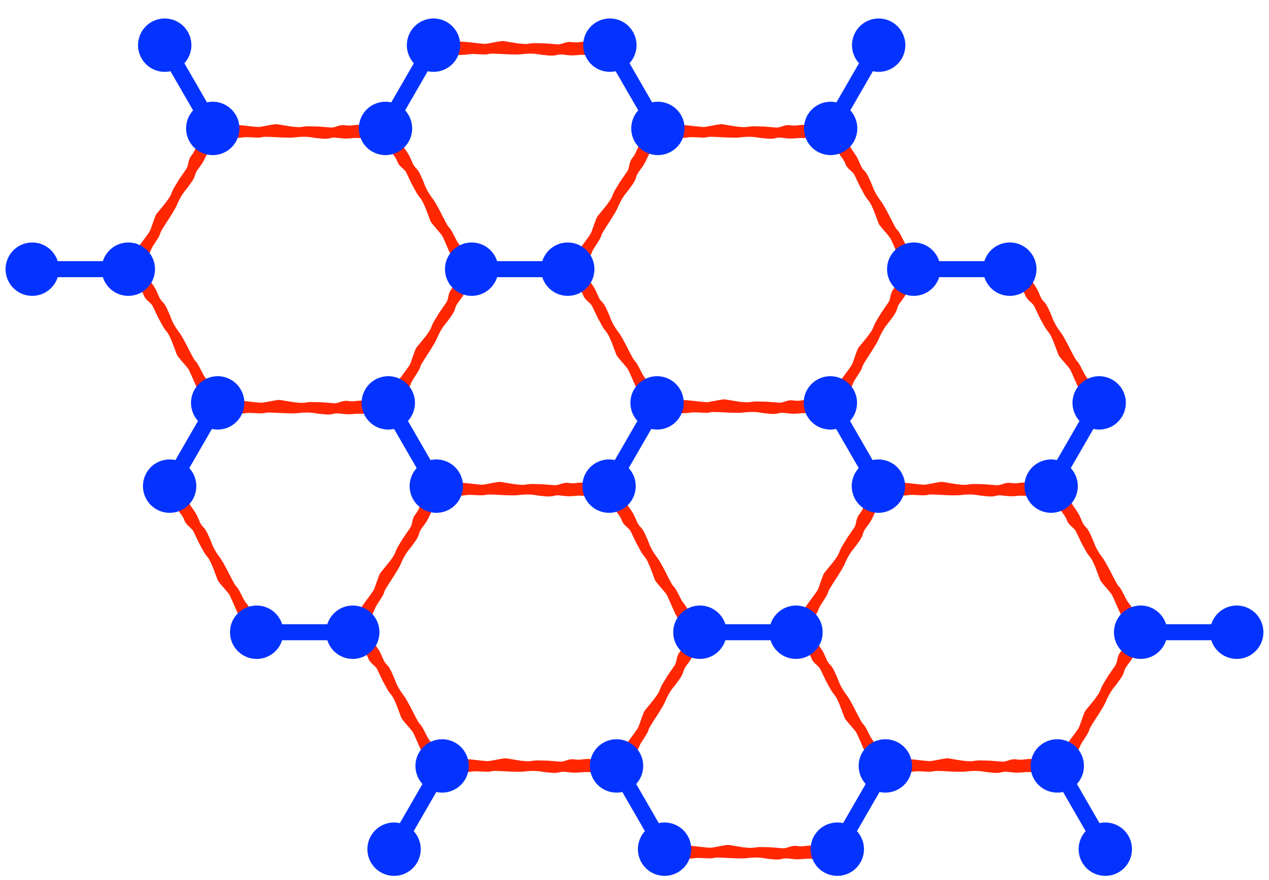

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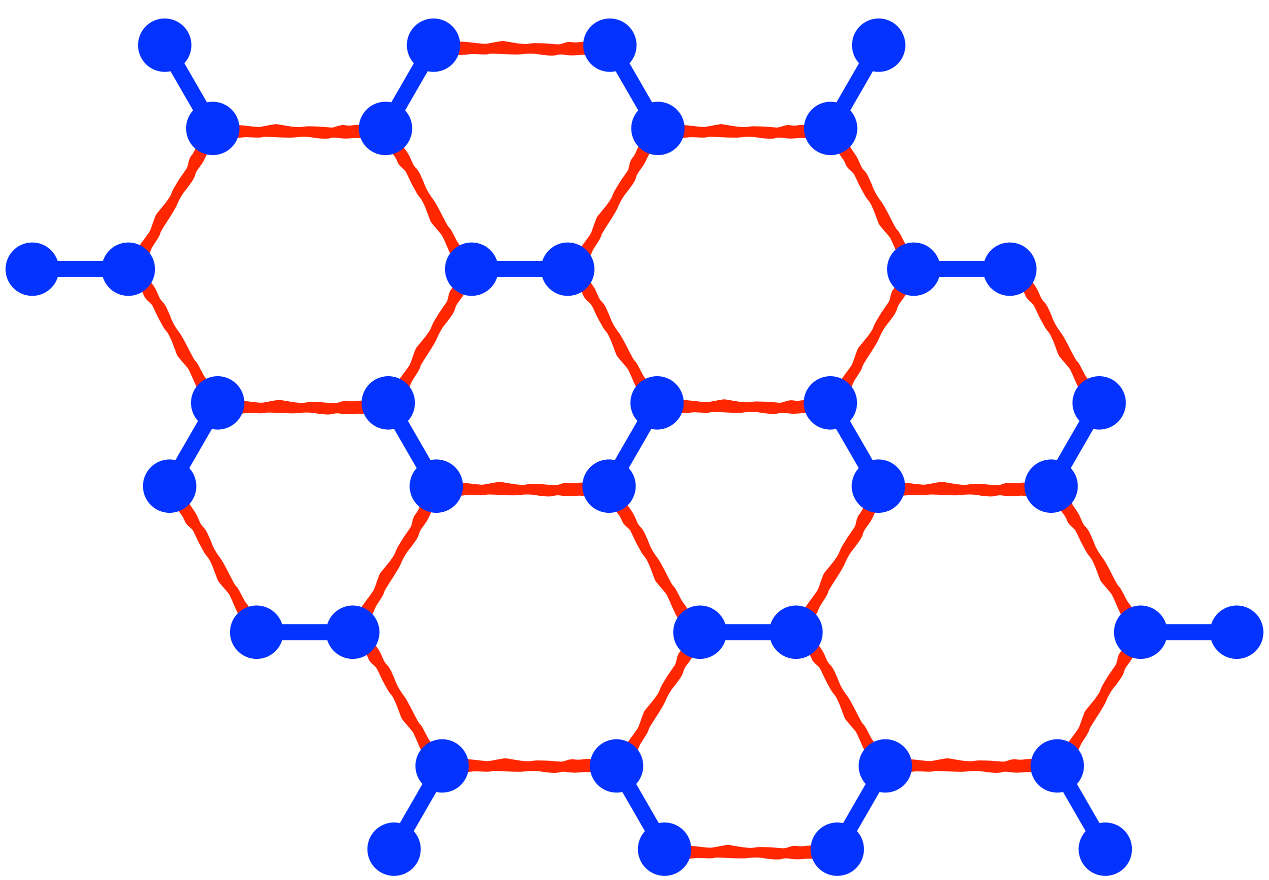

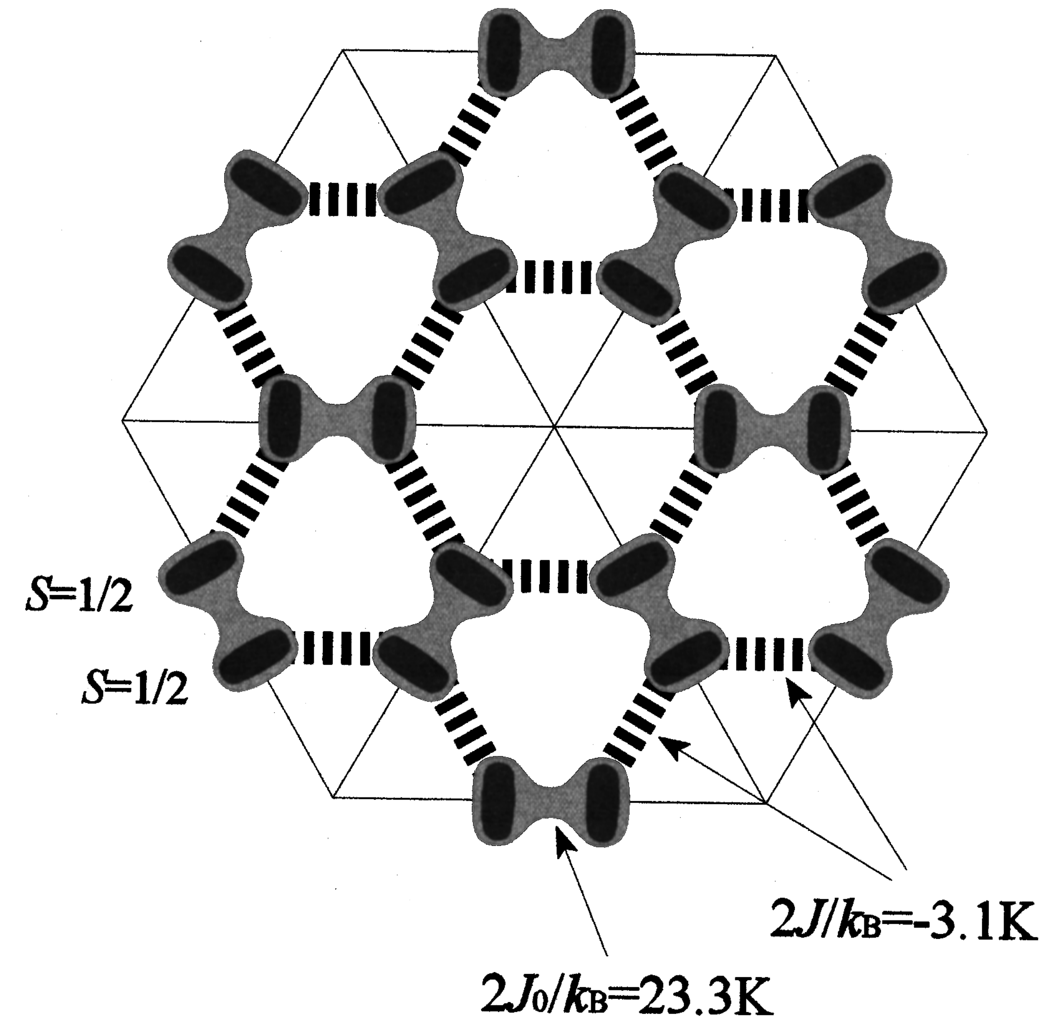

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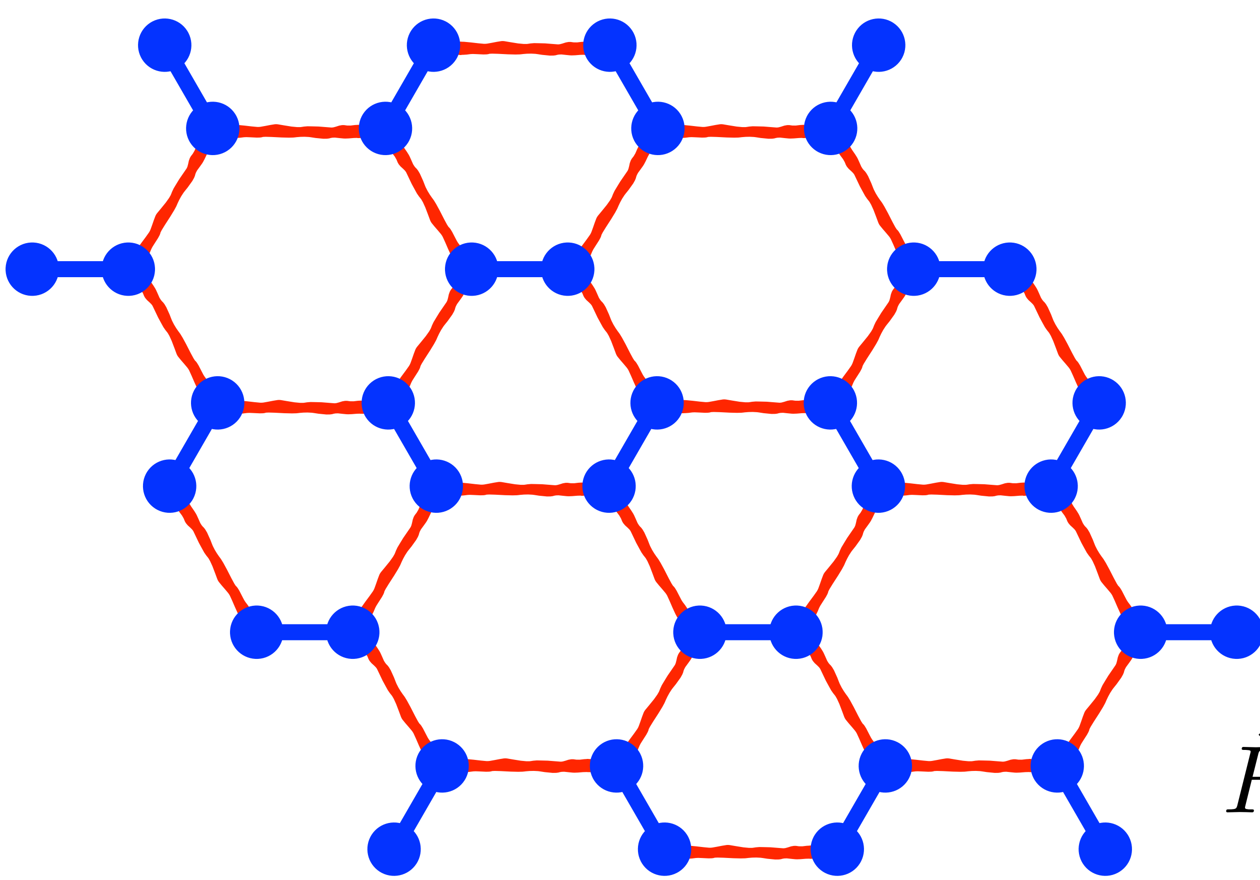

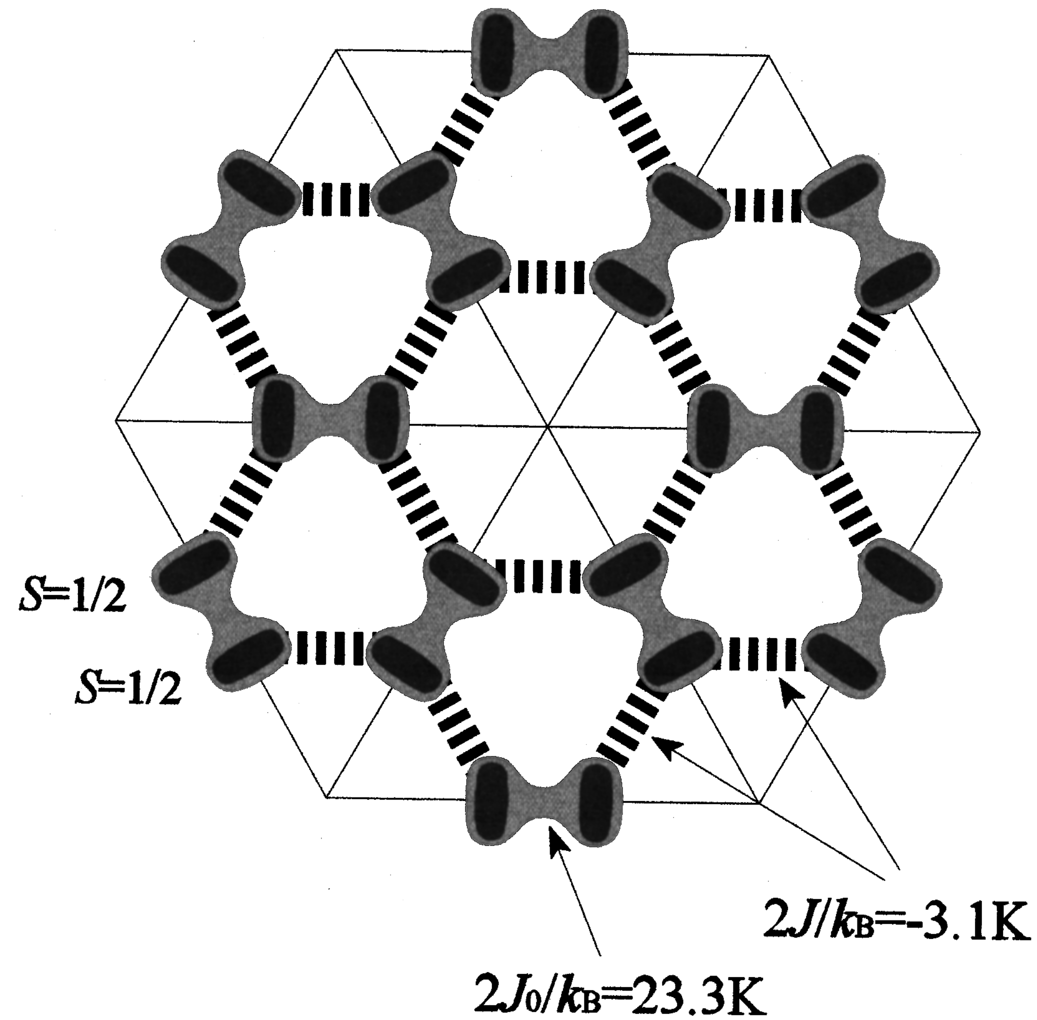

$$m-MPYNN.BF_4$$

$$\hat{H} = J_F \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_A \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

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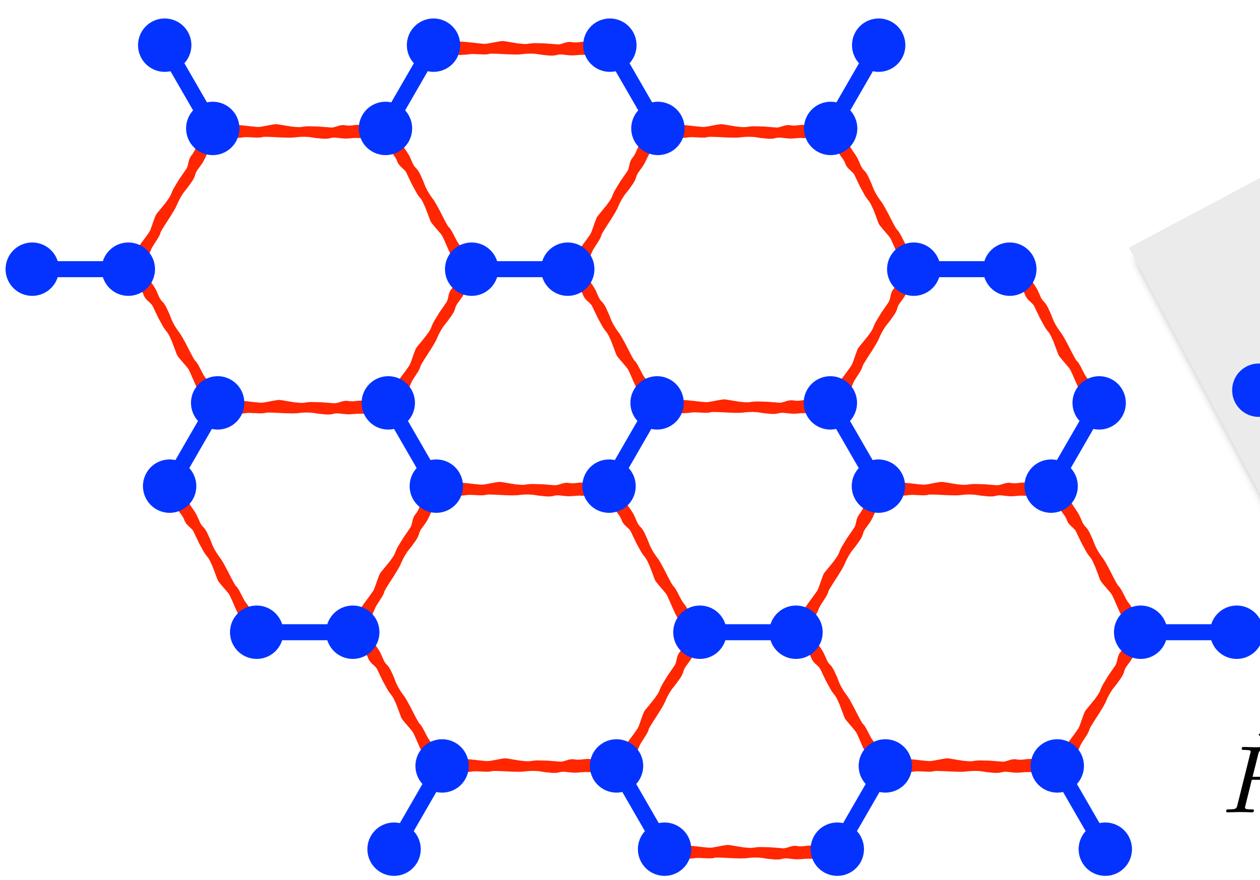

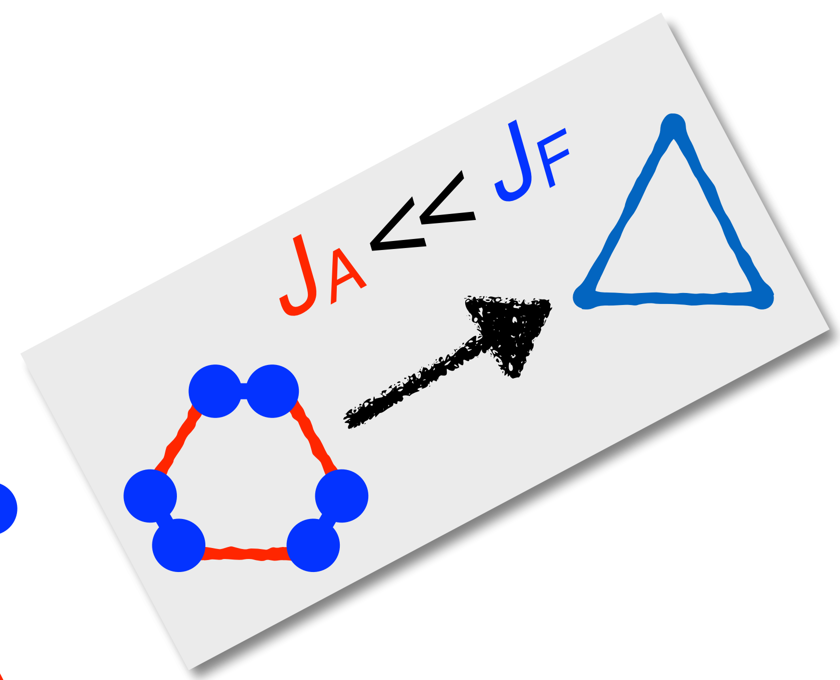

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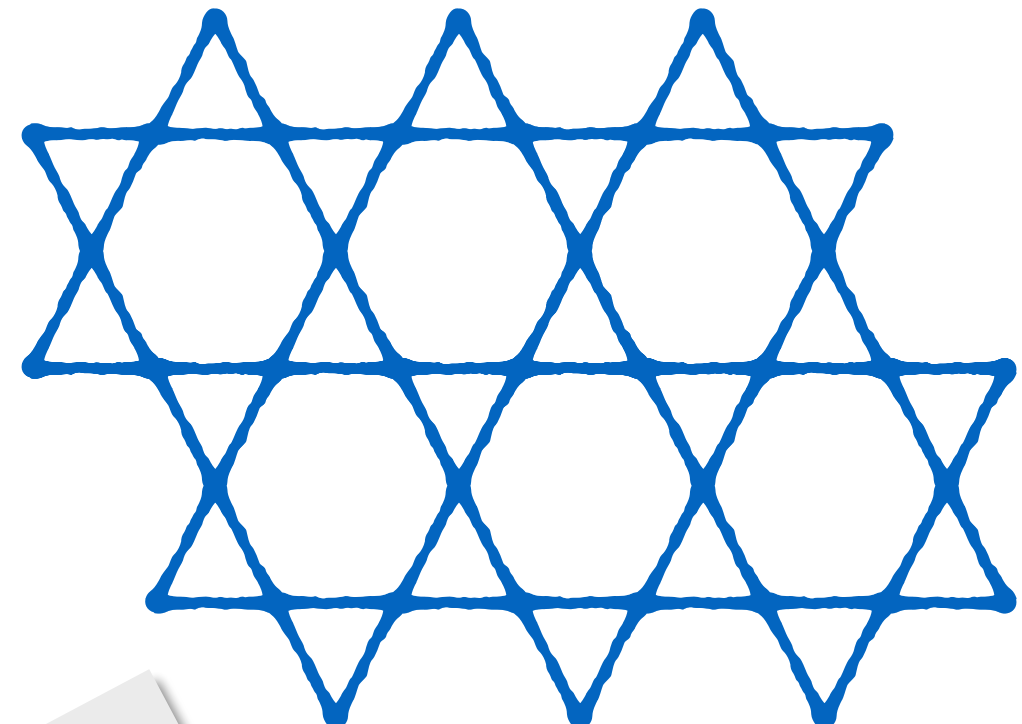

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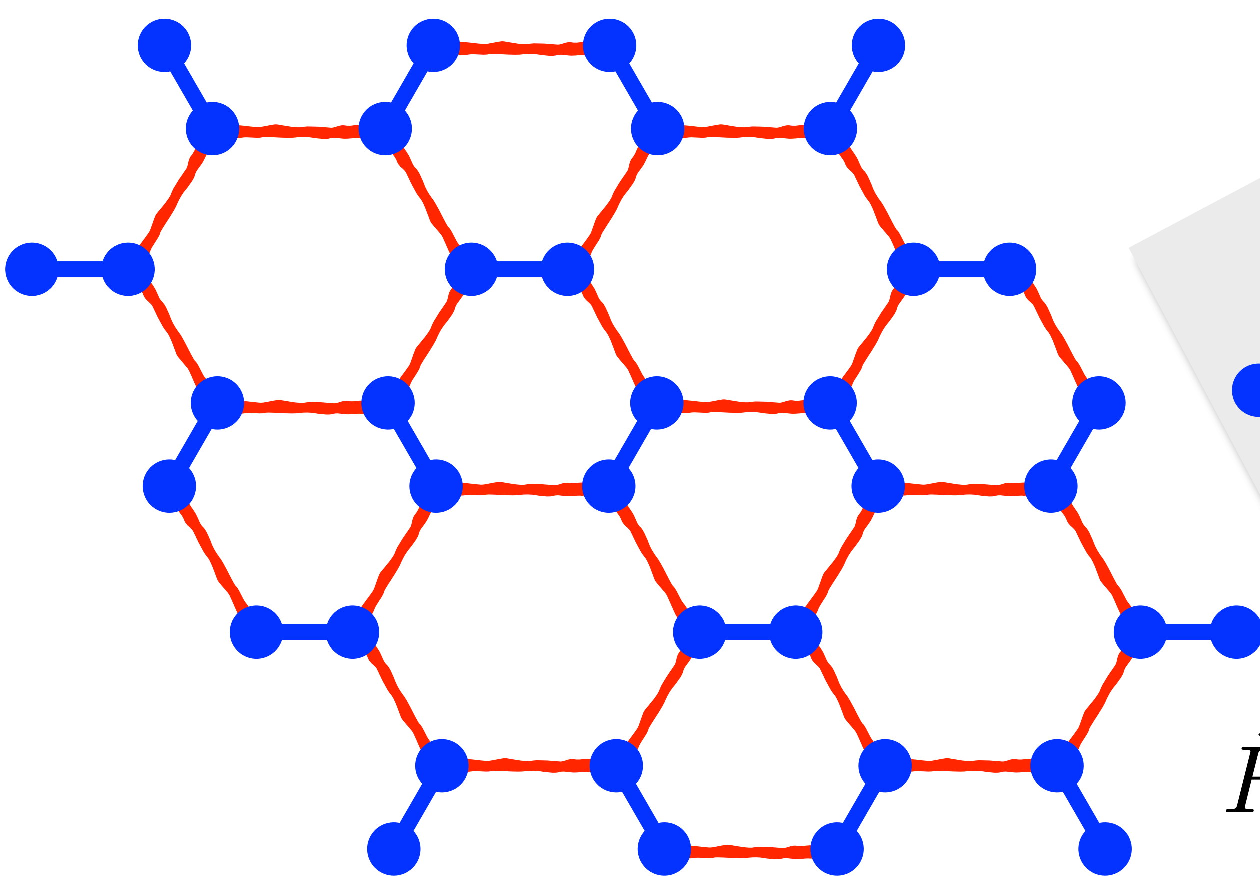

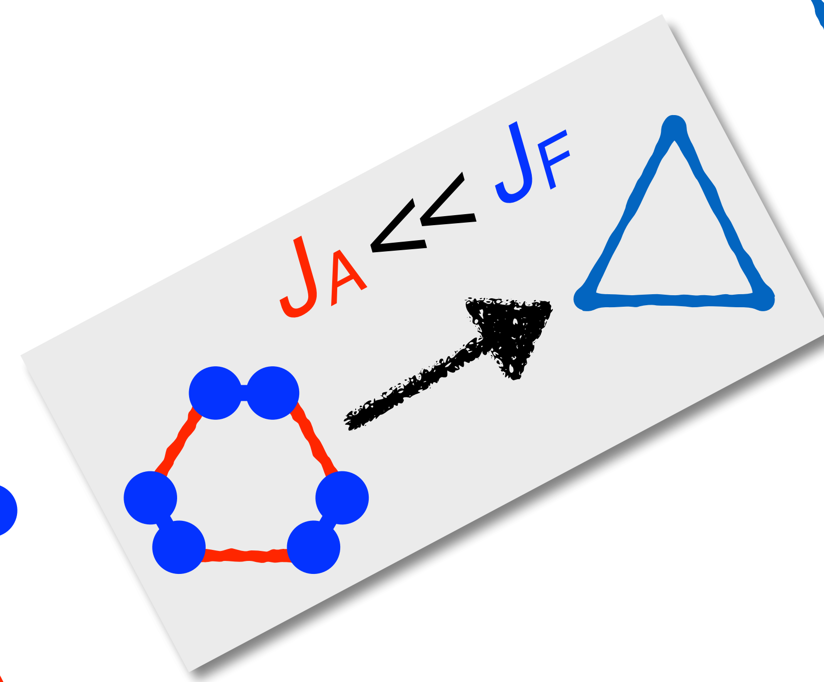

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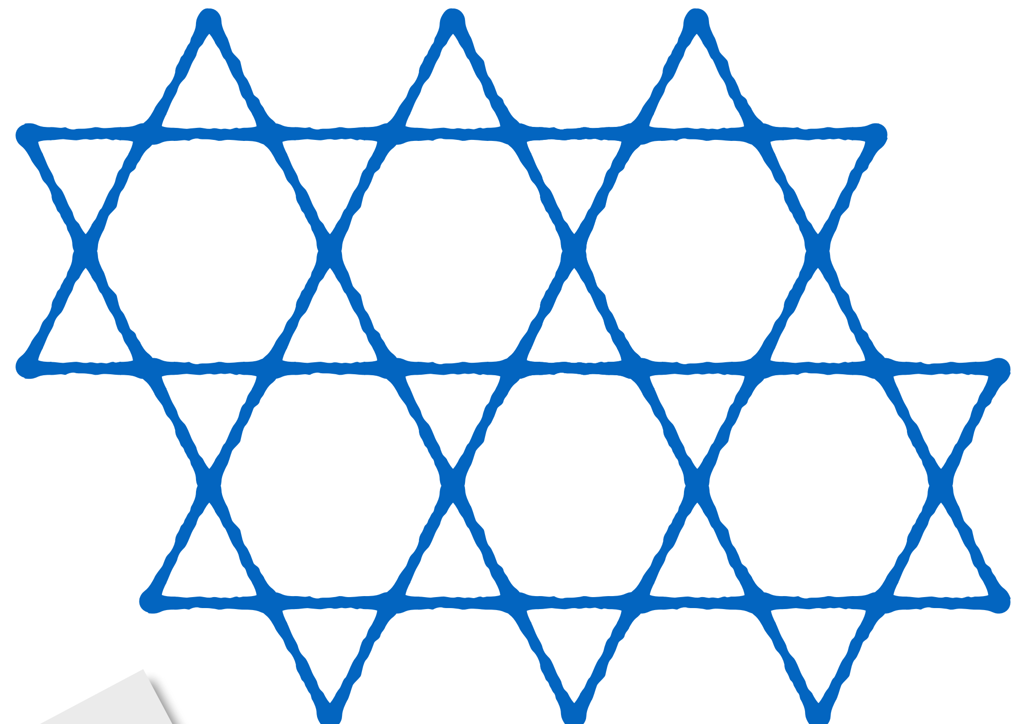
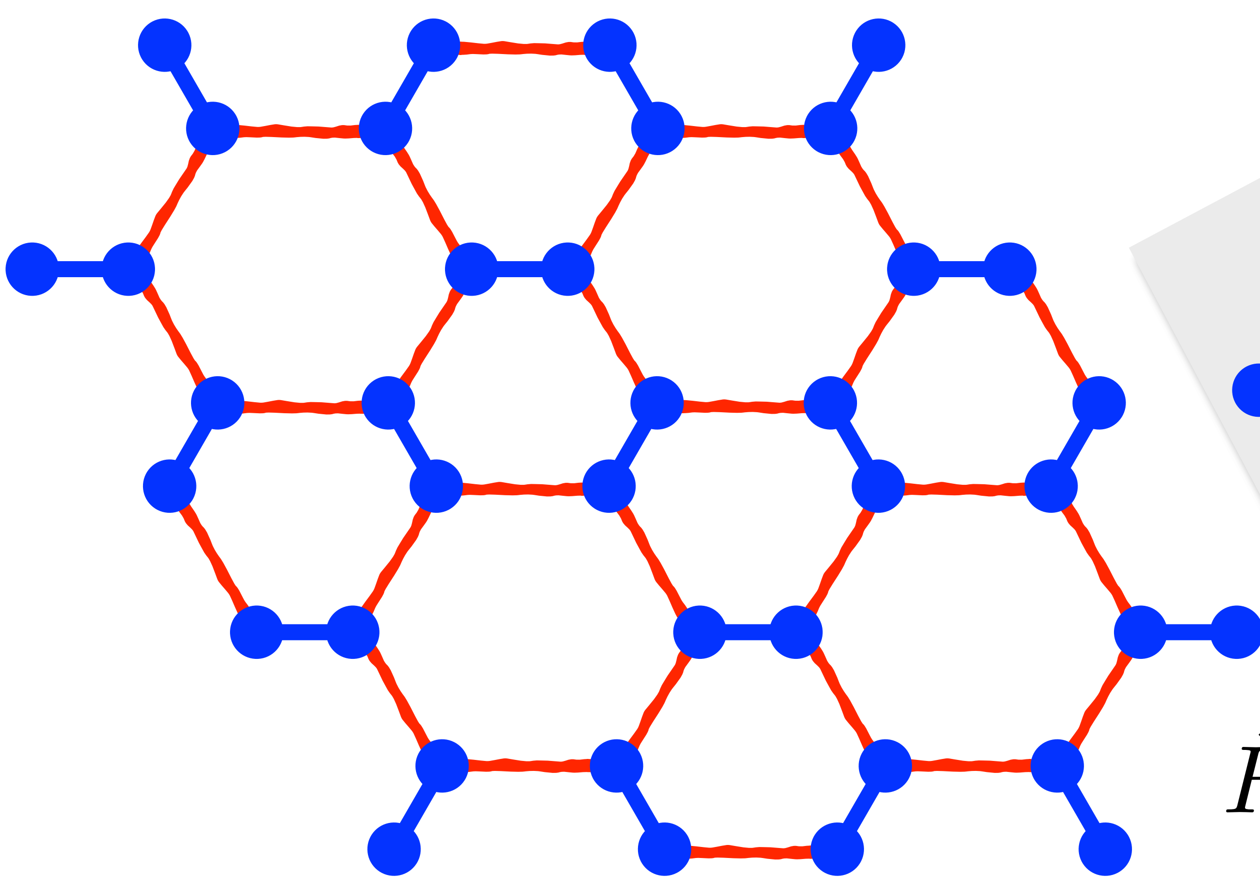
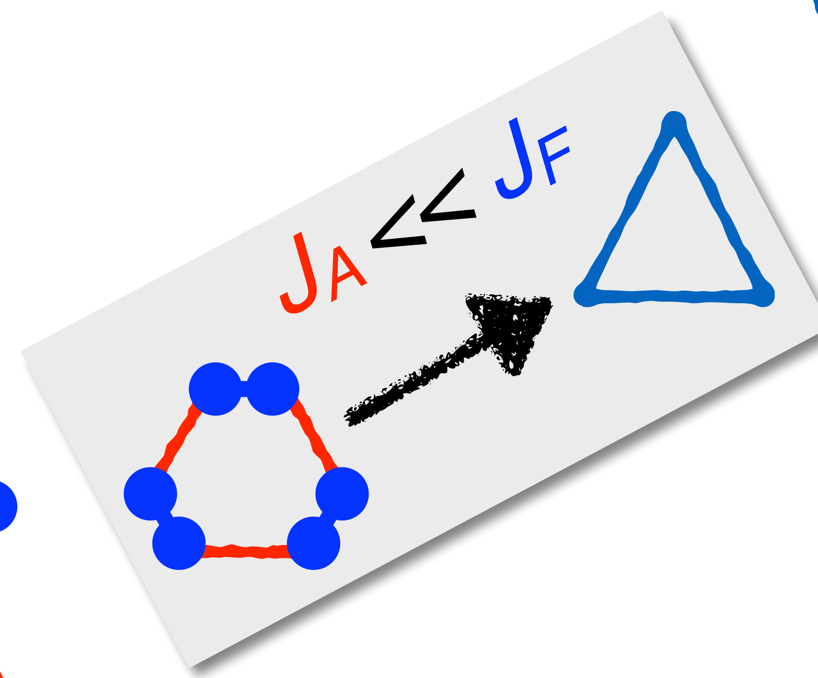


(spin-1 KHA)

"Hida Model"





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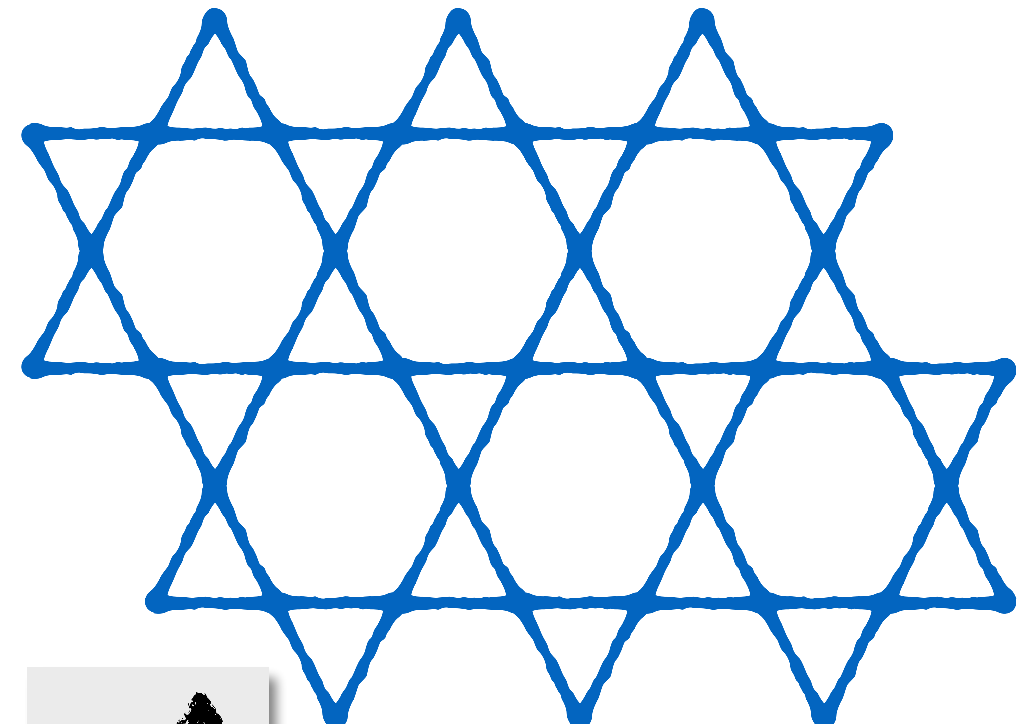

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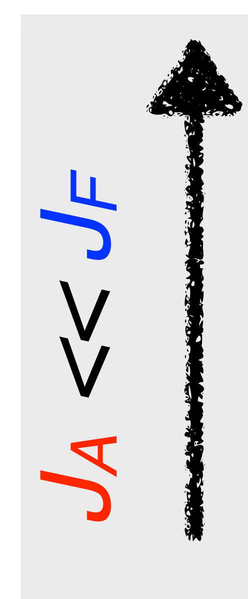

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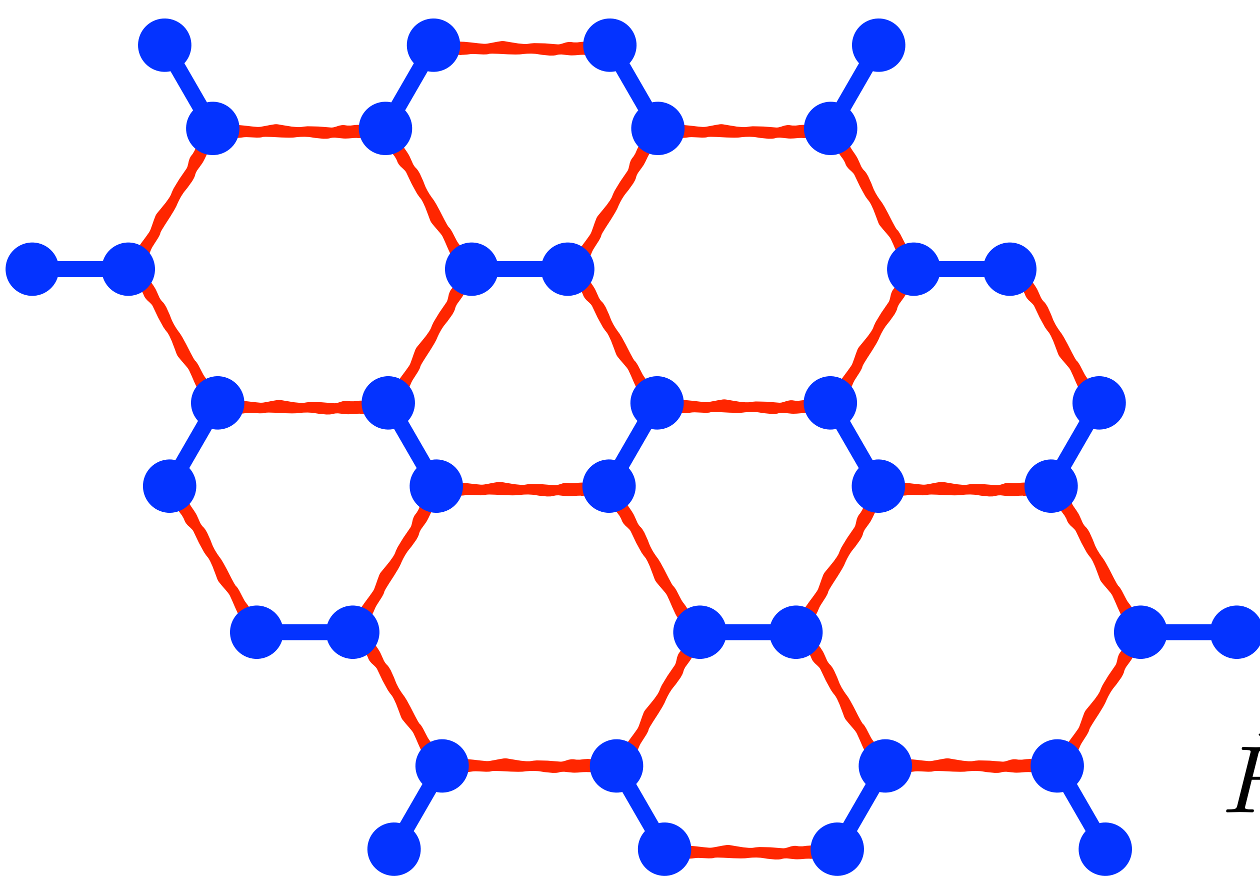

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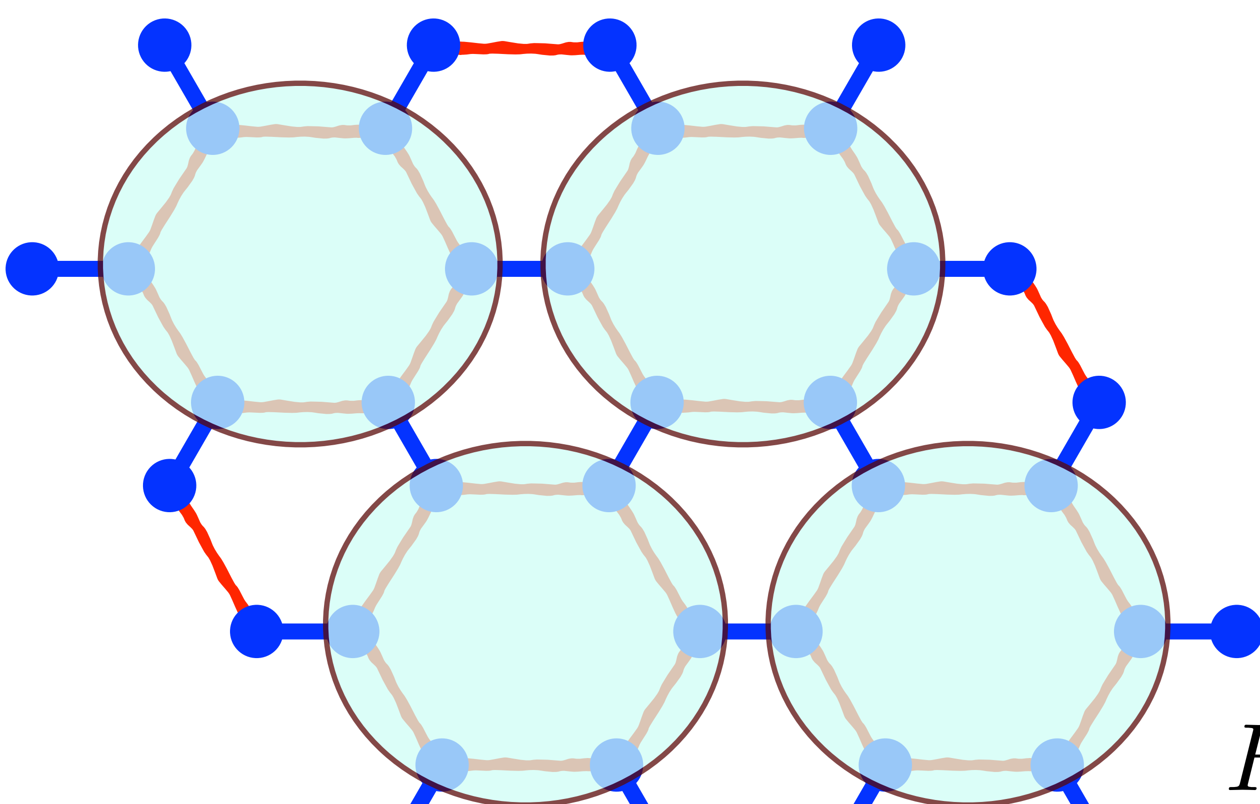
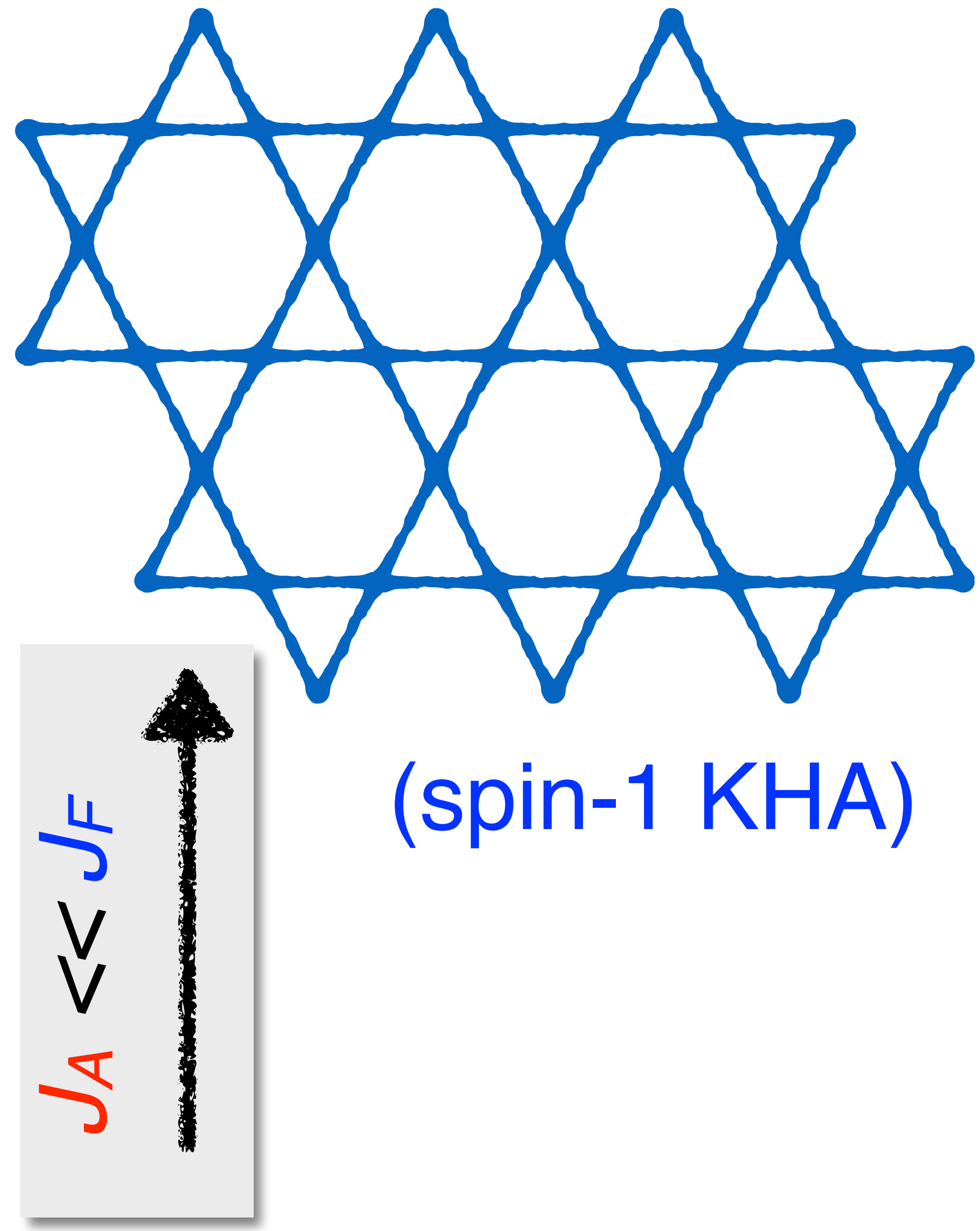
Spin-1 KHA

[Kazuo Hida, JPSJ (2000)]

Hida's ground state for spin-1 KHA

hexagonal singlets





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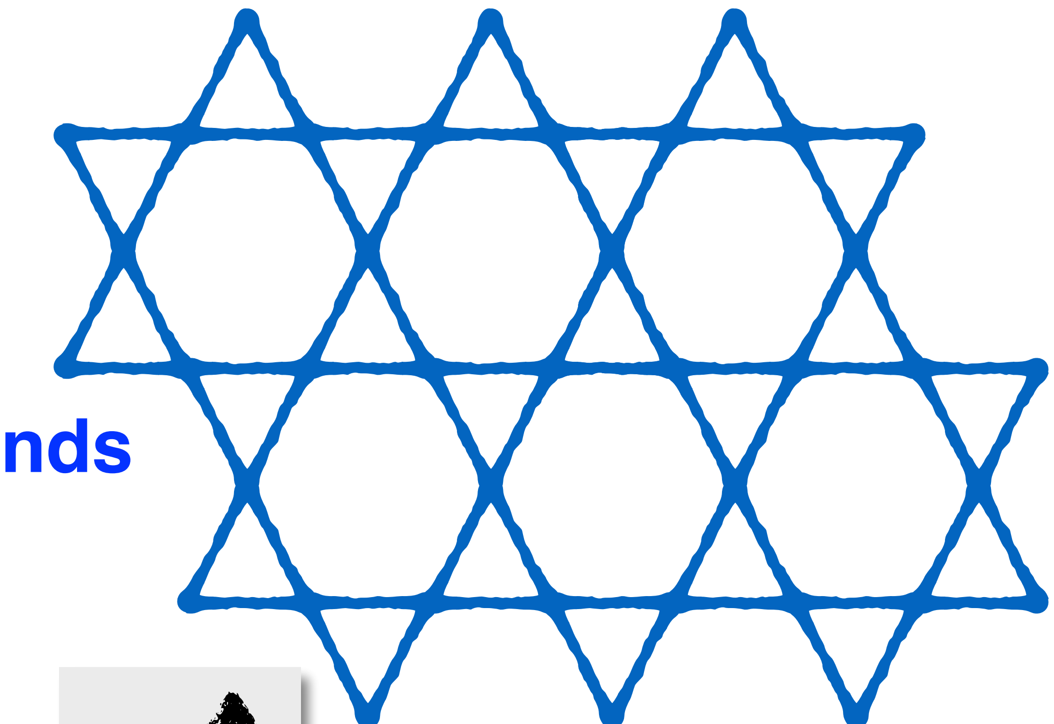
hexagonal singlets with symmetrized FM bonds



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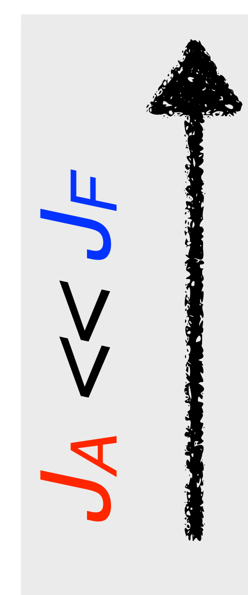

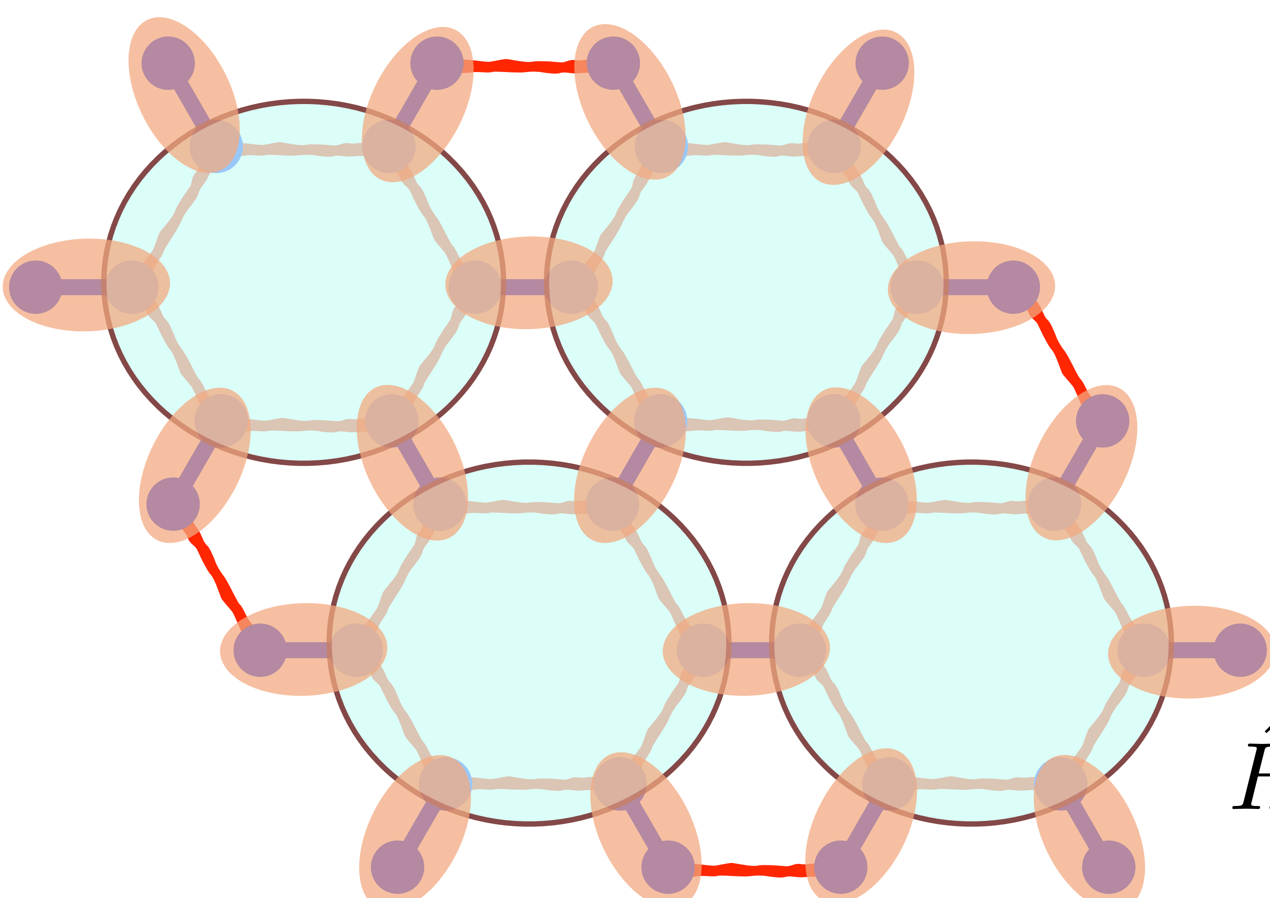

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Spin-1 KHA

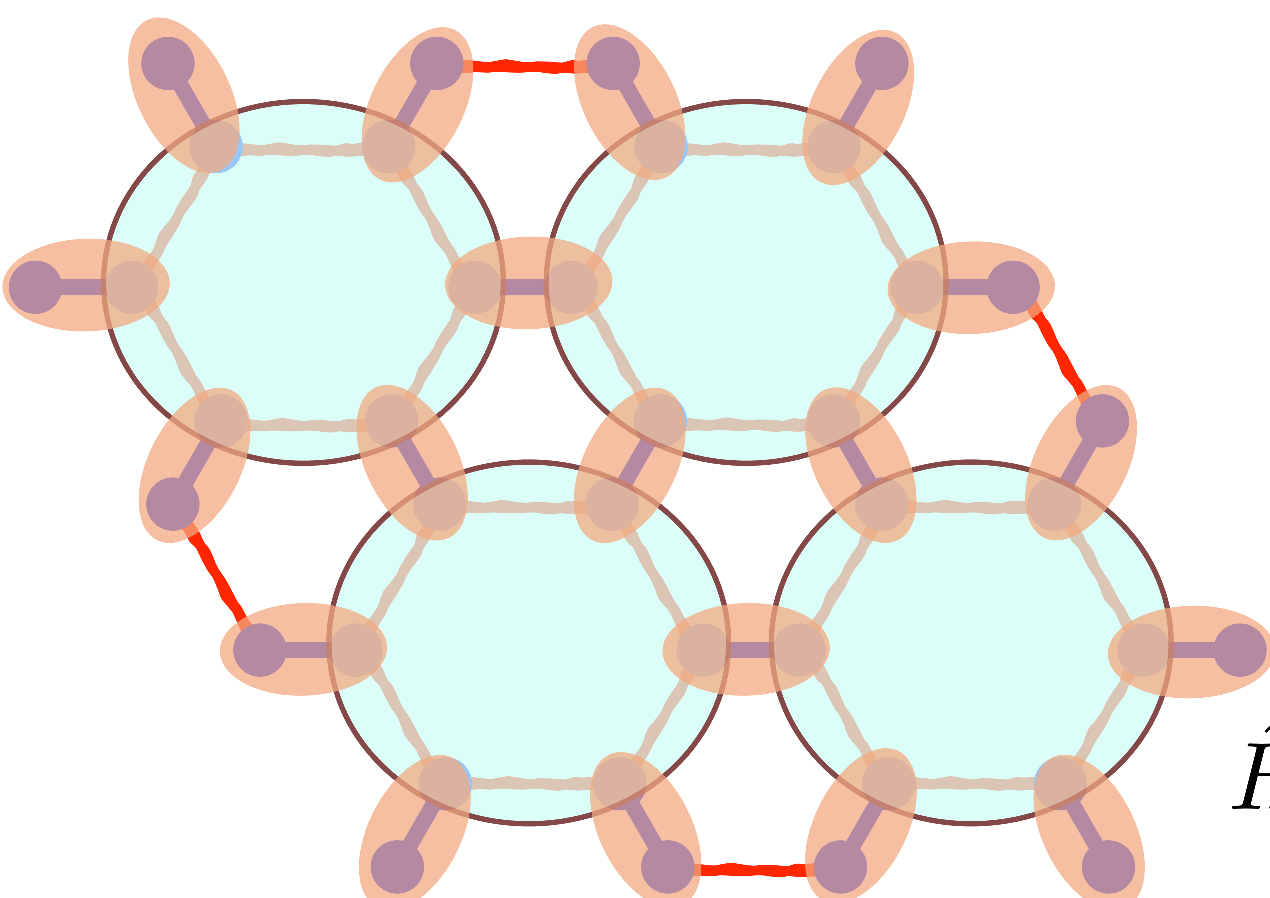
[Kazuo Hida, JPSJ (2000)]

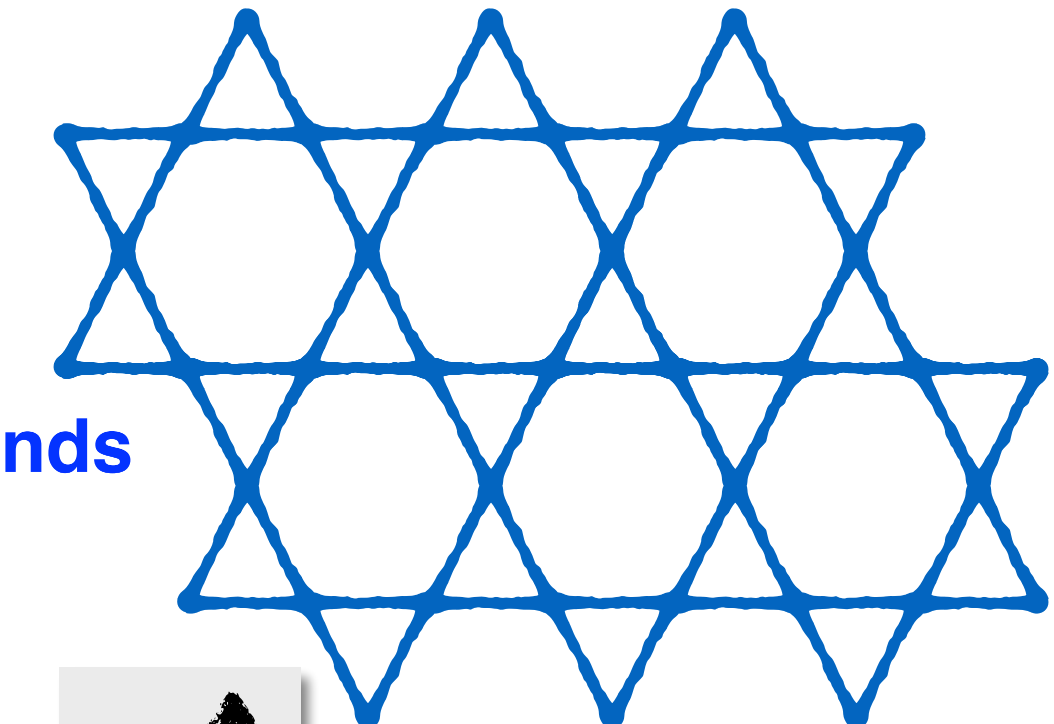
Hida's ground state for spin-1 KHA

hexagonal singlets with symmetrized FM bonds

(AKLT type)

HSS state





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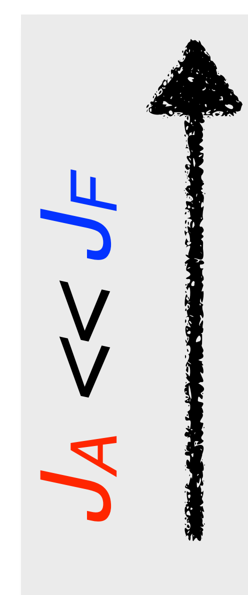

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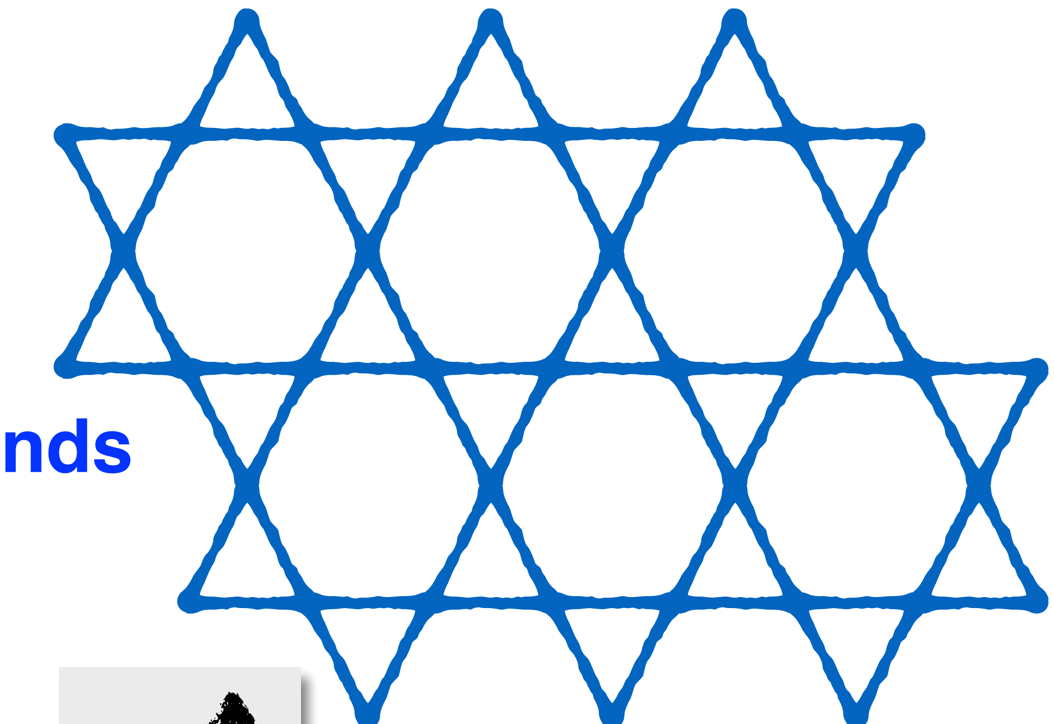

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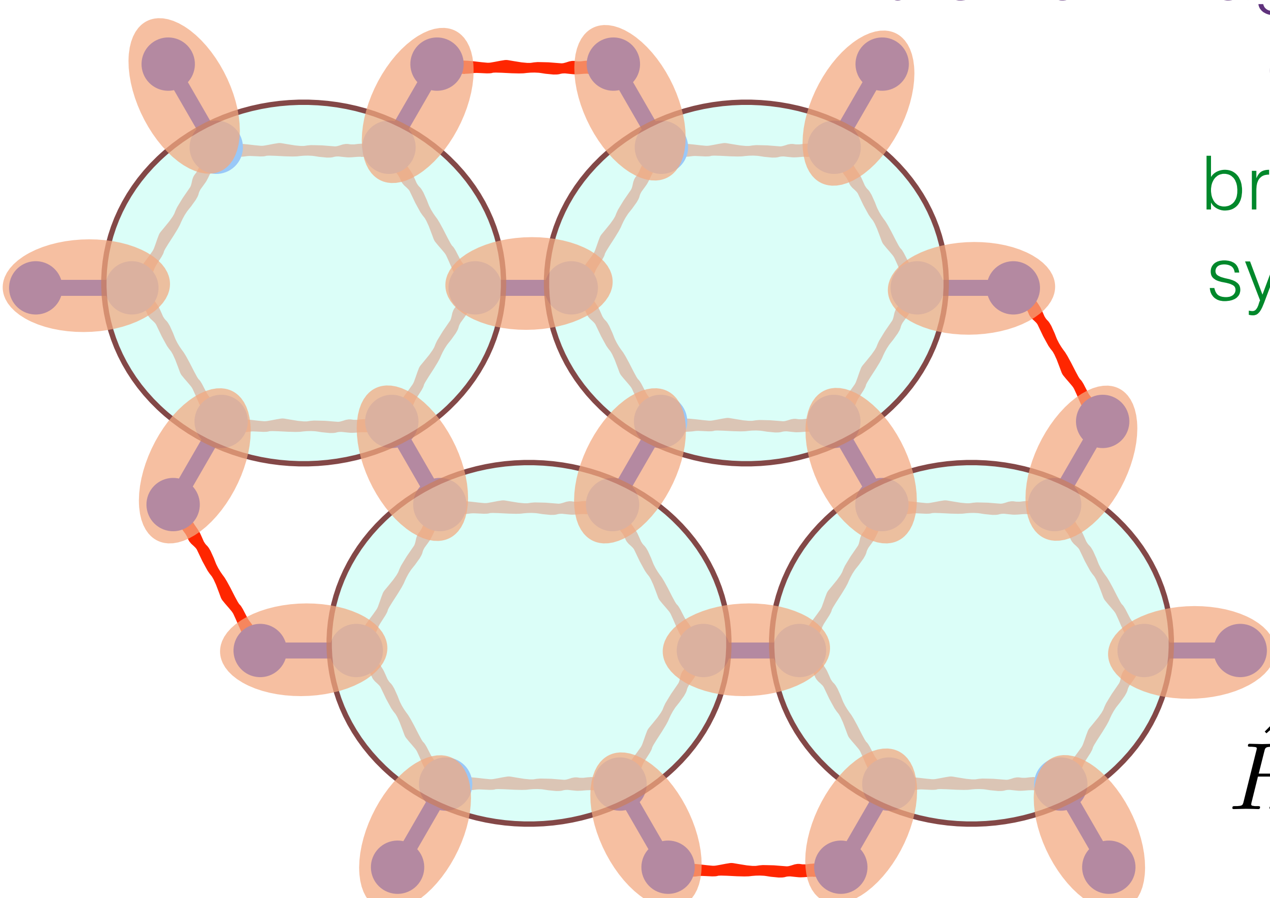
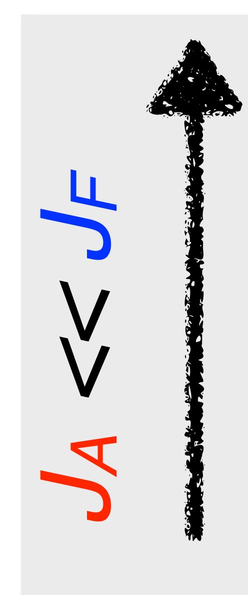


it is non-magnetic & gapped

breaks no symmetry



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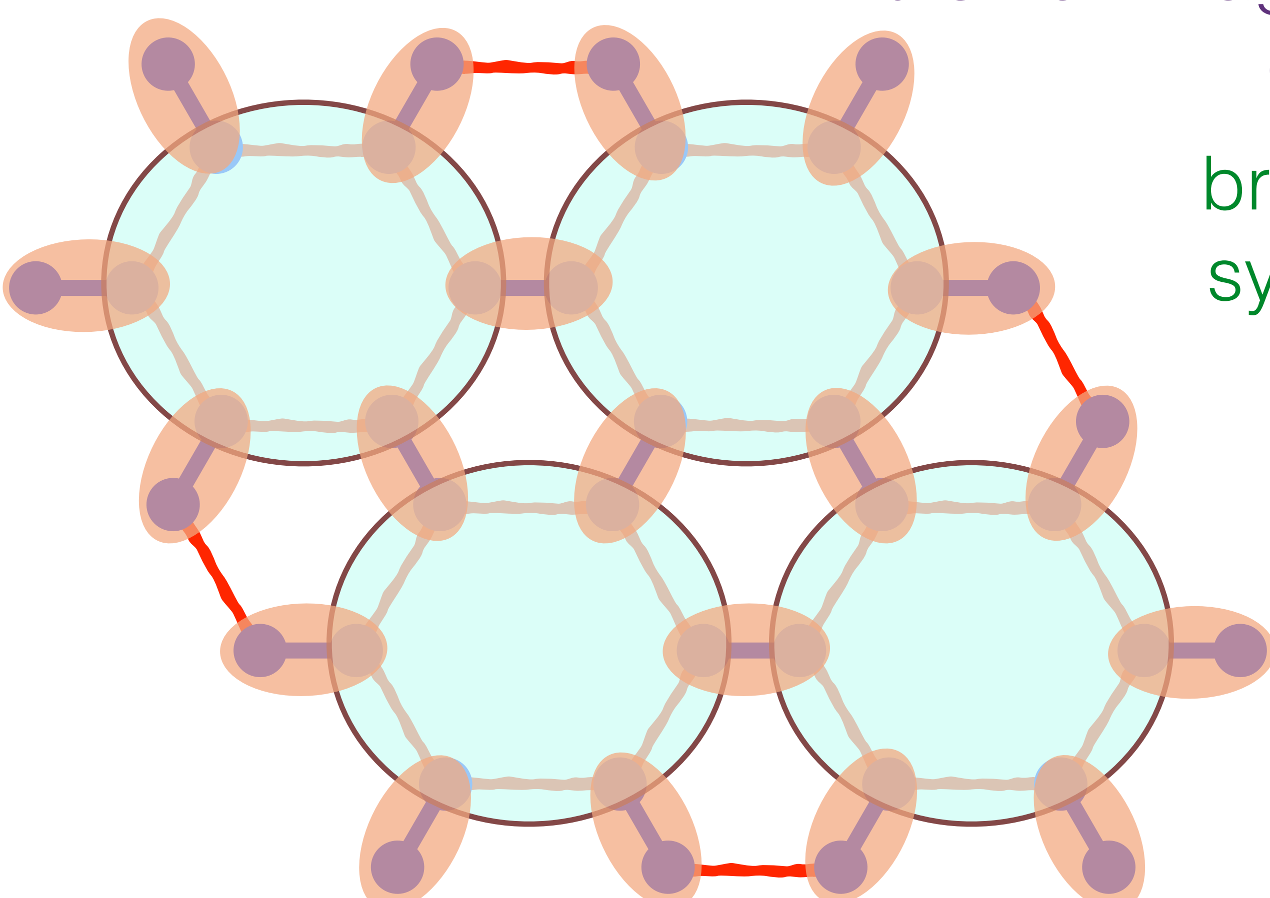

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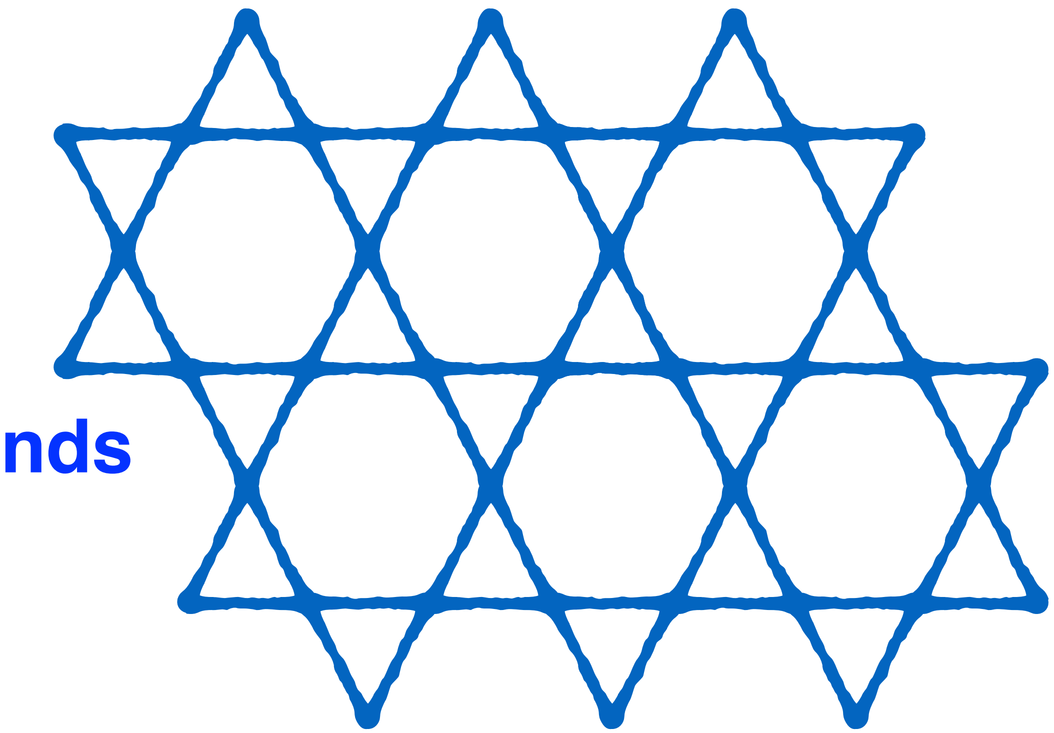


(spin-1 KHA)

However, the question of the ground state of spin-1 KHA has been revisited recently.

Spin-1 KHA

[Kazuo Hida, JPSJ (2000)]

Hida's ground state for spin-1 KHA

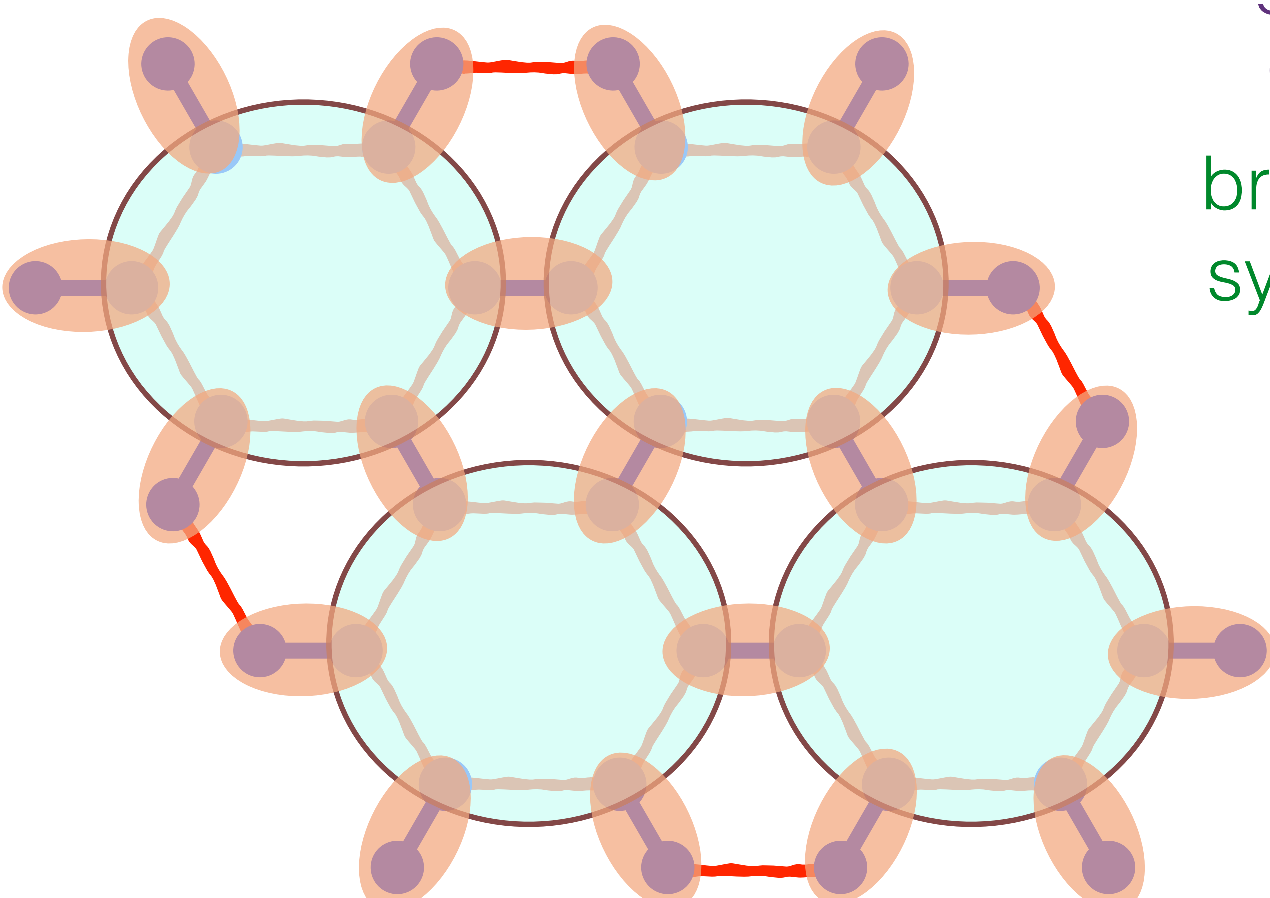
hexagonal singlets with symmetrized FM bonds

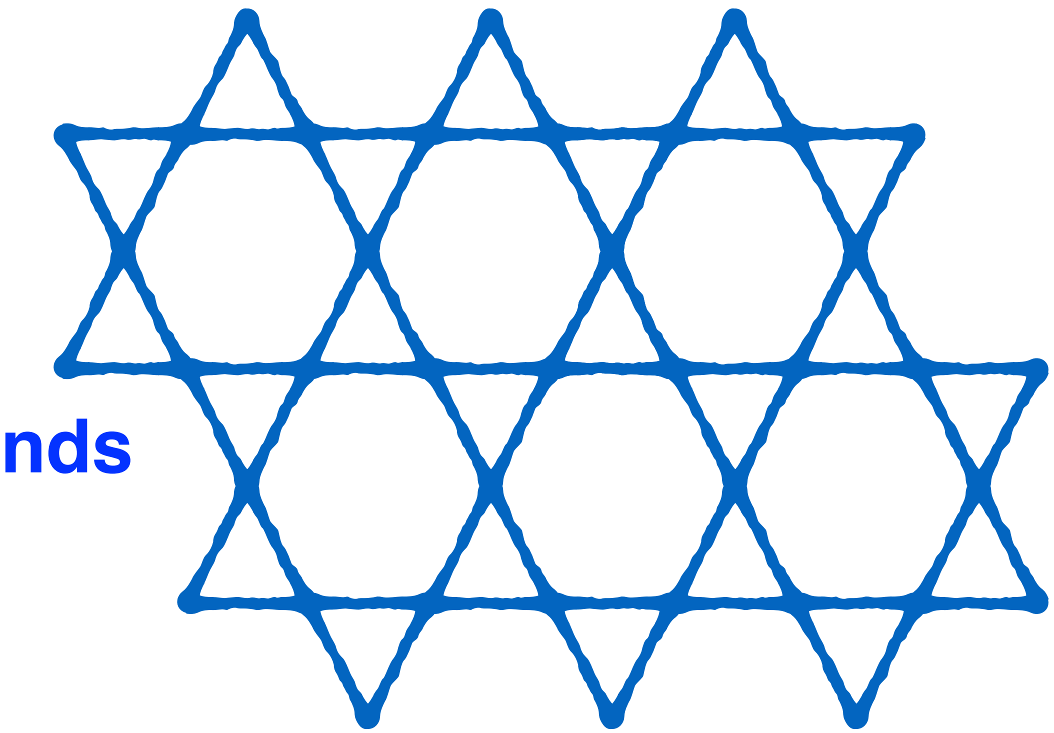
(AKLT type)

HSS state

it is non-magnetic & gapped

breaks no symmetry





(spin-1 KHA)

However, the question of the ground state of spin-1 KHA has been revisited recently.

and, energetically better candidate for the ground state has been found.

Spin-1 KHA

Spontaneously Trimerised Singlet (TS) state

Liu et al, PRB-Rapid (2015)

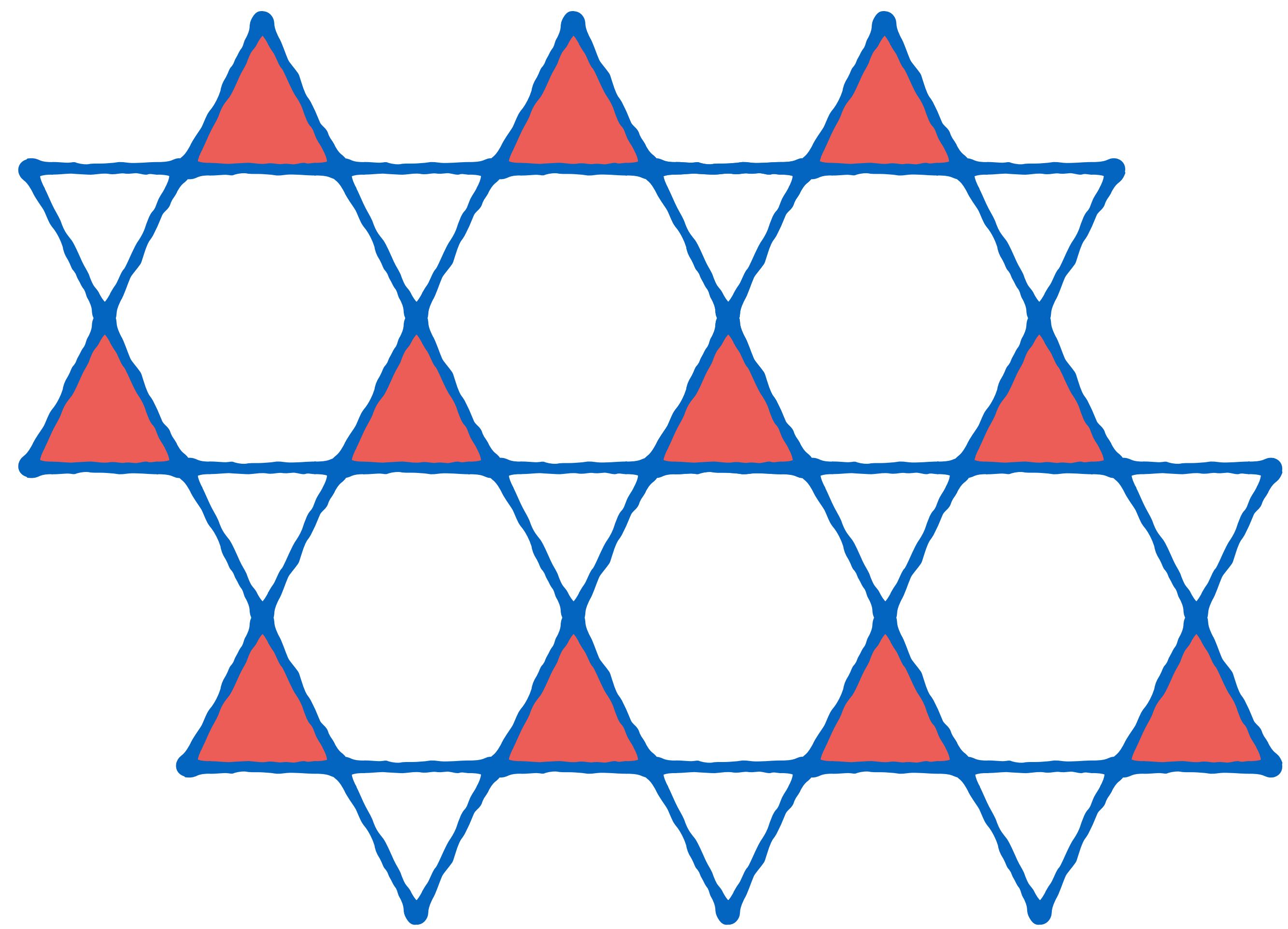
Picot and Poilblanc, PRL (2015)

Changlani and Läuchli, PRB (2015)

Ghosh, Verma and Kumar, PRB (2016)

Rajiv Singh et al (2016)

and others…



[Z. Cai et al, J. Phys. Condens. Matter. (2009)]

Spin-1 KHA

A Model on Trimerised Kagome Lattice

$$\hat{H} = J \sum_{\triangle} \vec{S}_i \cdot \vec{S}_j$$

$$+J' \sum_{\nabla} \vec{S}_i \cdot \vec{S}_j$$

P. Ghosh, A. K. Verma, and BK, PRB (2016)

Spin-1 KHA

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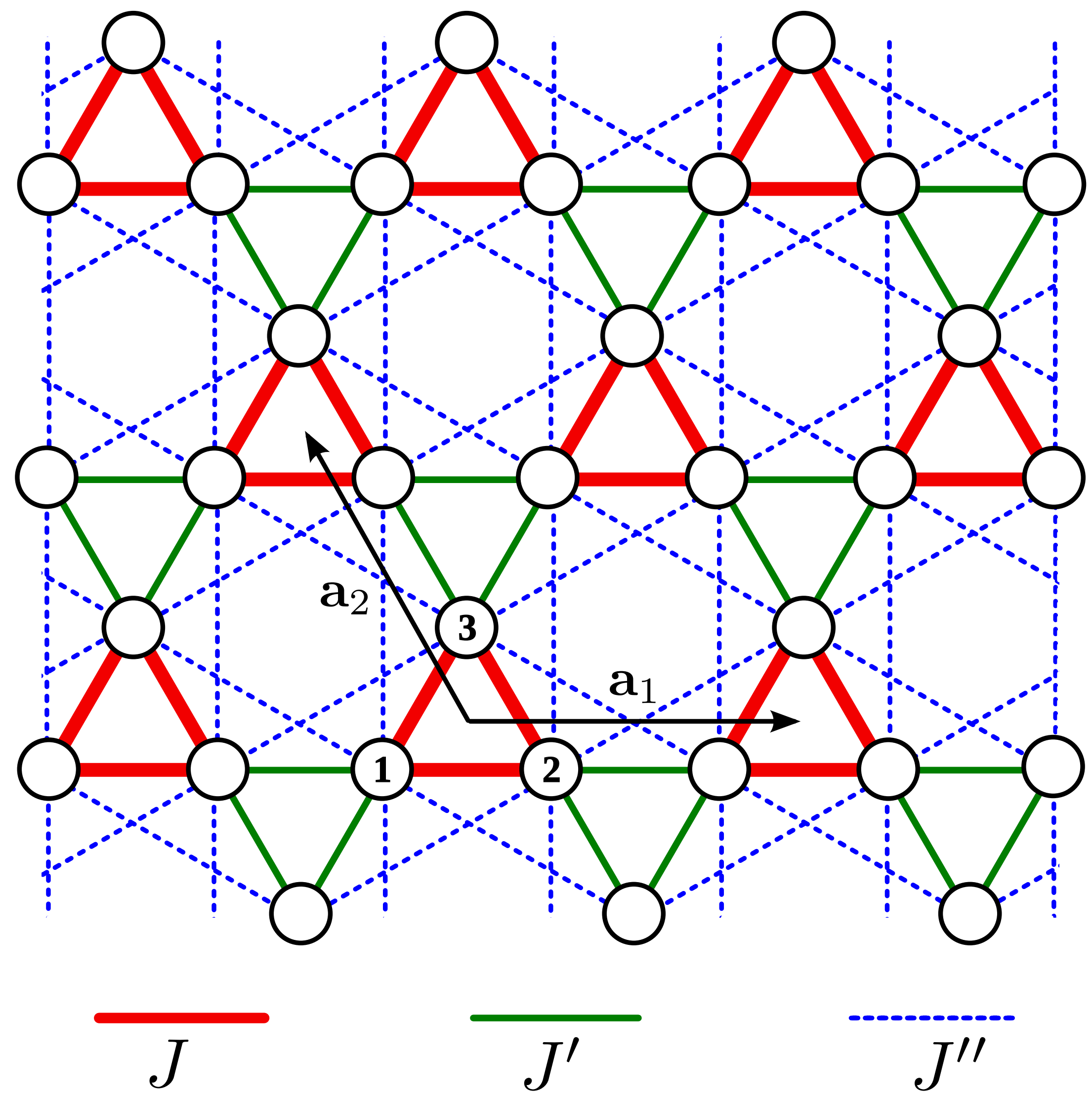
$$+J'' \sum_{\langle\langle i,j \rangle\rangle} \vec{S}_i \cdot \vec{S}_j$$

P. Ghosh, A. K. Verma, and BK, PRB (2016)

Spin-1 KHA

A Model on Trimerised Kagome Lattice

$$\hat{H} = J \sum_{\triangle} \vec{S}_i \cdot \vec{S}_j + J' \sum_{\nabla} \vec{S}_i \cdot \vec{S}_j + J'' \sum_{\langle\langle i,j \rangle\rangle} \vec{S}_i \cdot \vec{S}_j$$



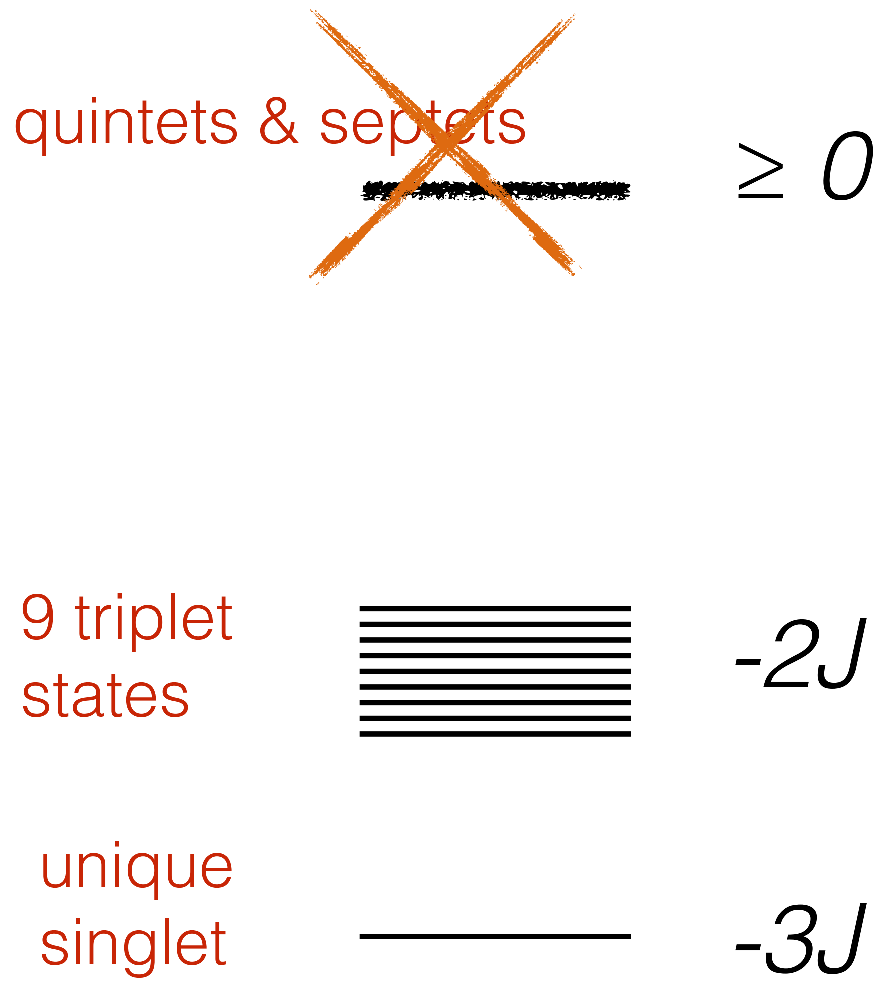
P. Ghosh, A. K. Verma, and BK, PRB (2016)

Spin-1 KHA

Plaquette Triplon Analysis

eigenstates of a spin-1 triangle

$$\hat{H}_{\triangle} = J(\vec{S}_1 \cdot \vec{S}_2 + \vec{S}_2 \cdot \vec{S}_3 + \vec{S}_3 \cdot \vec{S}_1)$$



plaquette operators

$$|s\rangle := \hat{s}^{\dagger}|\emptyset\rangle,$$

$$|t_{m\nu}\rangle := \hat{t}^{\dagger}_{m\nu}|\emptyset\rangle.$$

$$\hat{s}^{\dagger}\hat{s} + \sum_{m,\nu} \hat{t}^{\dagger}_{m\nu}\hat{t}_{m\nu} = 1.$$ (constraint)

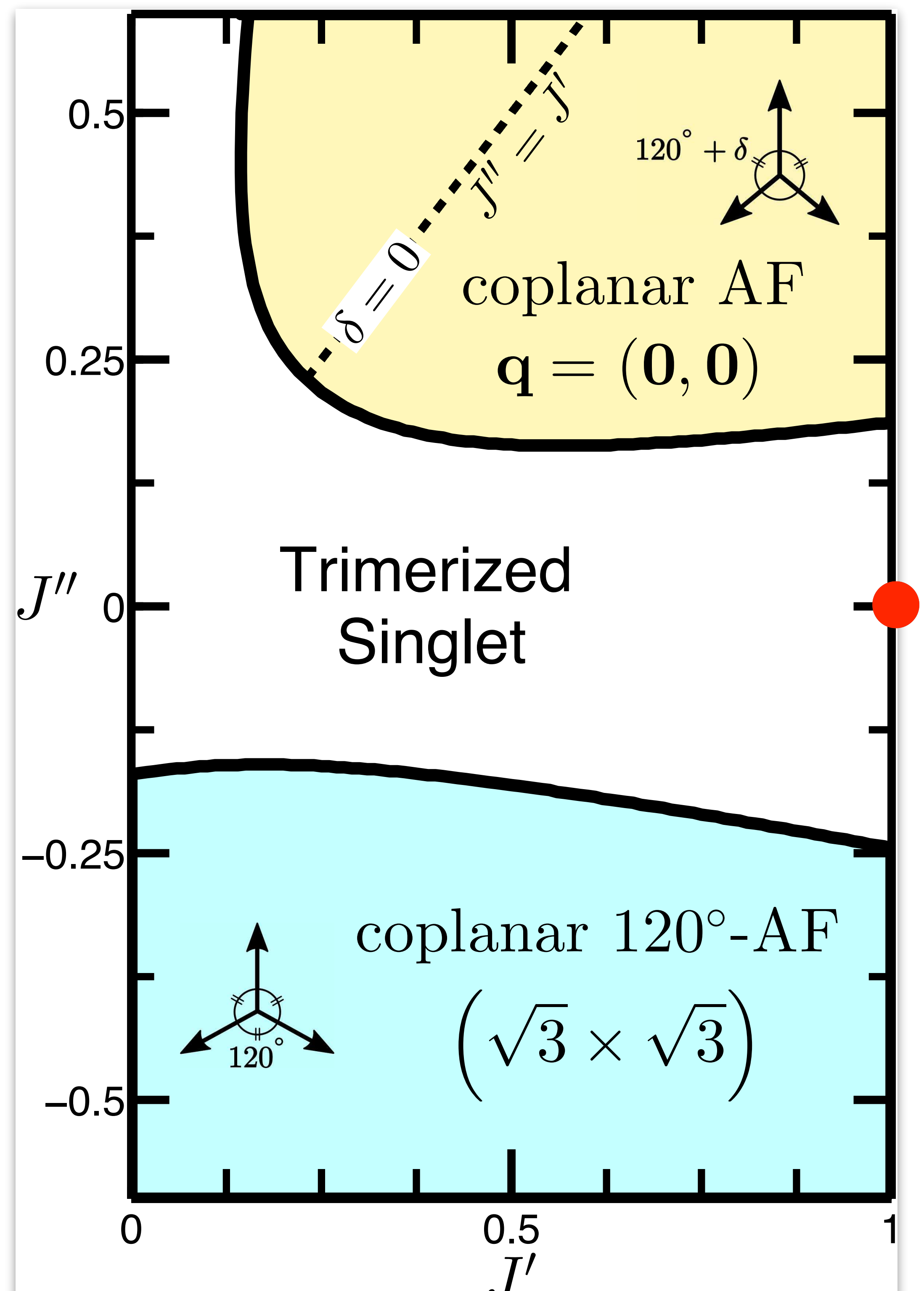
akin to the bond-operators for dimerised AF problems [Sachdev & Bhatt (1990); BK (2010)]

P. Ghosh, A. K. Verma, and BK, PRB (2016)

Spin-1 KHA

Quantum Phase Diagram

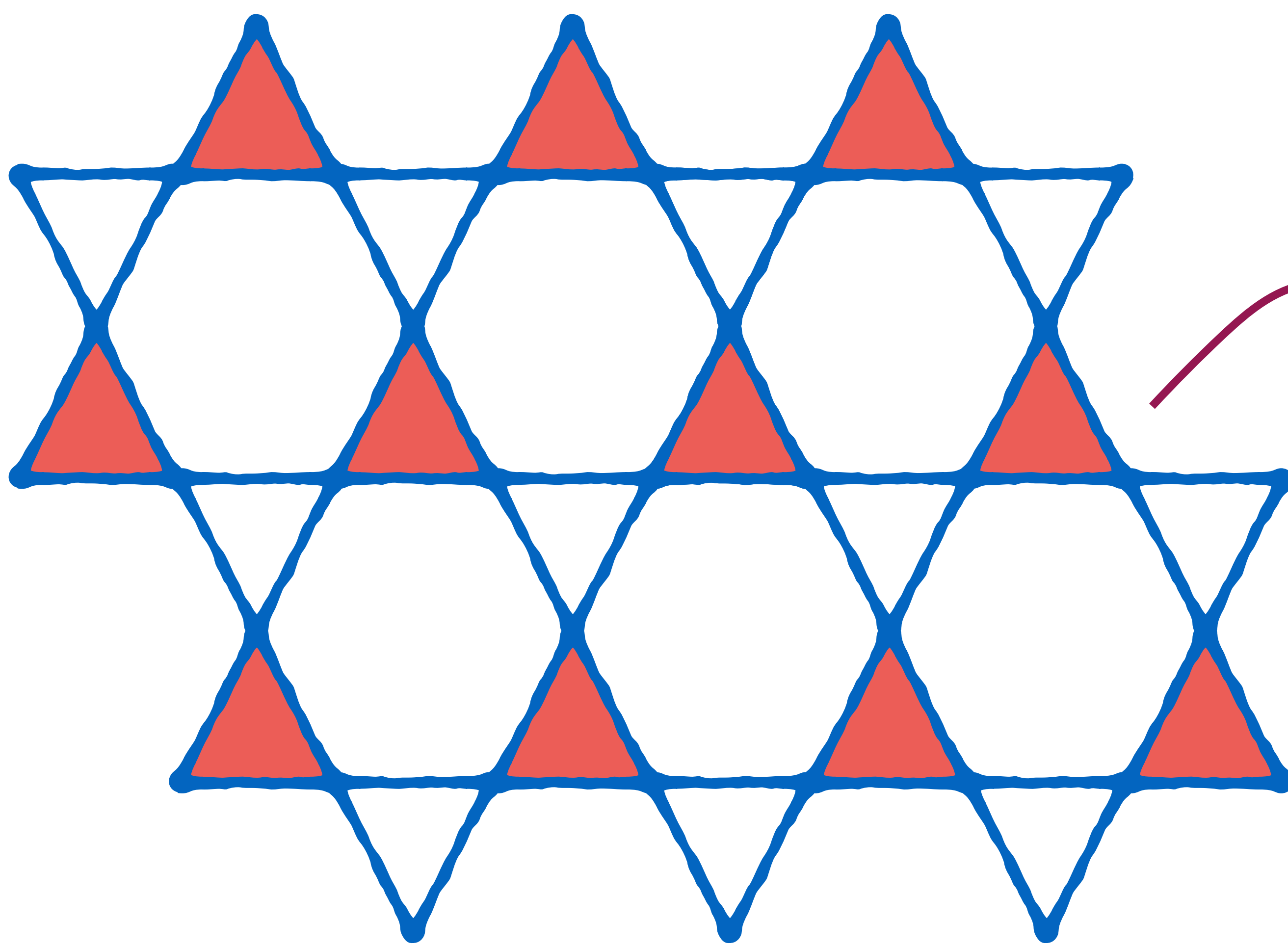
$$\hat{H} = J \sum_{\triangle} \vec{S}_i \cdot \vec{S}_j + J' \sum_{\triangledown} \vec{S}_i \cdot \vec{S}_j + J'' \sum_{\langle\langle i,j \rangle\rangle} \vec{S}_i \cdot \vec{S}_j$$

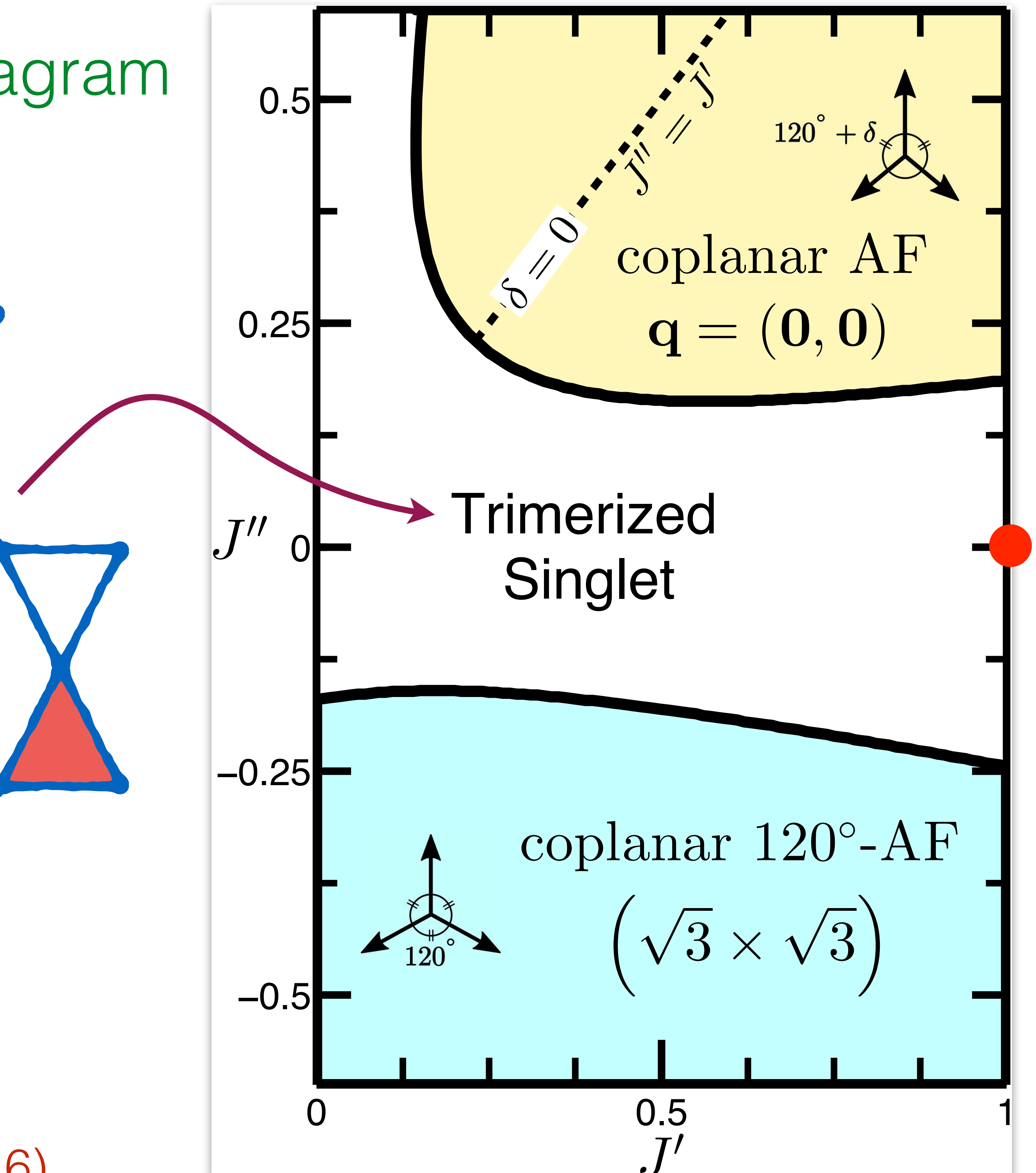


P. Ghosh, A. K. Verma, and BK, PRB (2016)

Spin-1 KHA

Quantum Phase Diagram





P. Ghosh, A. K. Verma, and BK, PRB (2016)

Spin-1 KHA

Magnetic Order with wave vector **q**

$$\mathbf{m}_j(\mathbf{r}) = m_j(\cos[\varphi_j - \mathbf{q}\cdot\mathbf{r}], \sin[\varphi_j - \mathbf{q}\cdot\mathbf{r}], 0)$$

$$(m_1, \varphi_1) = \left(2\bar{s}\sqrt{\frac{n_c}{3(1+\zeta)}}, \frac{\pi}{2}\right),$$

$$(m_2, \varphi_2) = \left(m_1\frac{\sqrt{1+3\zeta}}{2}, \varphi_1 + \frac{2\pi}{3} + \delta\right)$$

$$(m_3, \varphi_3) = \left(m_2, \varphi_1 - \frac{2\pi}{3} - \delta\right).$$

$$\delta = \tan^{-1}[\sqrt{3}(1-\sqrt{\zeta})/(1+3\sqrt{\zeta})]$$

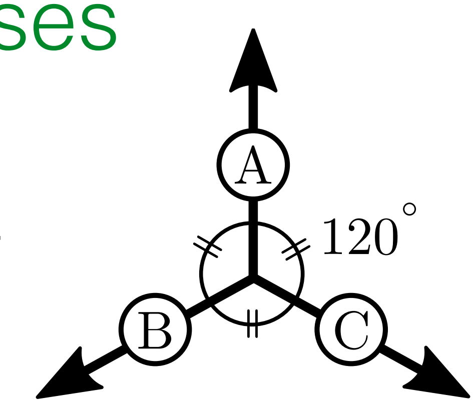
$$\zeta = n_{c1}/n_{c\bar{1}}$$

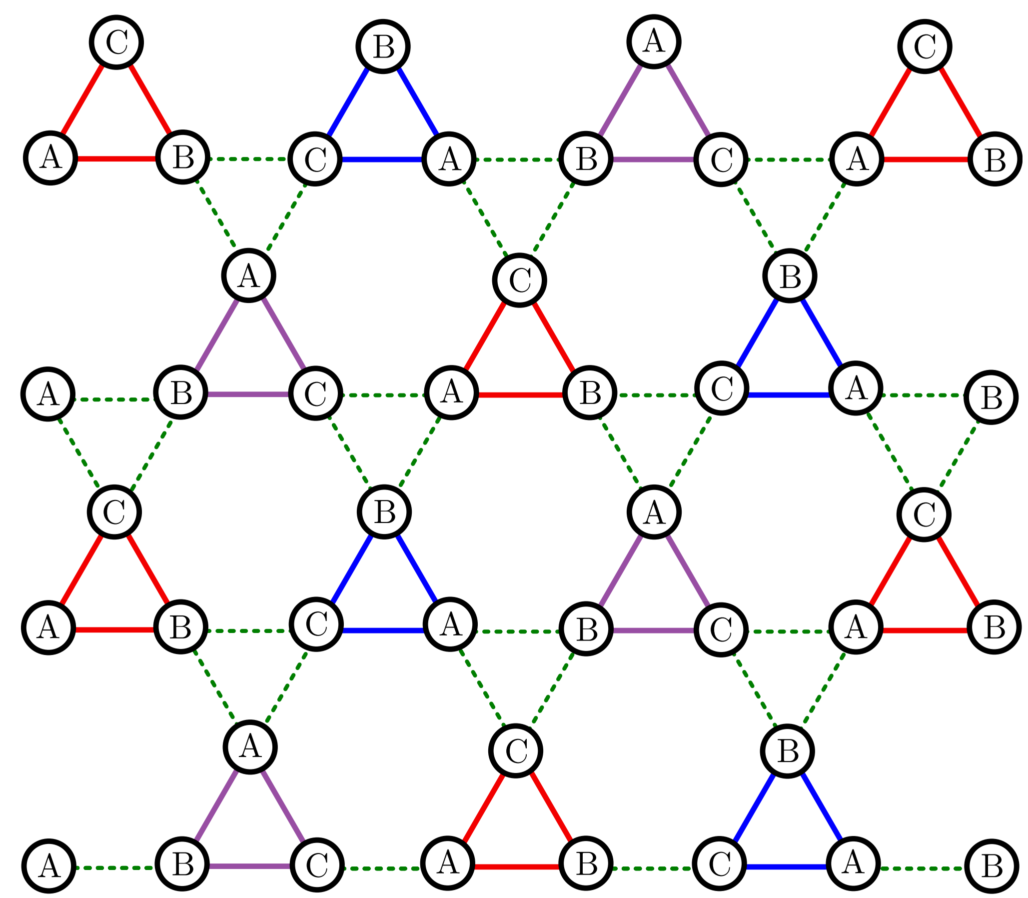
P. Ghosh, A. K. Verma, and BK, PRB (2016)

Spin-1 KHA

Magnetic Order in the Two Phases

$\sqrt{3} \times \sqrt{3}$



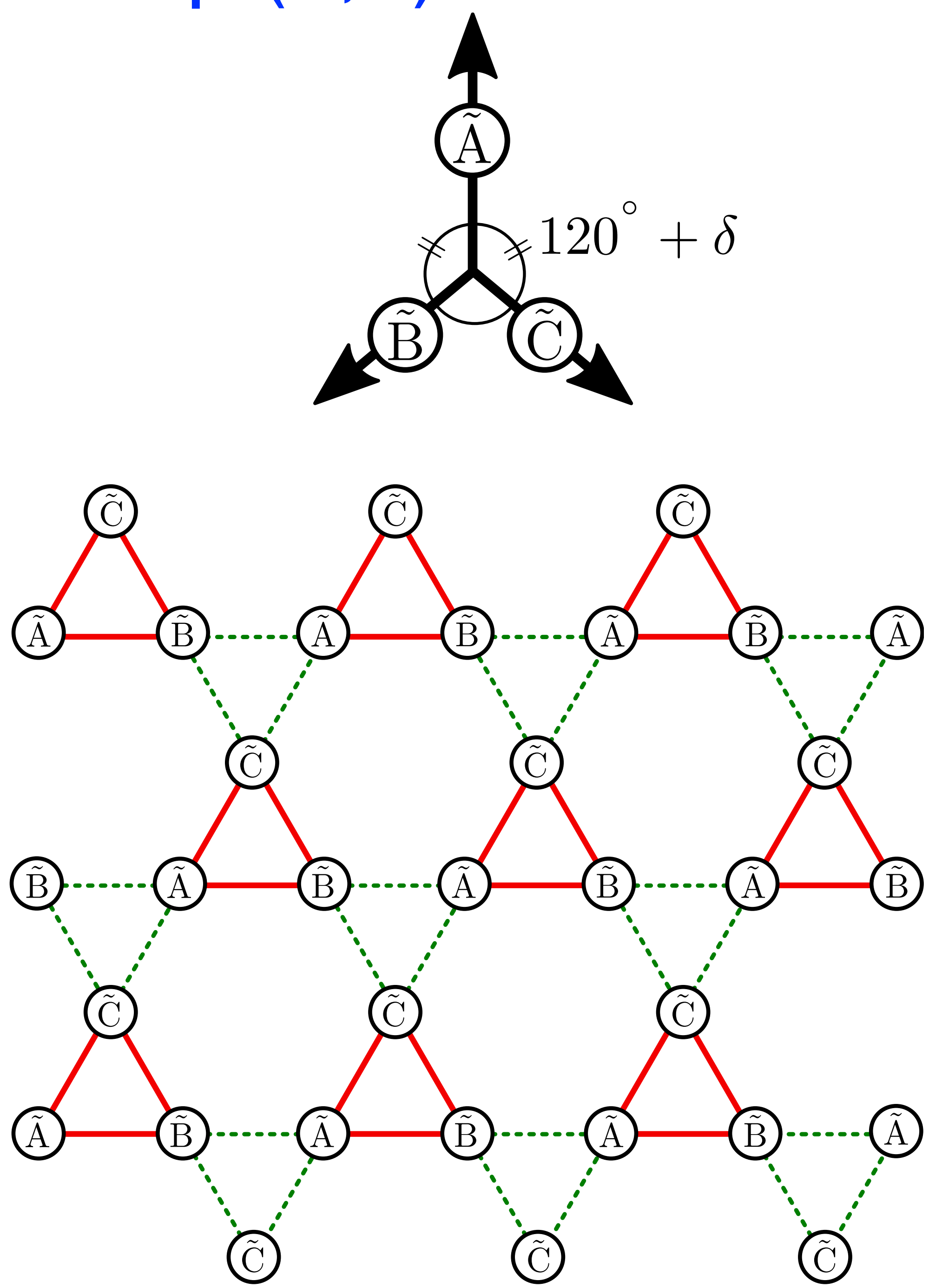


P. Ghosh, A. K. Verma, and BK, PRB (2016)

Spin-1 KHA

Magnetic Order in the Two Phases

Novel q=(0,0) order



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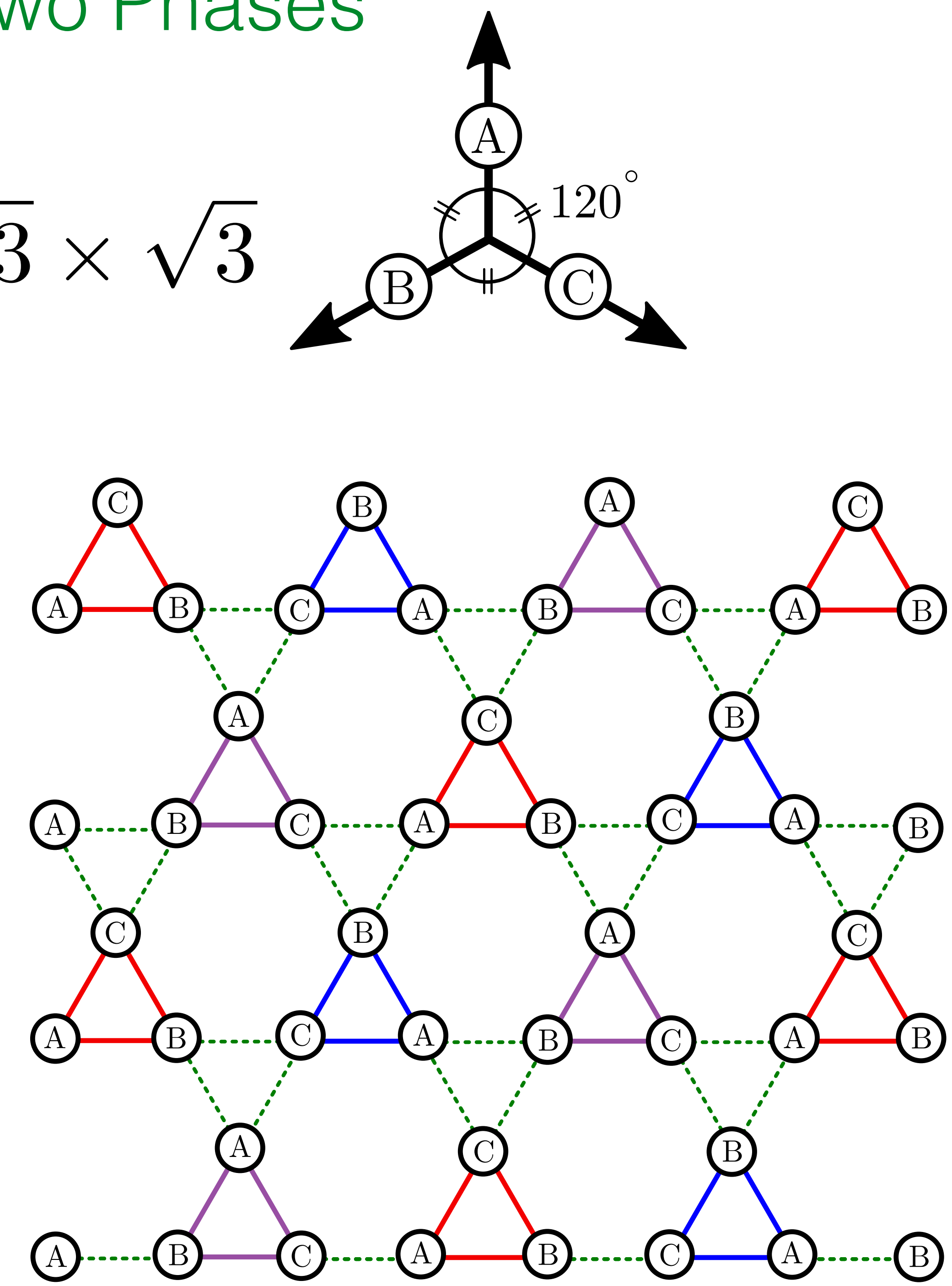
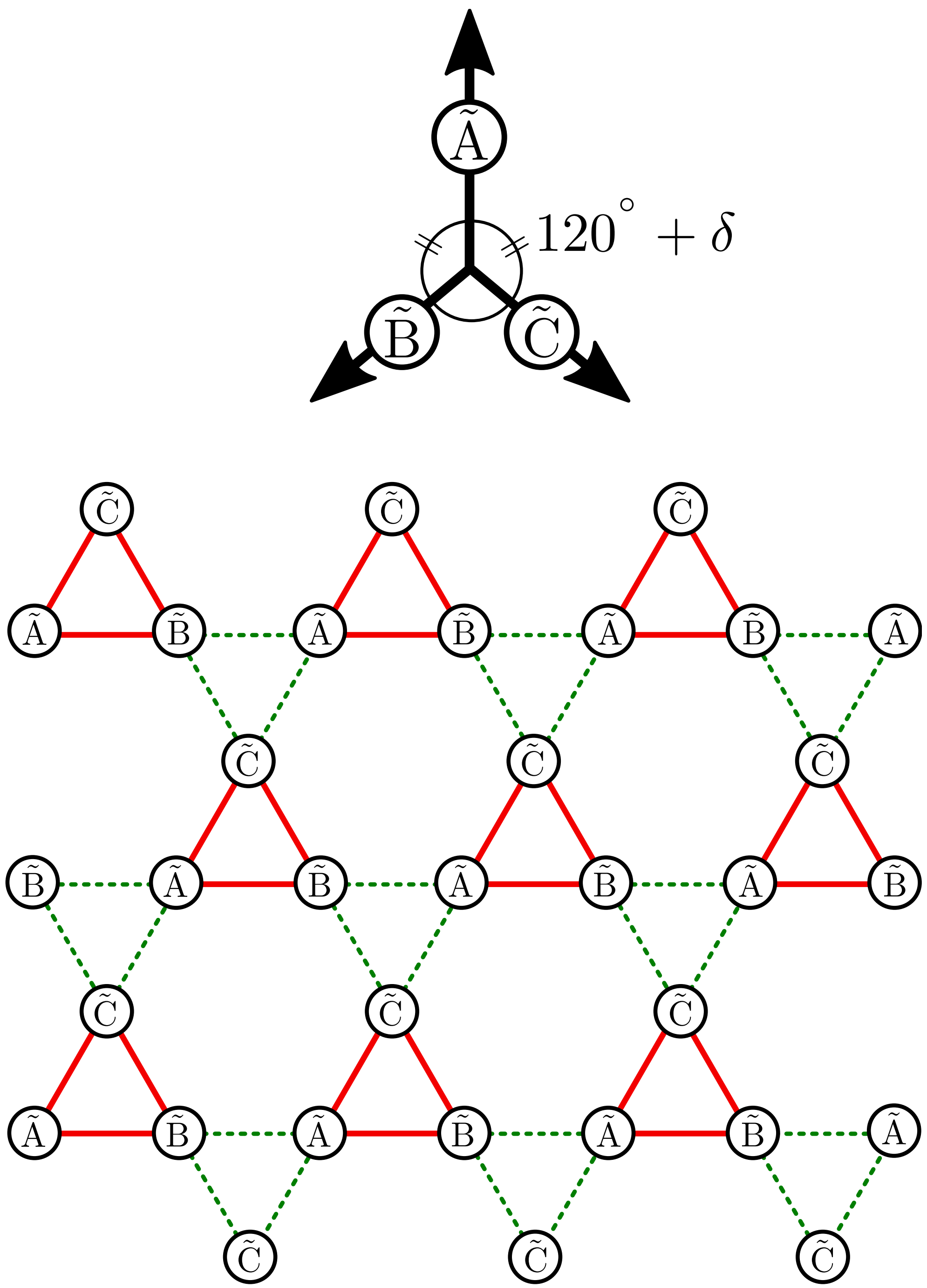
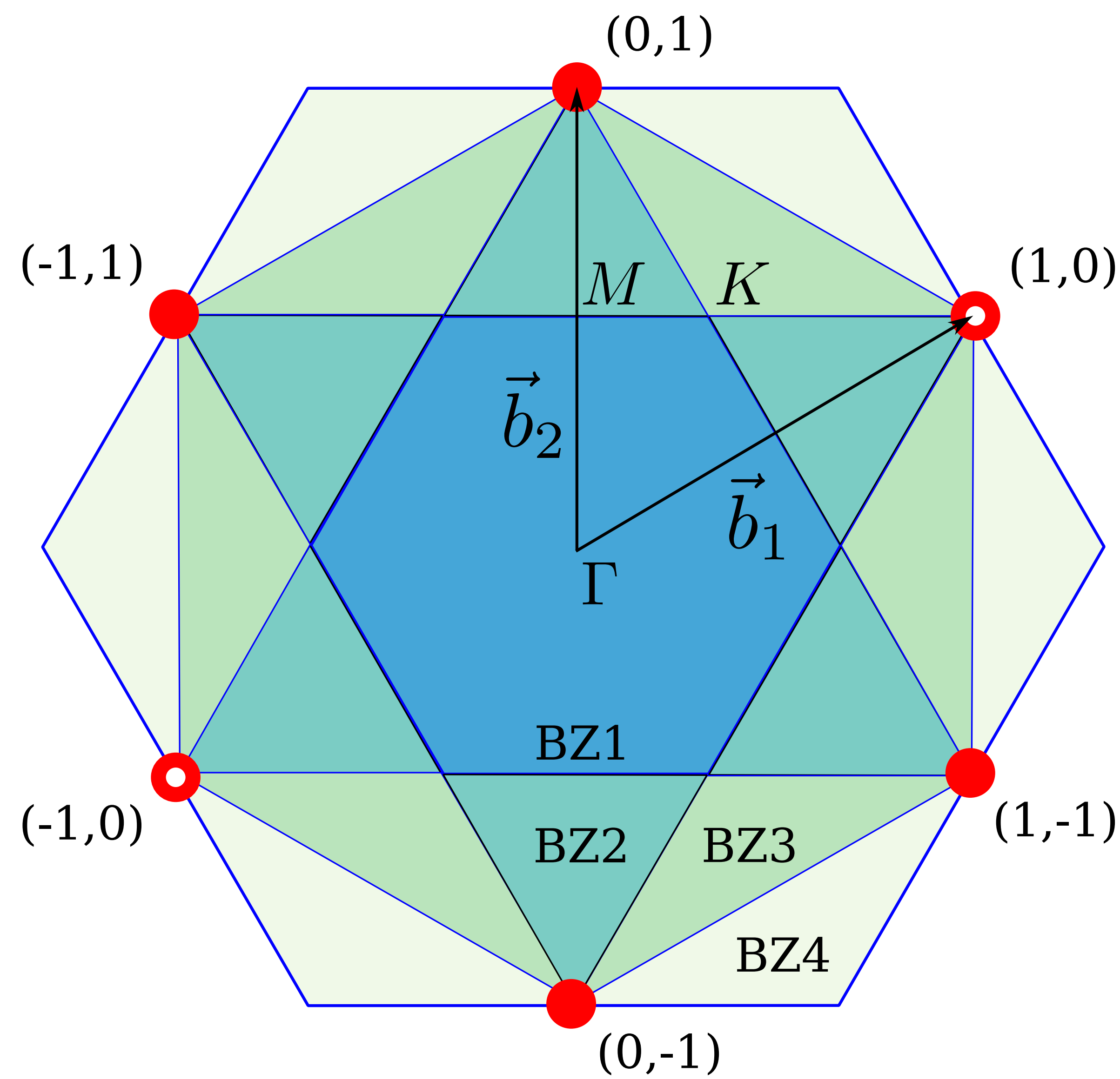


P. Ghosh, A. K. Verma, and BK, PRB (2016)

Spin-1 KHA

Structure factor of q=(0,0) order with δ≠0





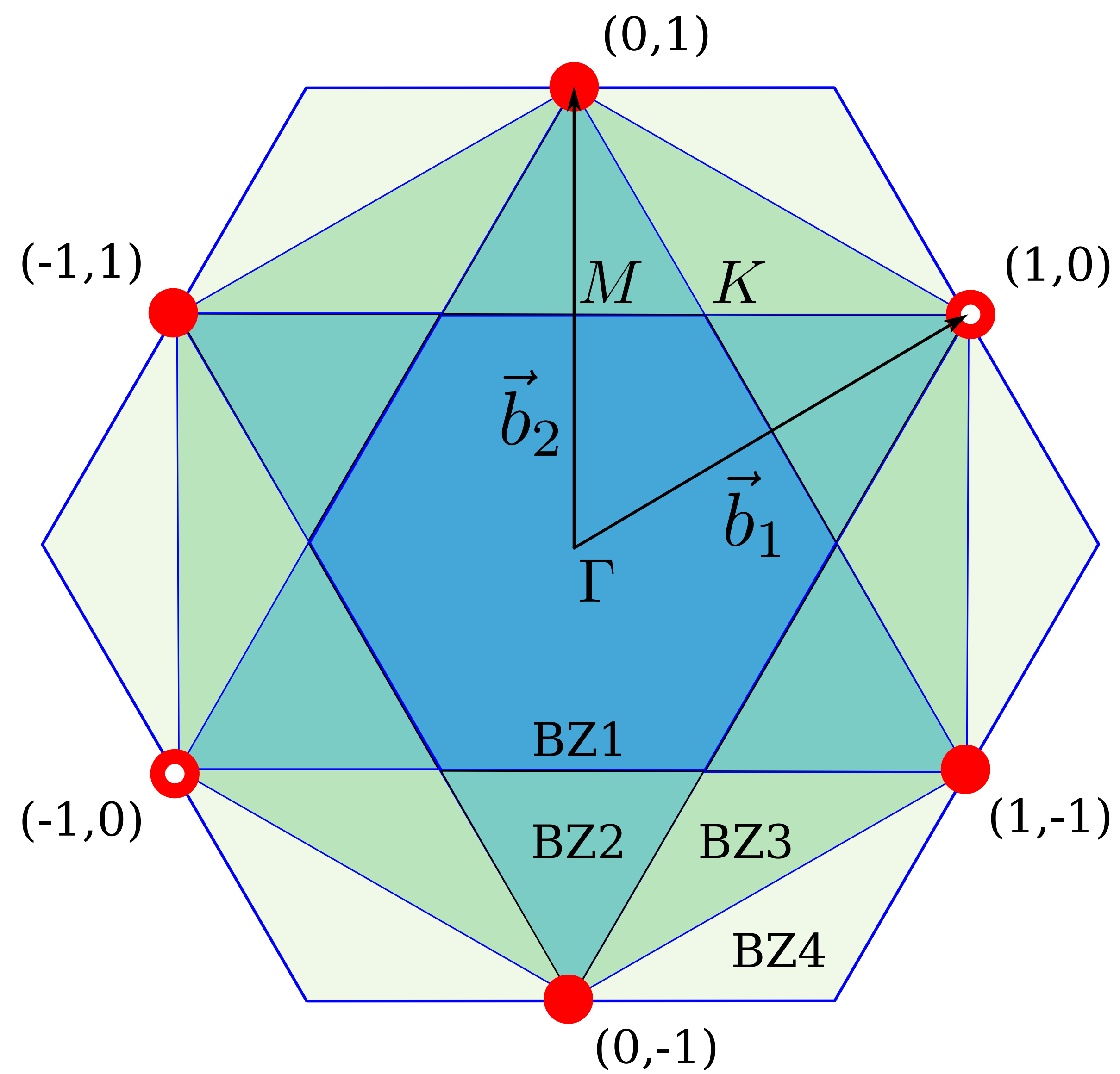
P. Ghosh, A. K. Verma, and BK, PRB (2016)

Spin-1 KHA

Structure factor of q=(0,0) order with δ≠0

experimental measure of δ

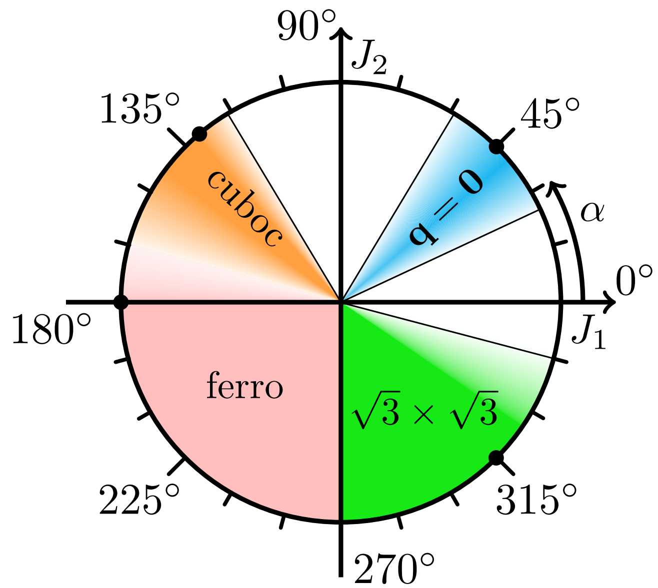
$$\frac{I_{(1,0)}}{I_{(0,1)}} = \frac{4}{1+3\zeta} = 4\sin^2\left(\frac{\pi}{6}+\delta\right)$$



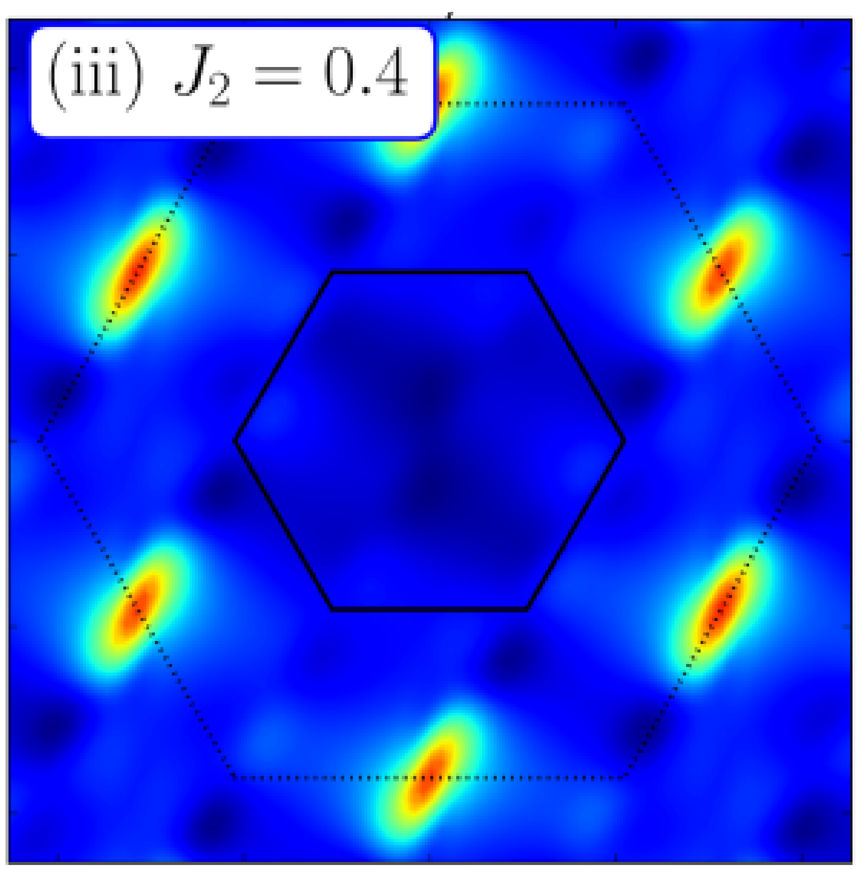
P. Ghosh, A. K. Verma, and BK, PRB (2016)

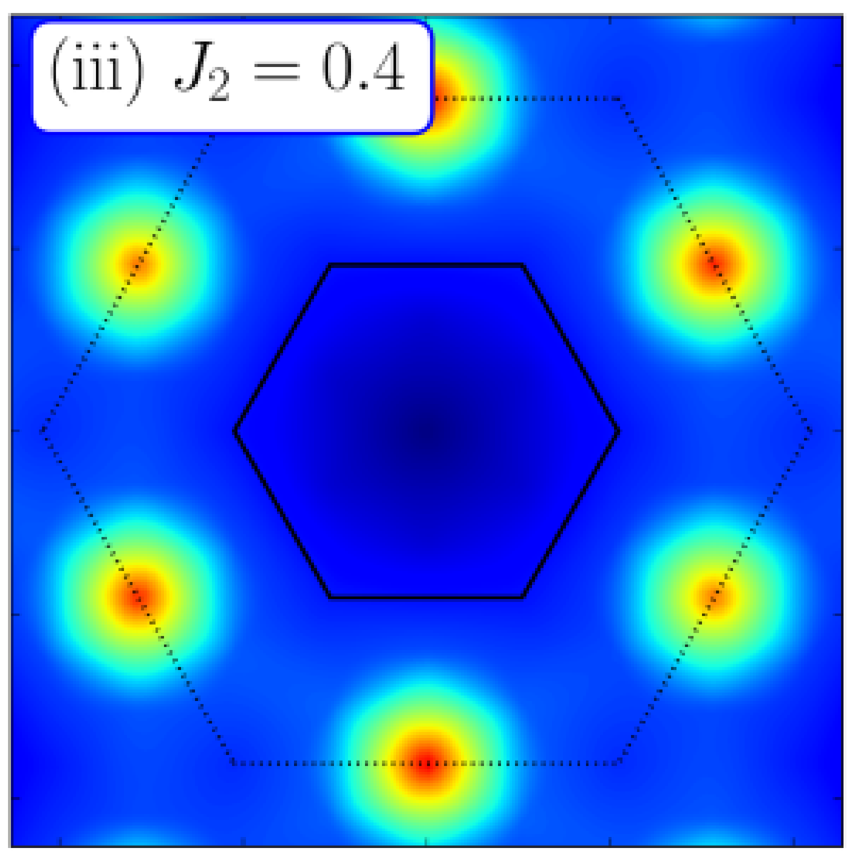
Structure factor for q=(0,0) order

Spin-1/2



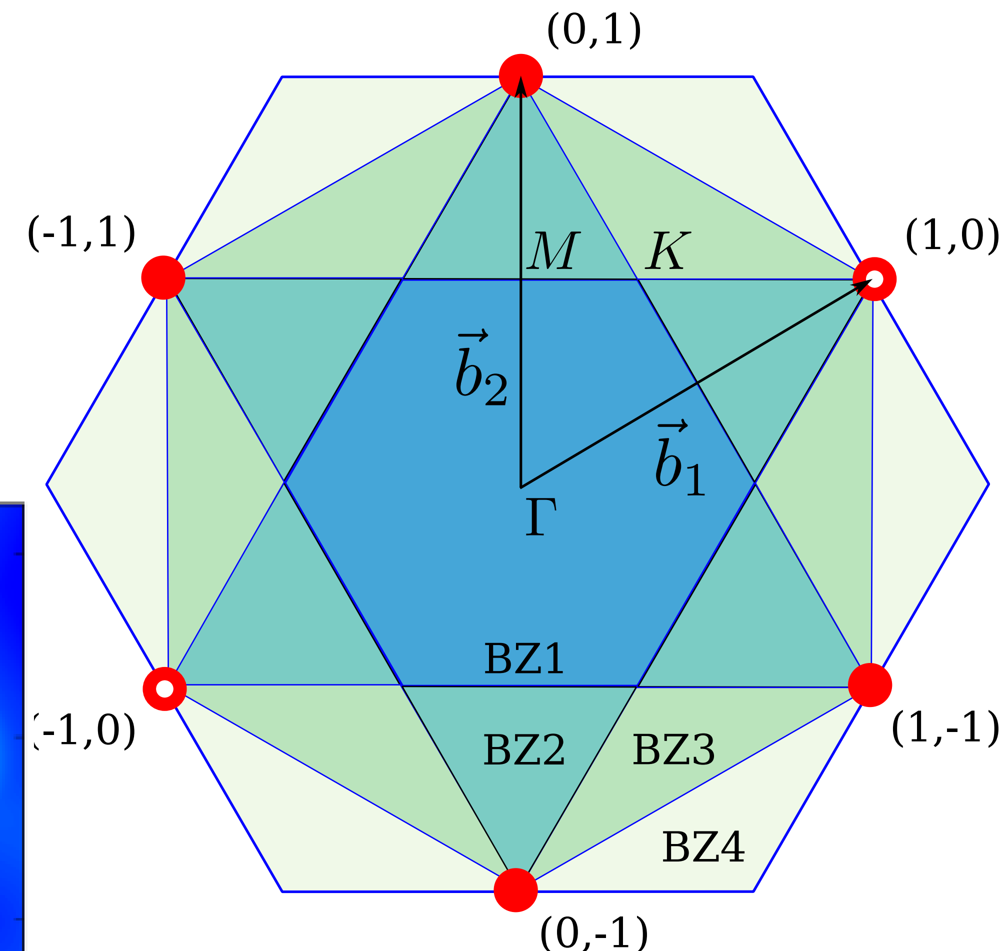
FRG; Suttner et al, PRB-Rapid (2014)





DMRG; Kolley et al, PRB (2015)

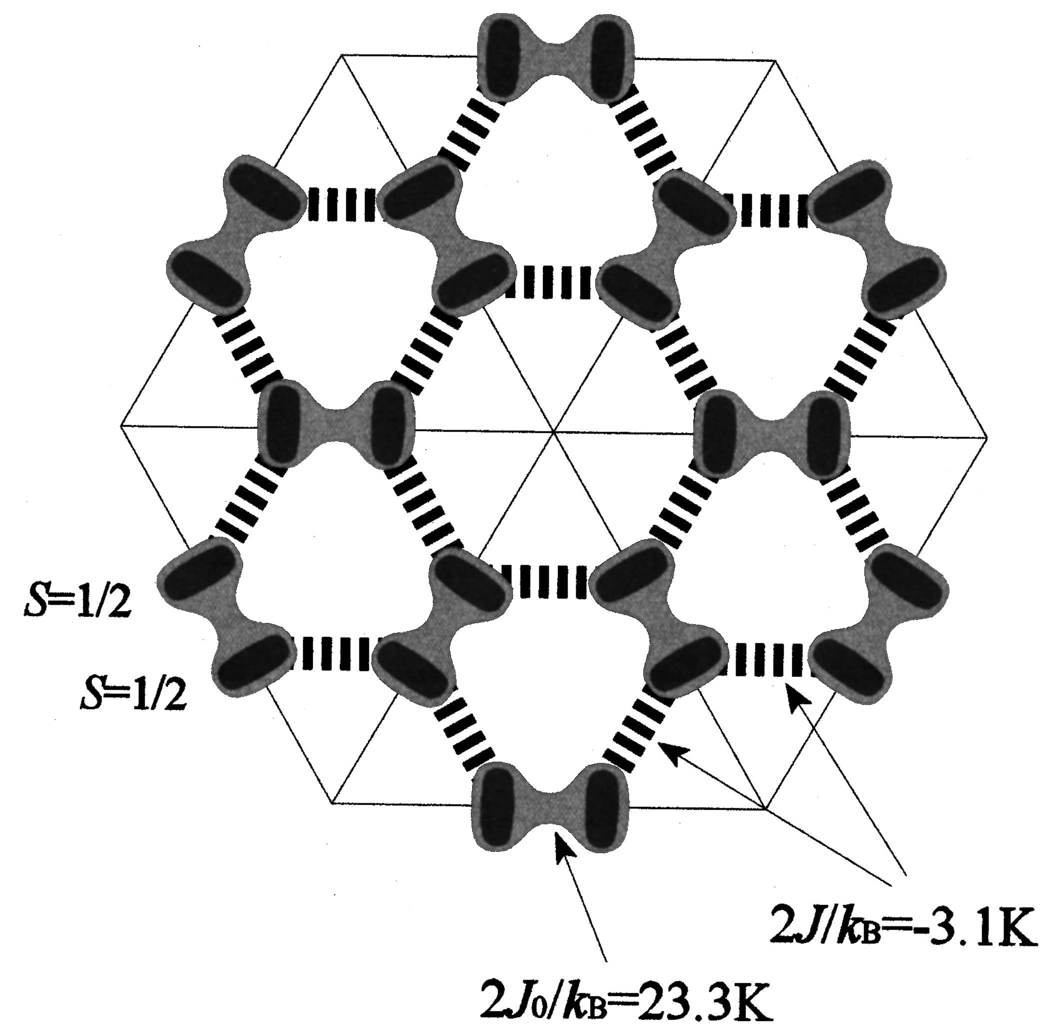
Spin-1: δ≠0



P. Ghosh, A. K. Verma, and BK, PRB (2016)

The m-MPYNN.X Organic Salts

What state do they realize?



$$m - MPYNN.BF_4$$

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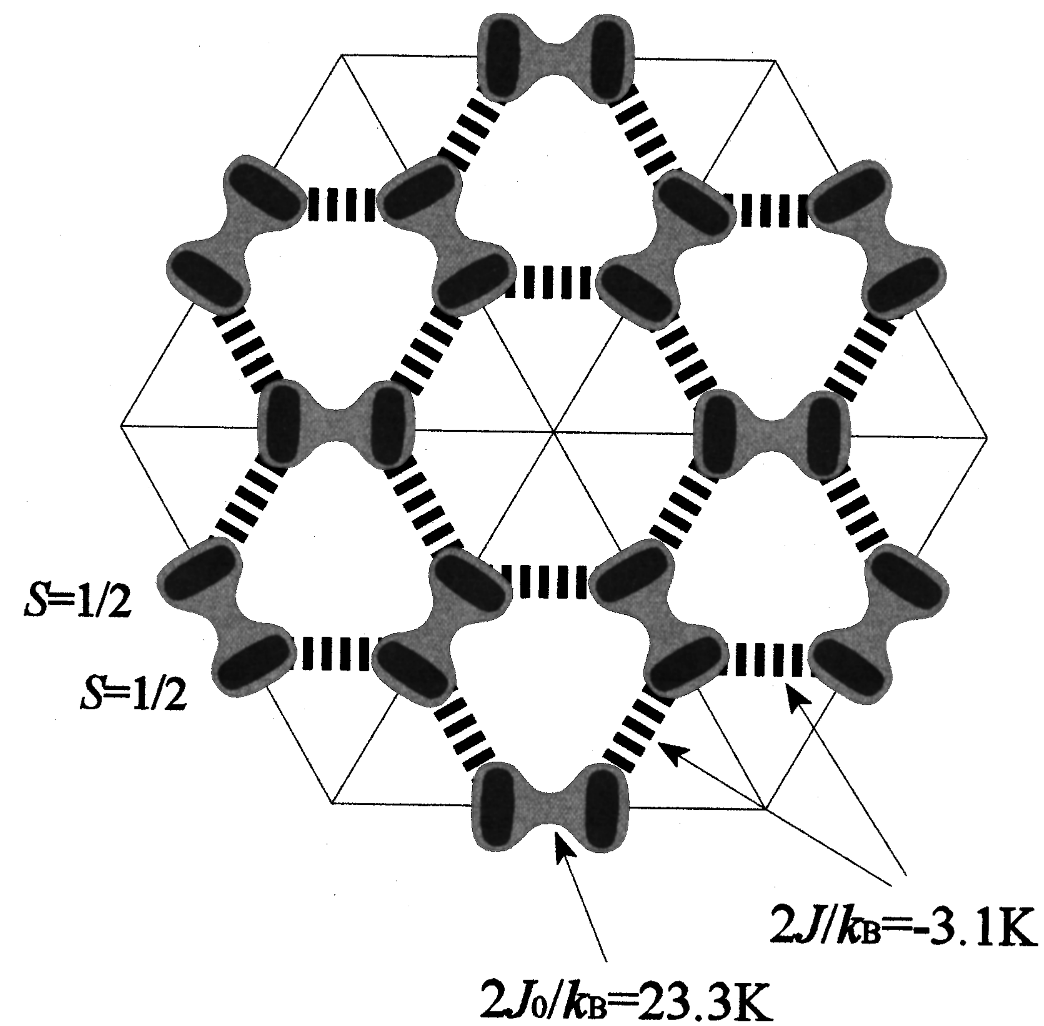
- Trimerized singlet state, or
- the HSS state of Hida?



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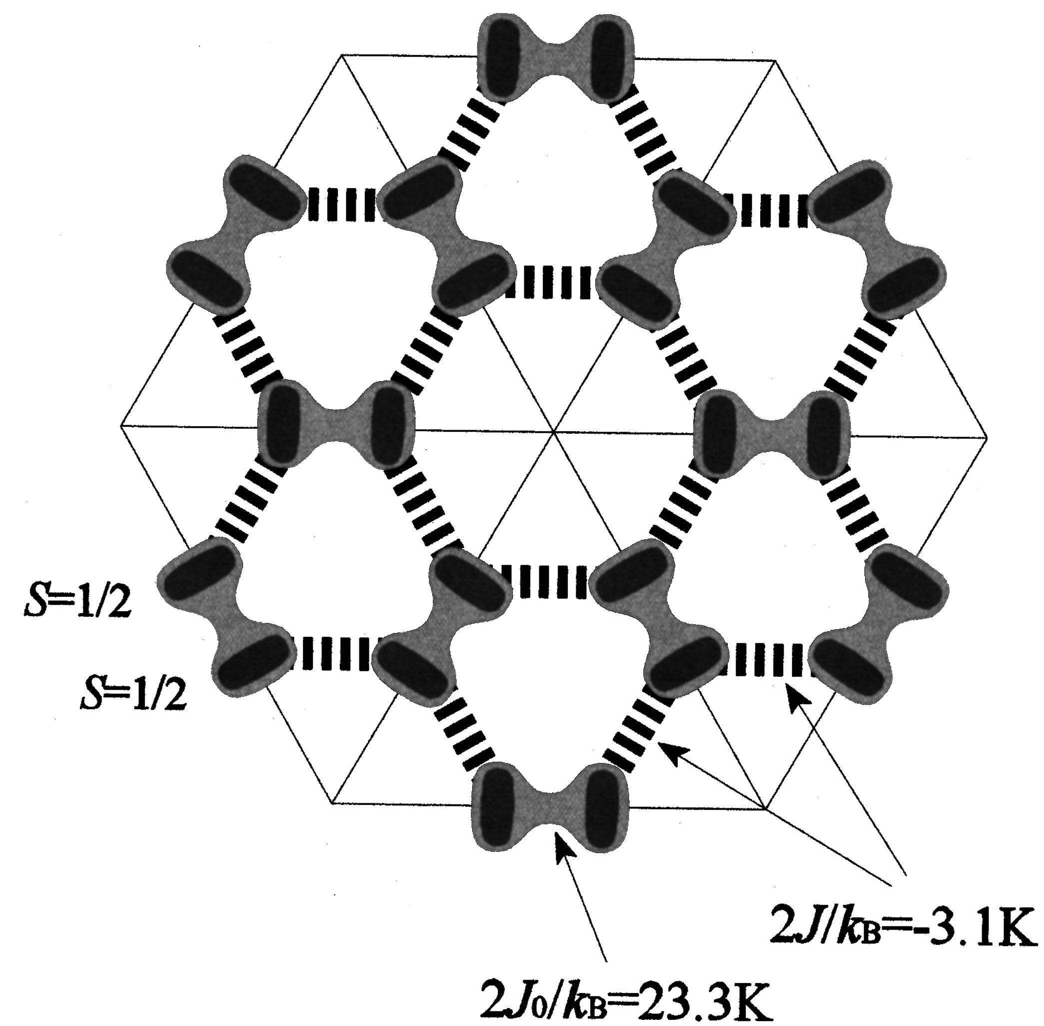
X	I	BF_4	$(BF_4)_{0.72}I_{0.28}$	ClO_4
J_A	1.6 K	3.11 K	1.20 K	0.19 K
J_F	− 10.2 K	− 23.26 K	− 11.3 K	− 10.5 K
J_F/J_A	− 6.375	− 7.479	− 9.416	− 55.263



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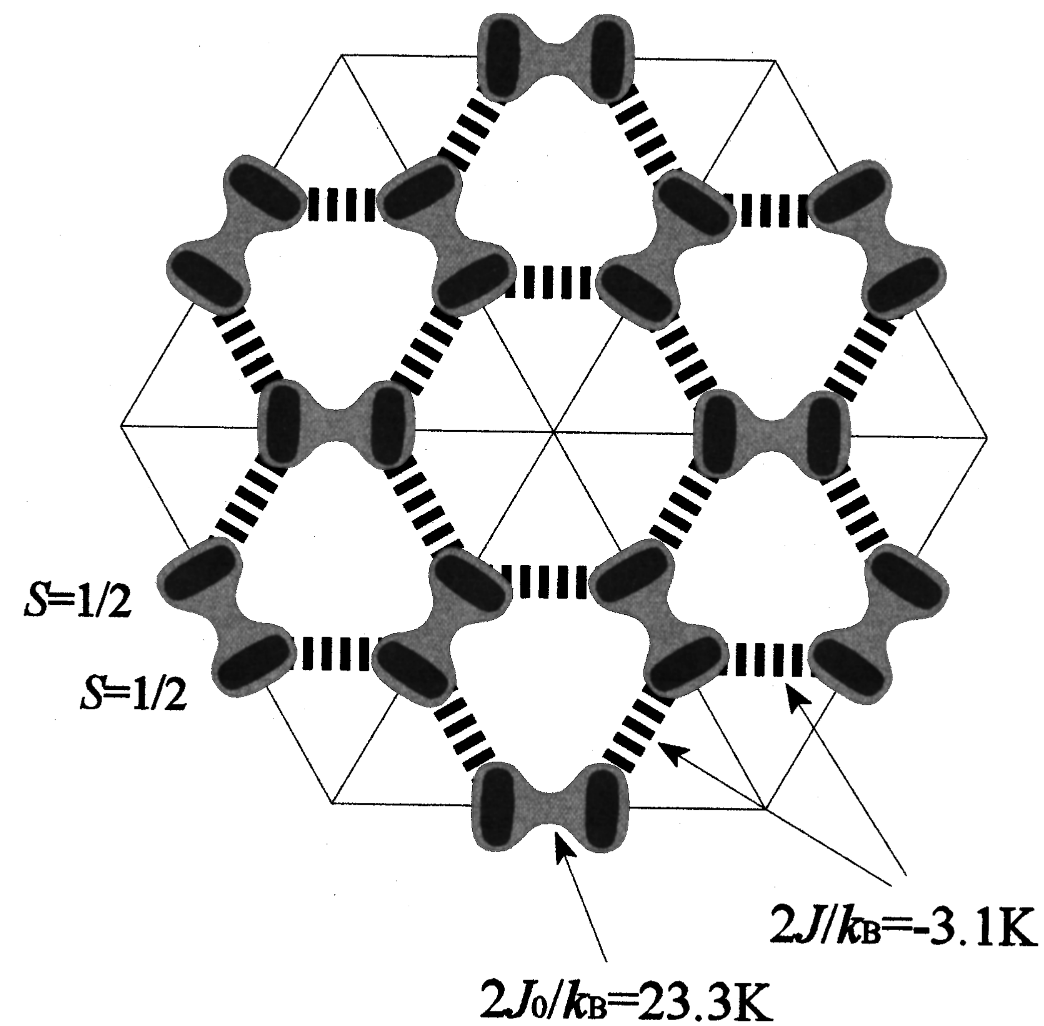

$m - MPYNN.BF_4$

How does the ground state of the Hida model evolve with J_F/J_A ?

How does the ground state evolve with J_F/J_A ?

Candidate states.

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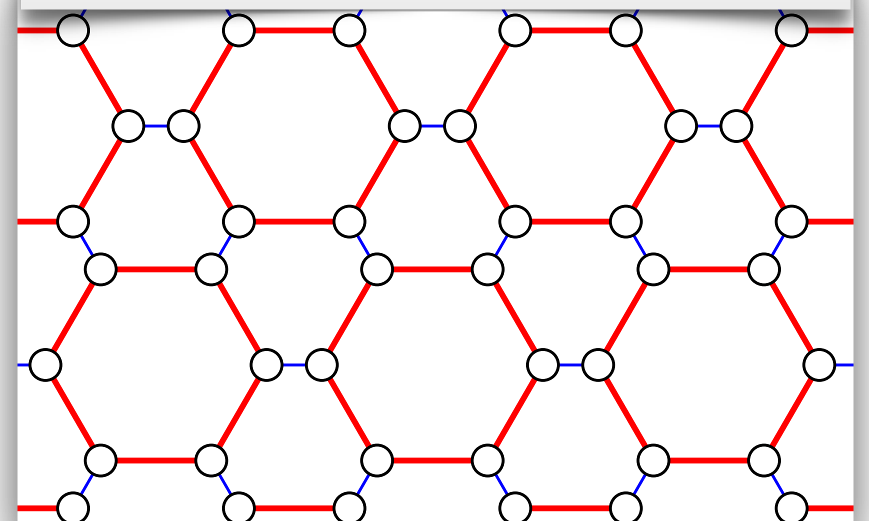
Candidate states.

hexagonal singlet (HS)



small $|J_F|/J_A$

Different from the HSS state. No symmetrisation on FM bonds.

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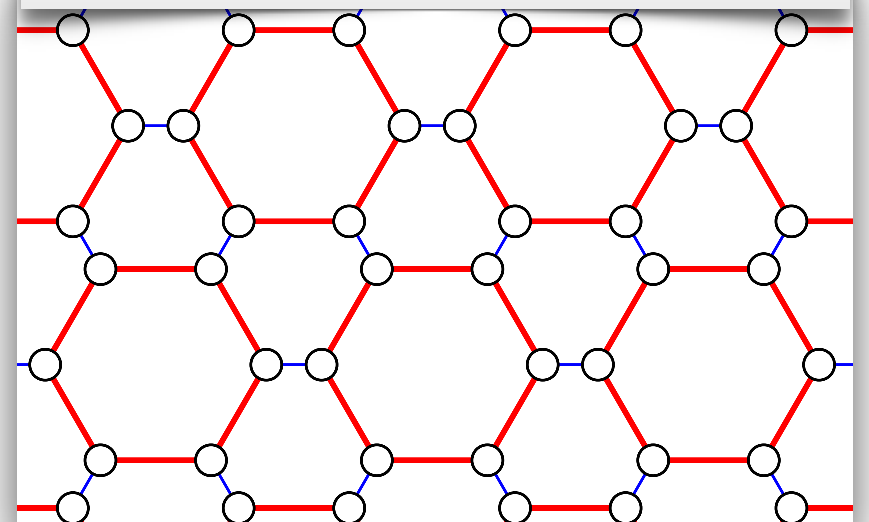

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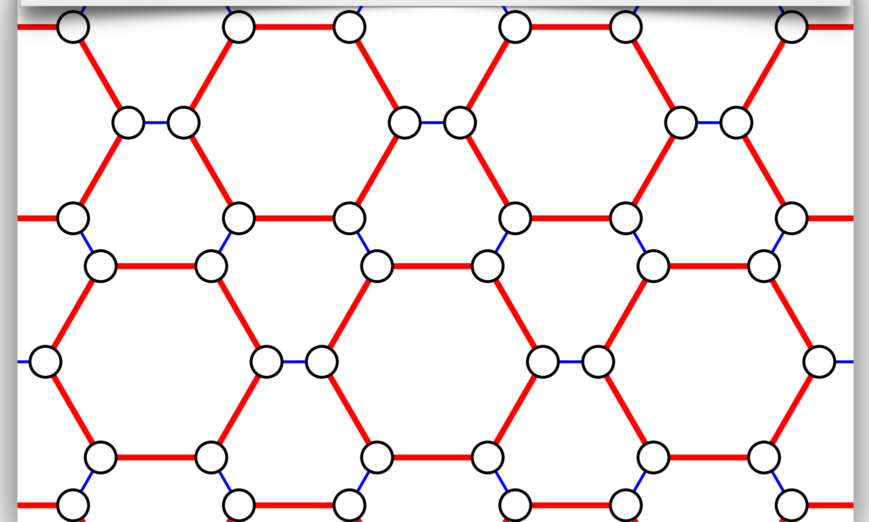

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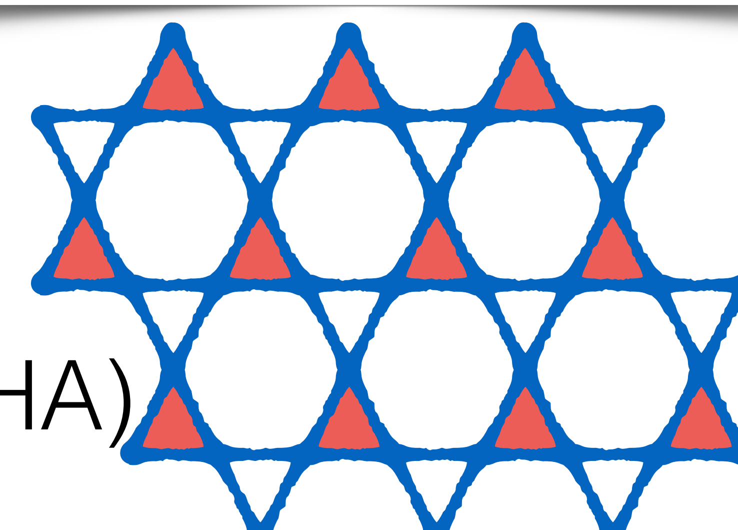
strong $|J_F|/J_A$

trimerised singlet (TS)



(spin-1 KHA)

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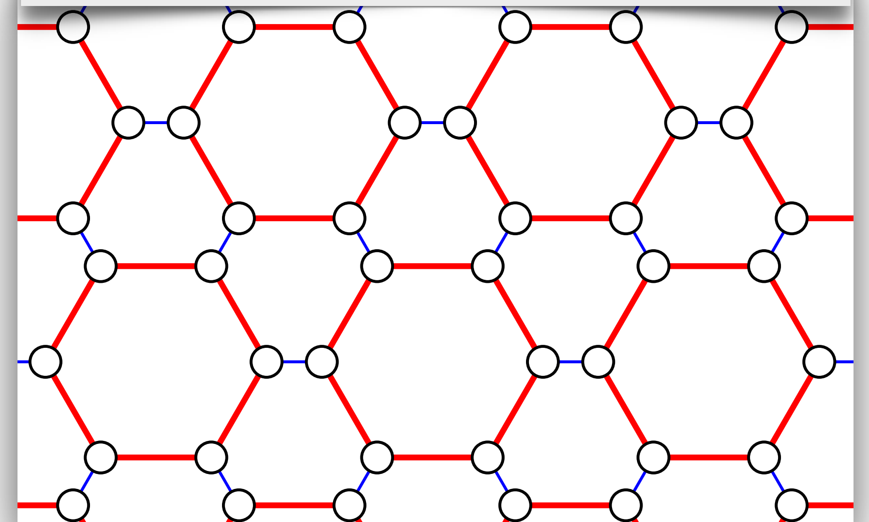

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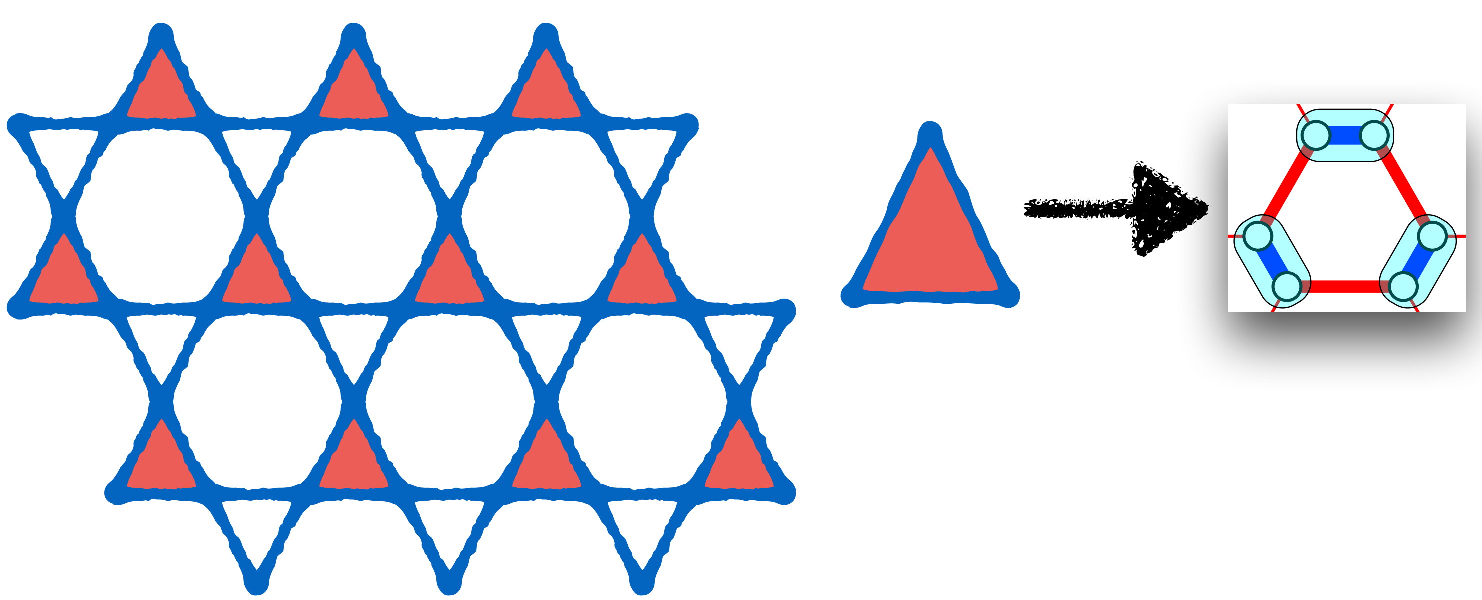

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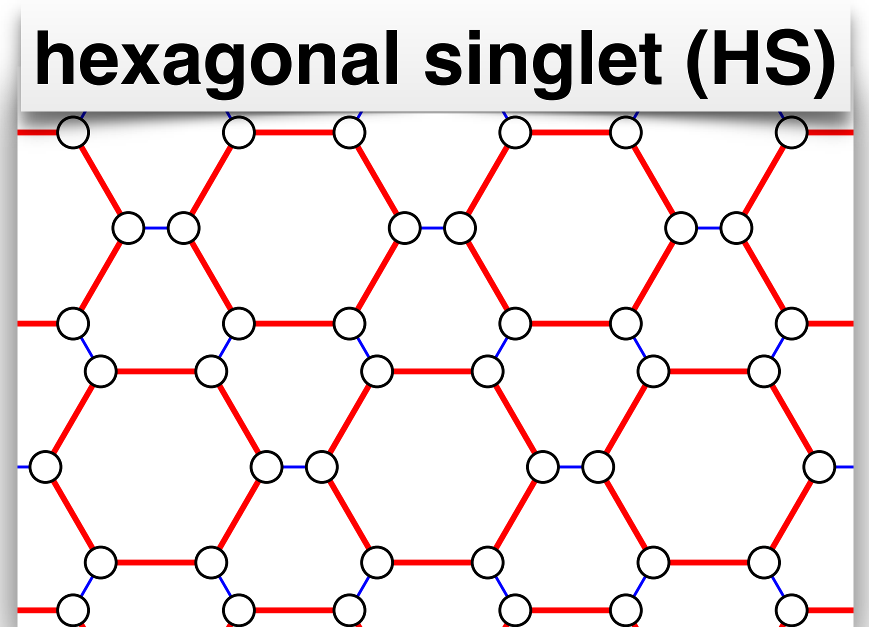

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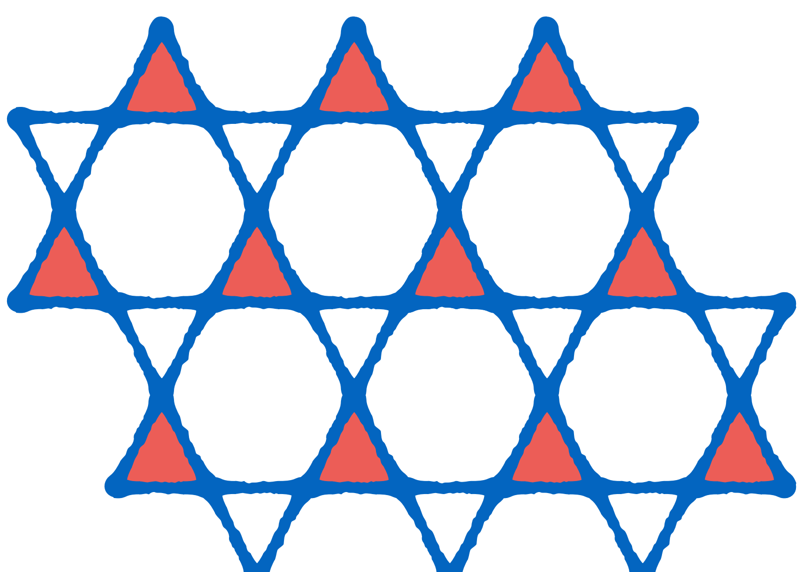

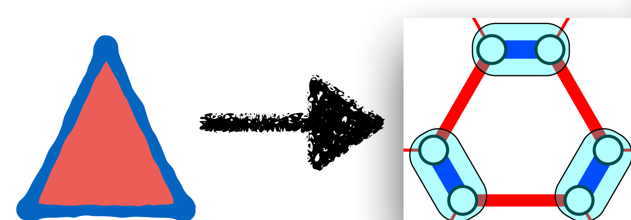

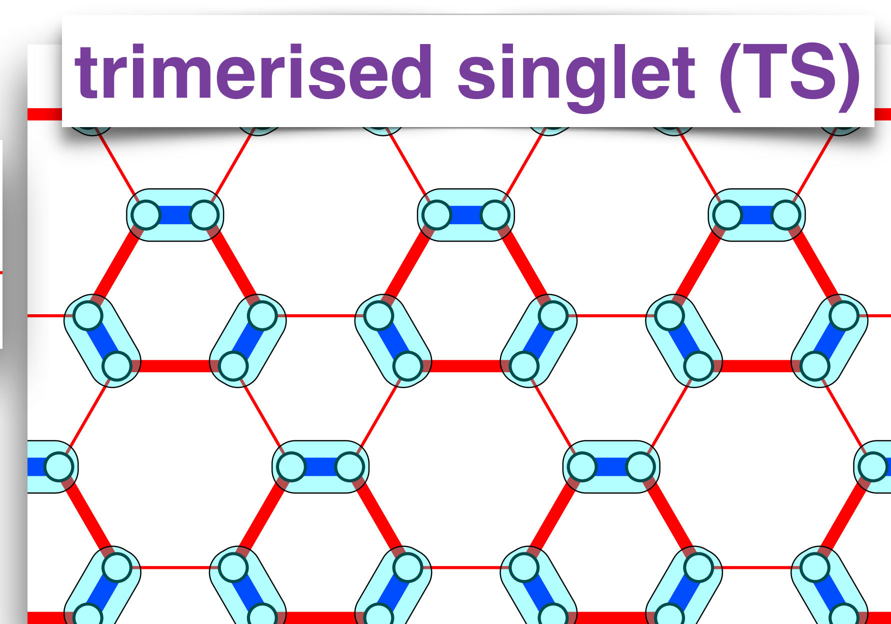

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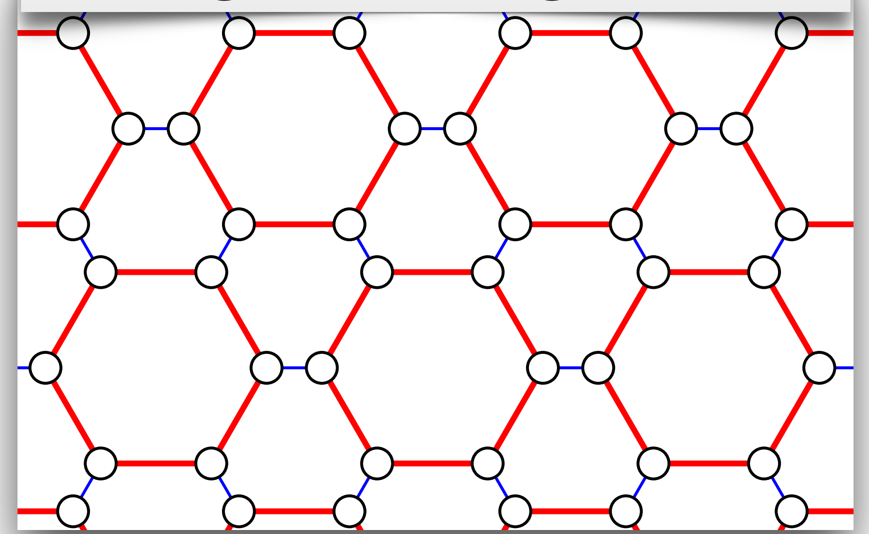


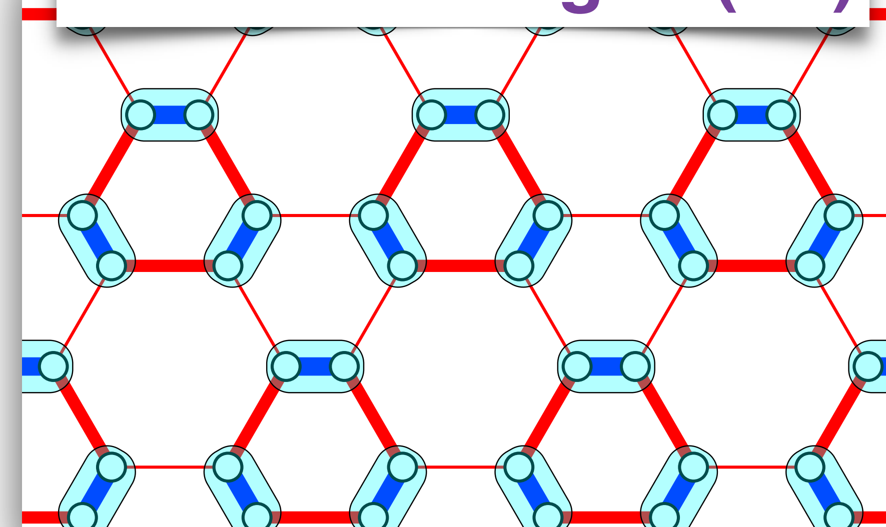
Different from the HSS state. No symmetrisation on FM bonds.

small $|J_F|/J_A$

intermediate $|J_F|/J_A$??

strong $|J_F|/J_A$

trimerised singlet (TS)



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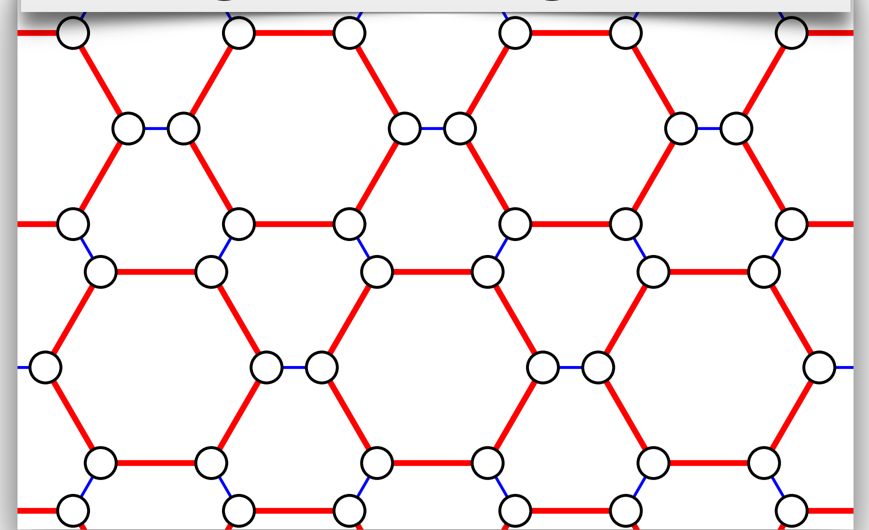

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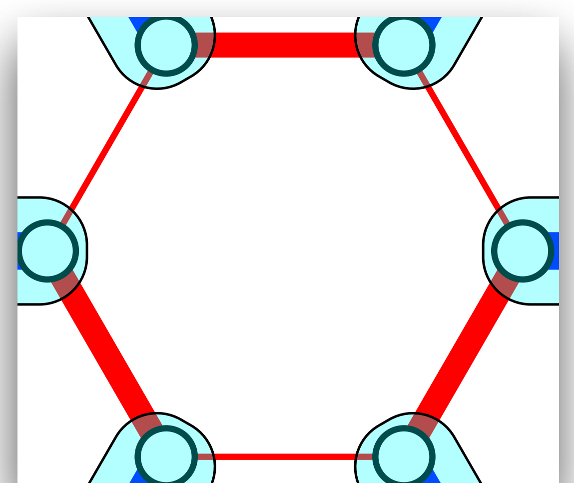
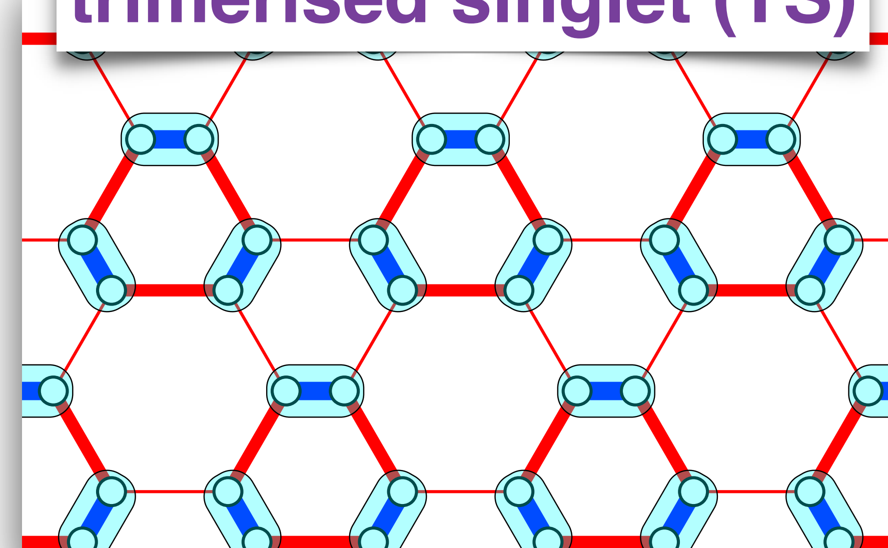


Antiferromagnetic hexagons are dimerized.

trimerised singlet (TS)



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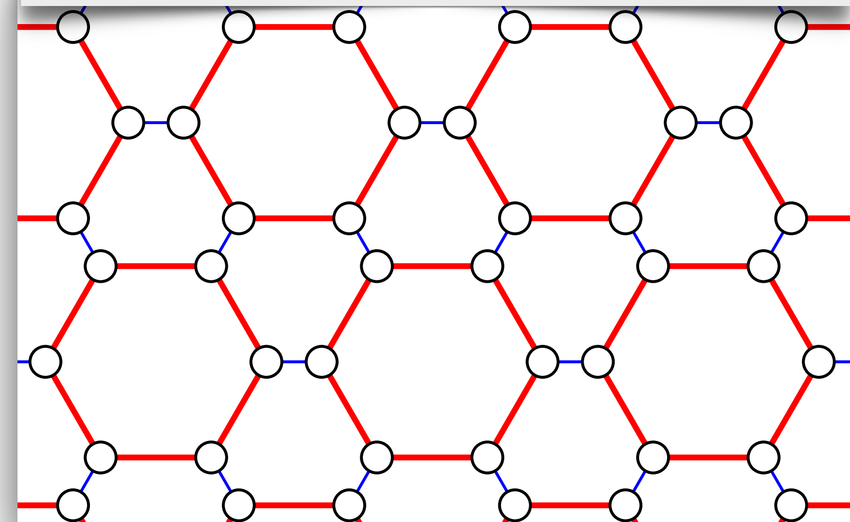
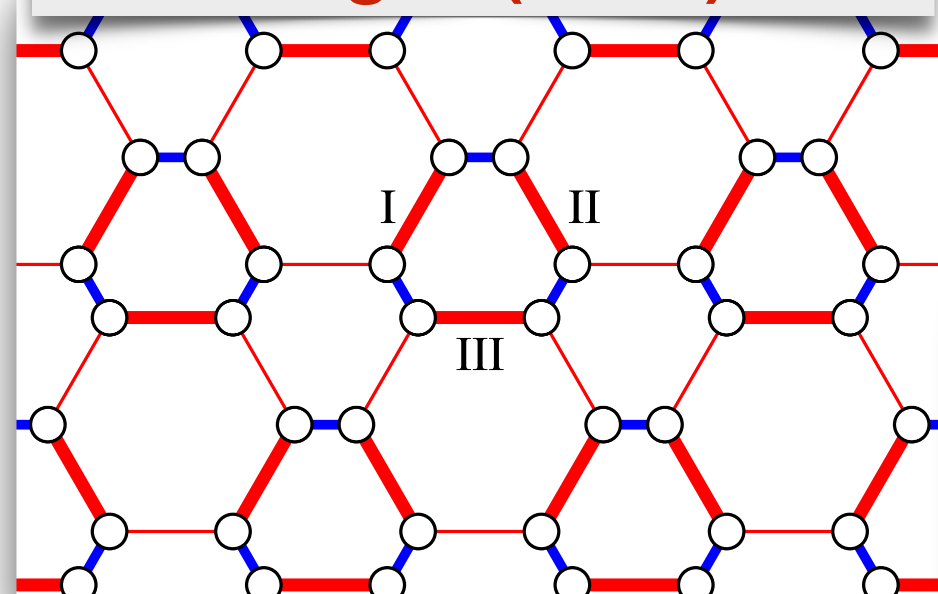
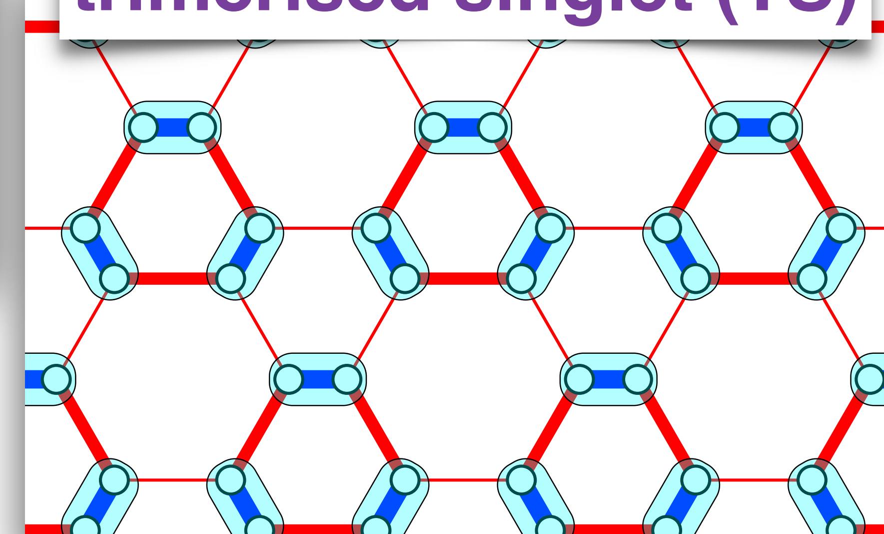


Different from the HSS state. No symmetrisation on FM bonds.

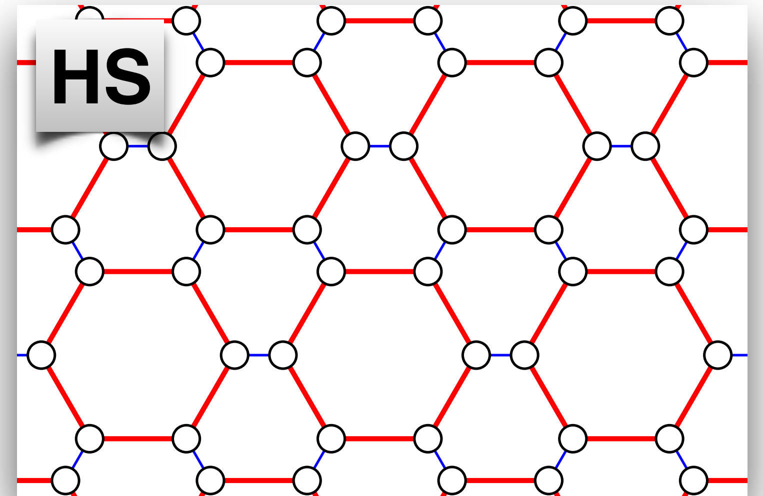
dimerised hexagonal singlet (D-HS)

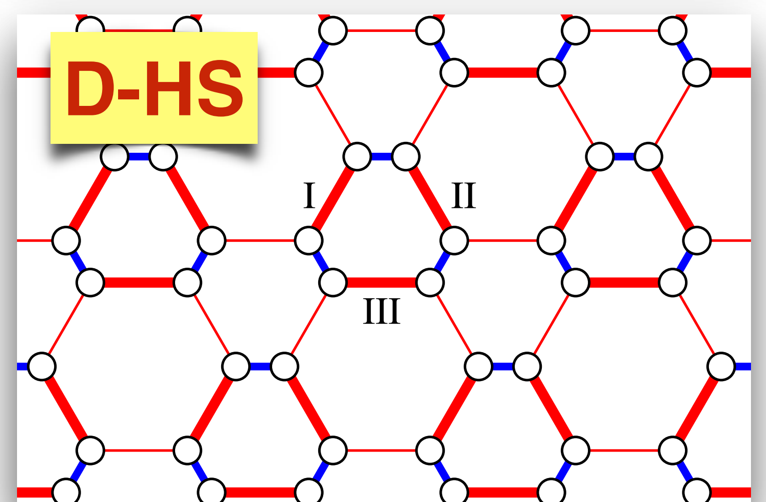


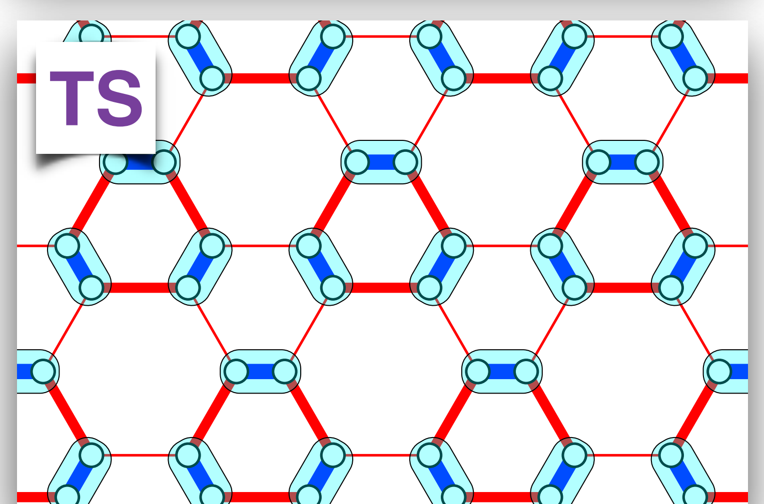
trimerised singlet (TS)



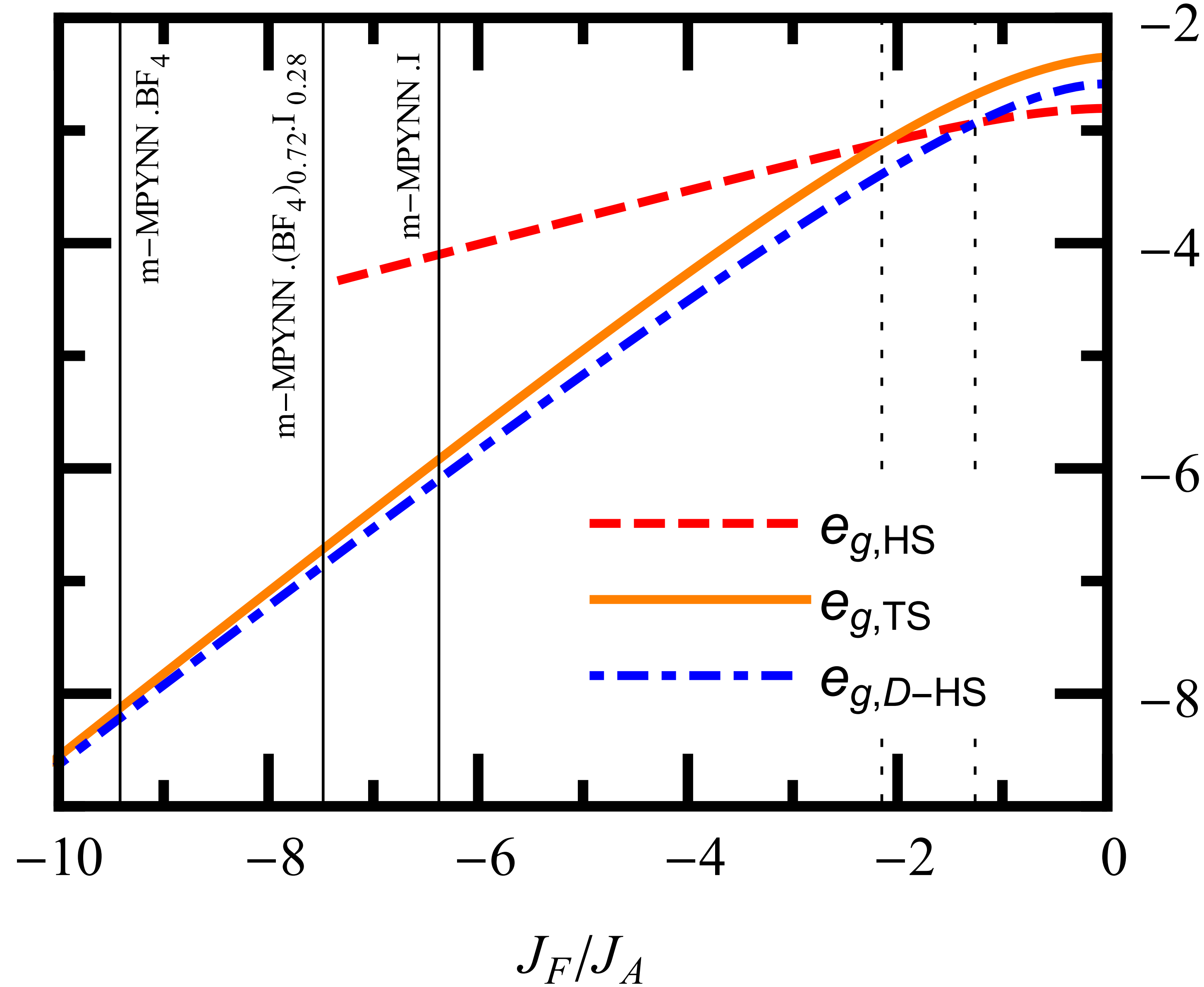
Possible Ground States of Hida Model







Comparison of their energies
(from triplon analysis)

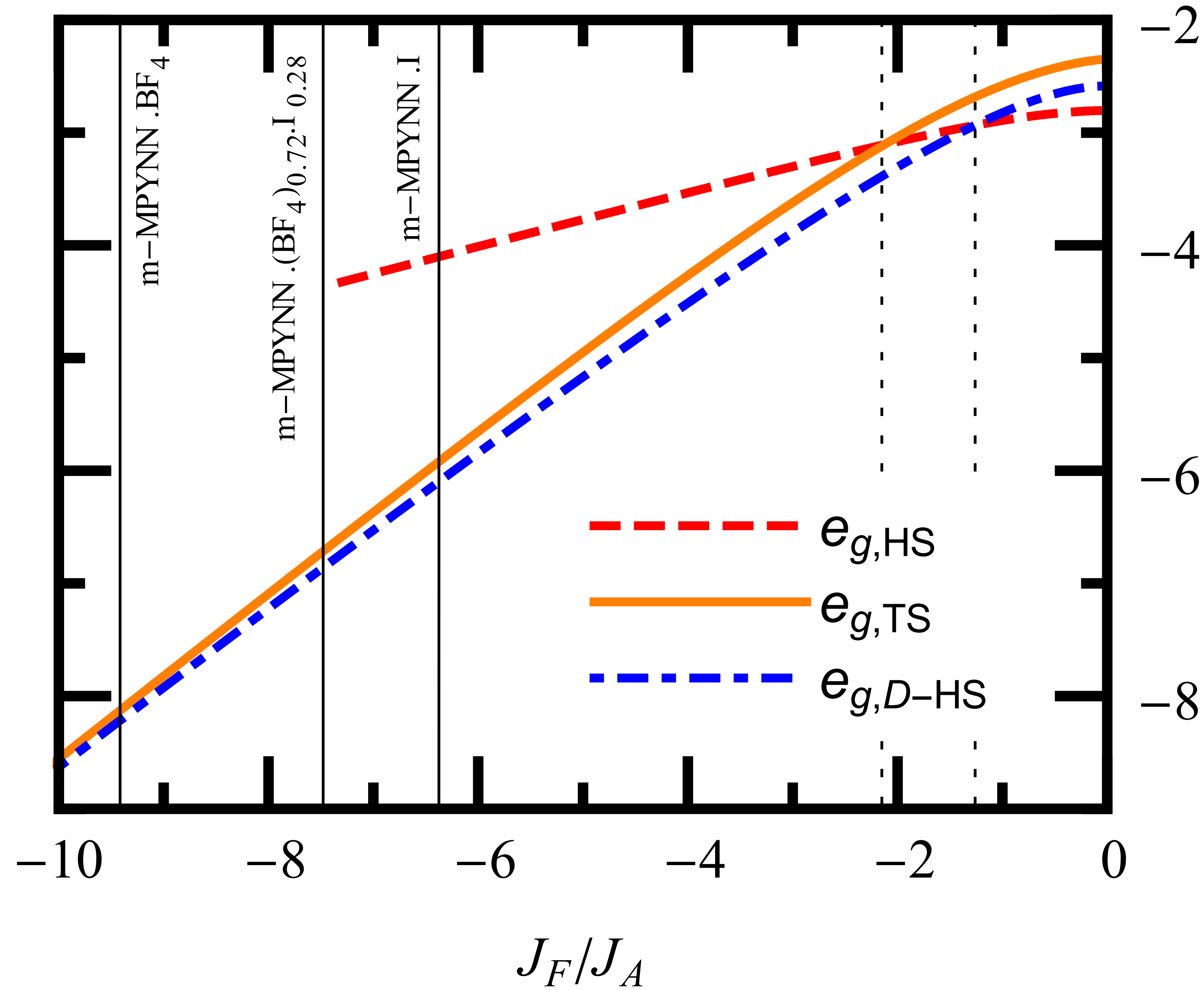


P. Ghosh and BK, PRB 97, 014413 (2018)

Possible Ground States of Hida Model

It suggests that the m-MPYNN.X family of organic salts realise the D-HS (TS) phase at low temperatures.

Comparison of their energies
(from triplon analysis)



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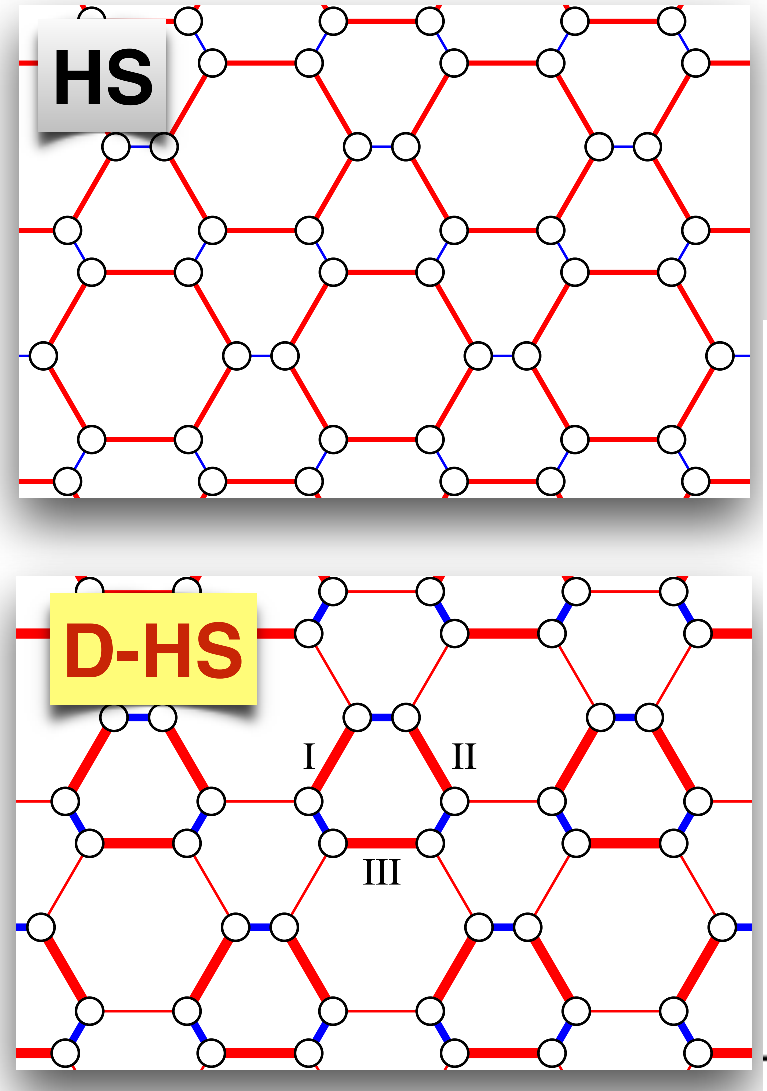
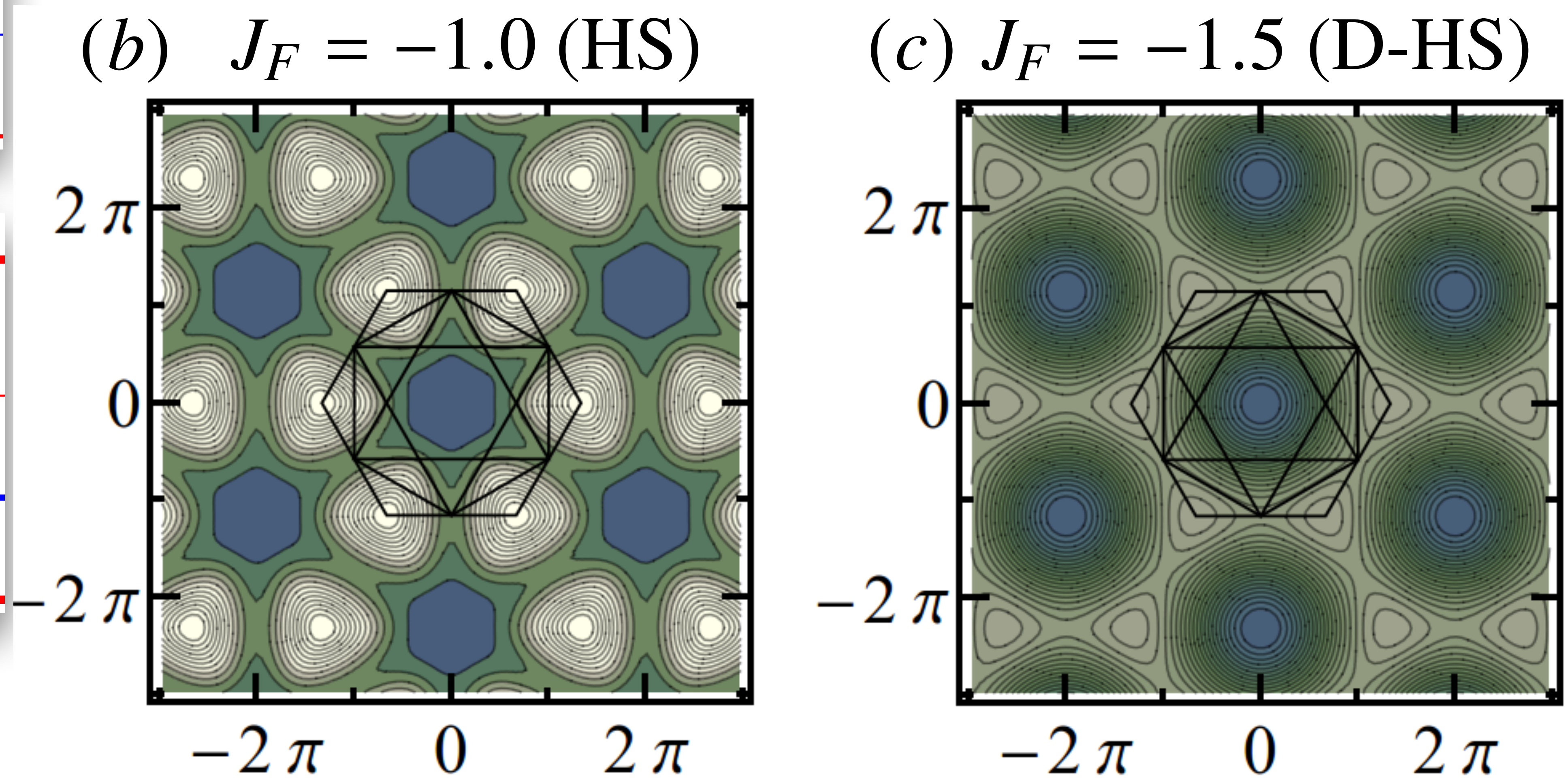
Possible Ground States of Hida Model



Comparing Spin Structure Factors of HS and D-HS

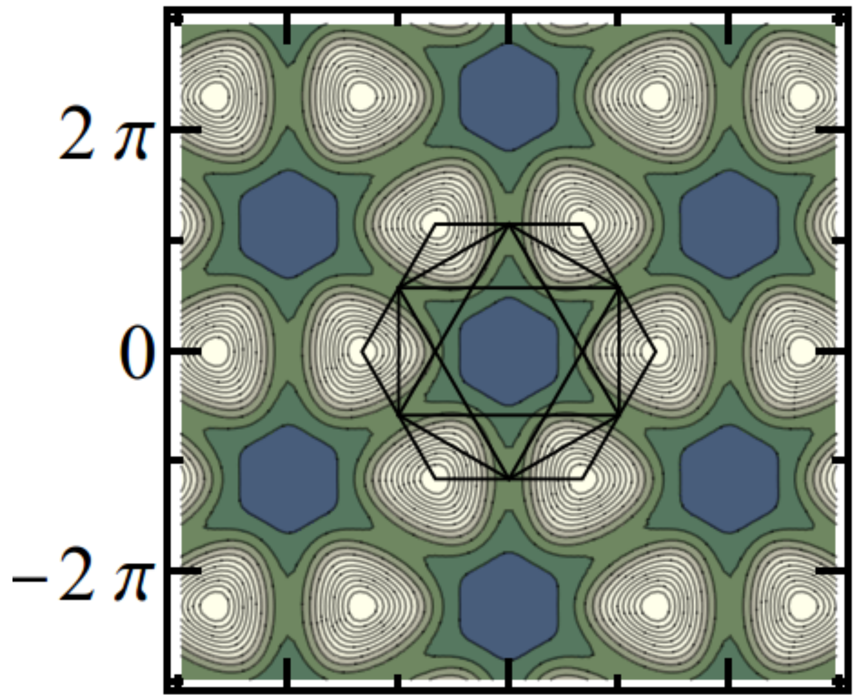
(from triplon analysis)



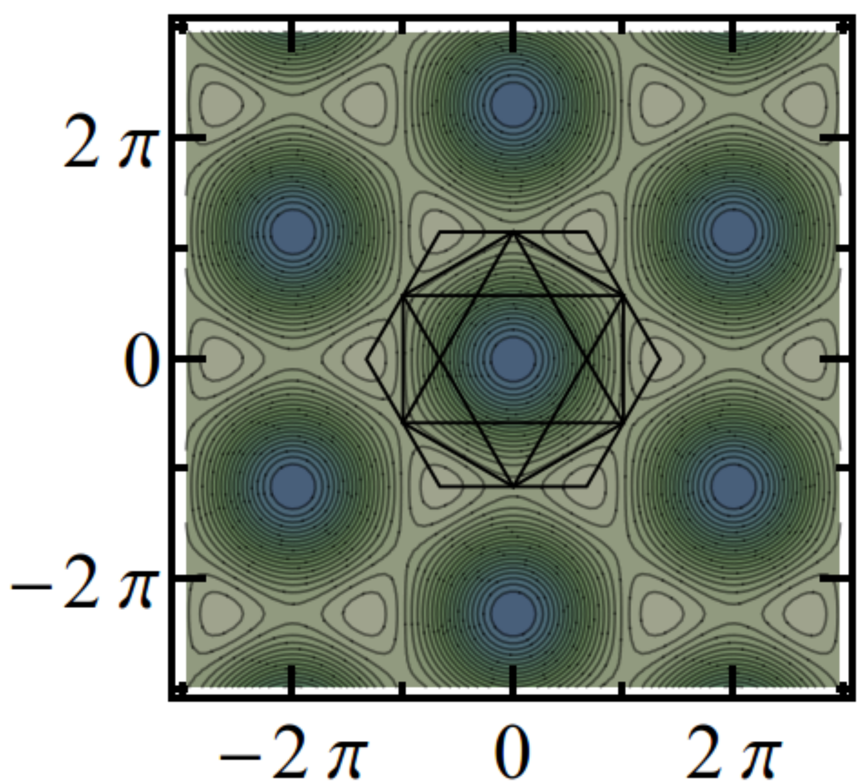
P. Ghosh and BK, PRB 97, 014413 (2018)

Possible Ground States of Hida Model

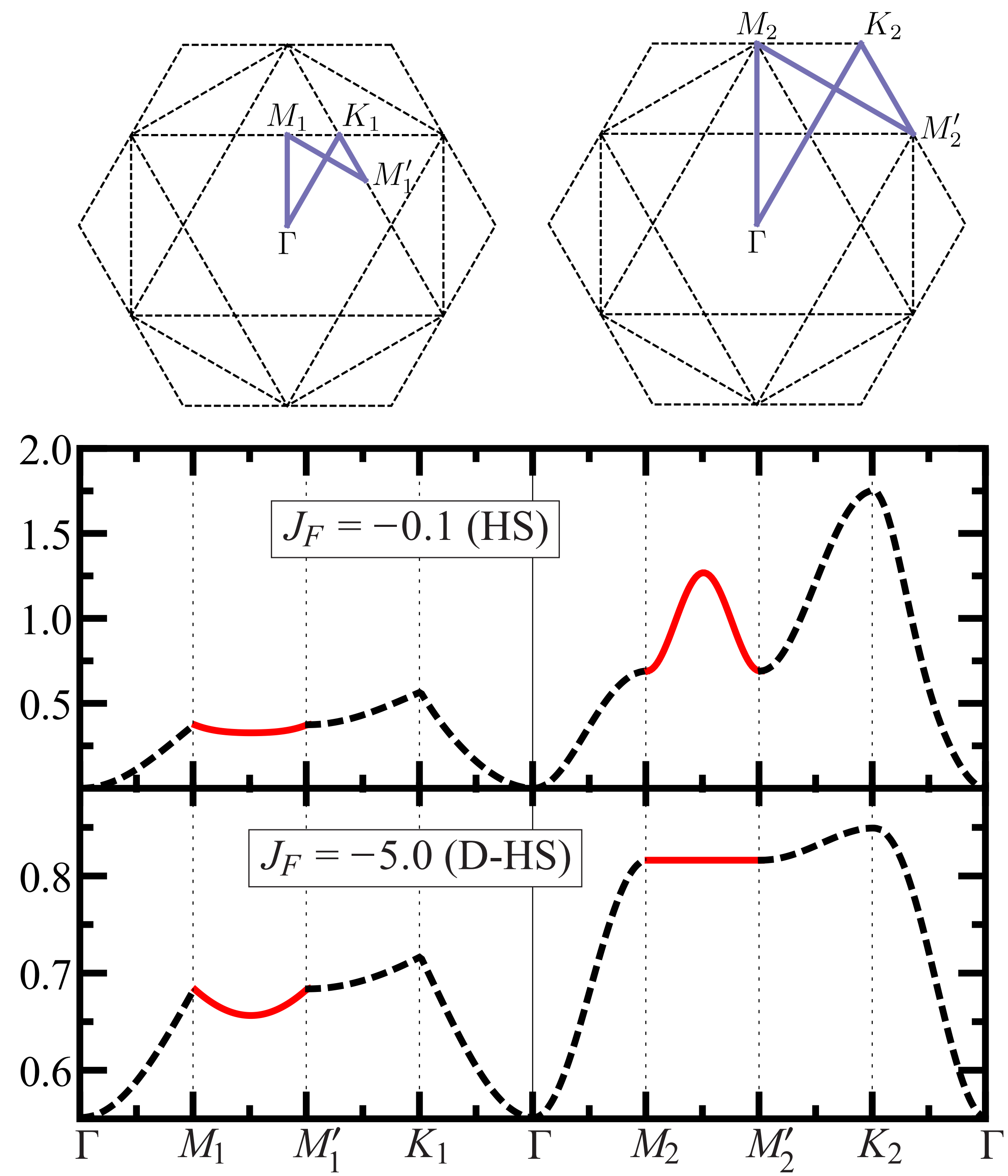
$J_F = -1.0$ (HS)



$J_F = -1.5$ (D-HS)



Static Structure Factors of HS and D-HS phases



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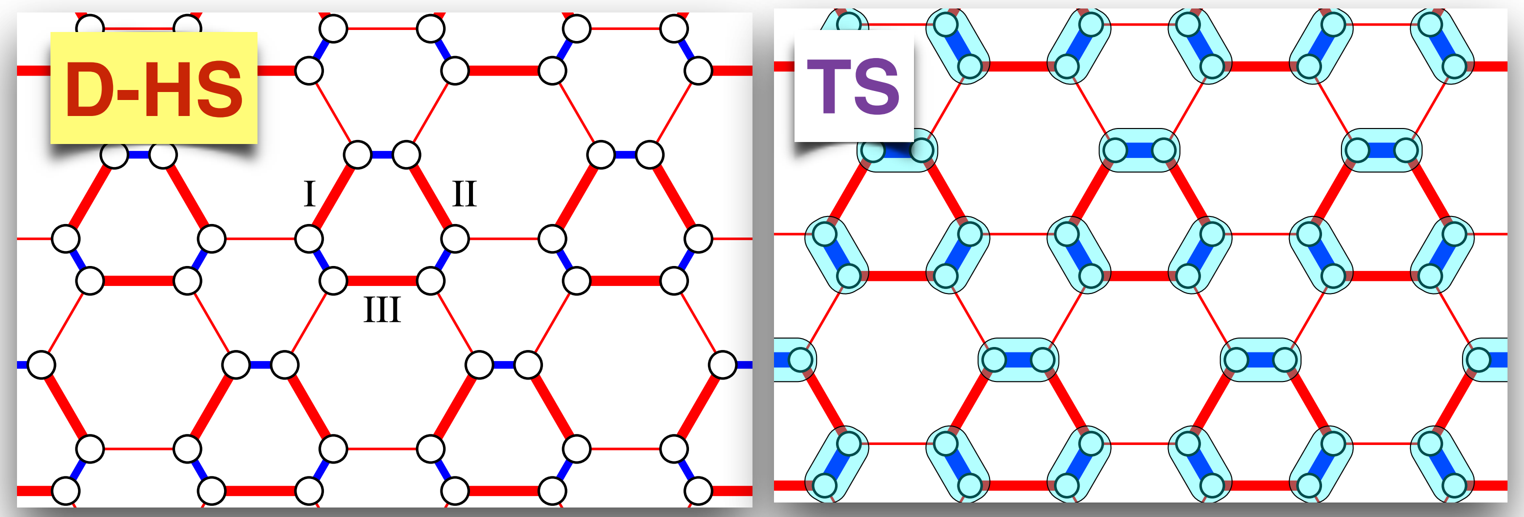
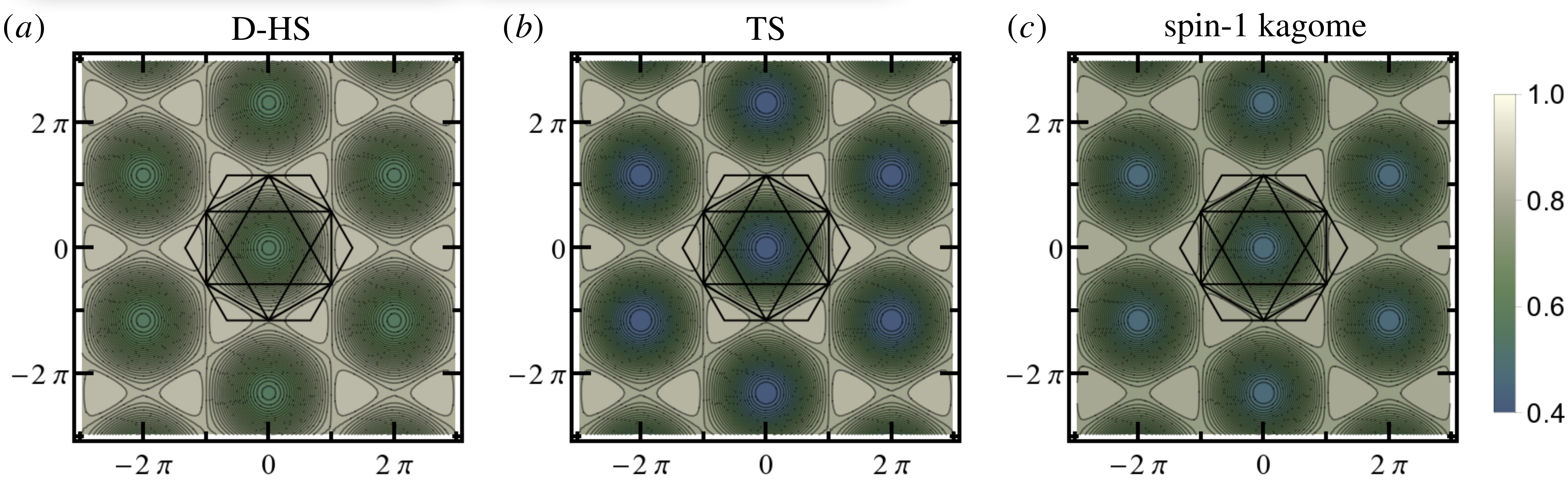
Possible Ground States of Hida Model

Comparing Spin Structure Factors of D-HS and TS



(from triplon analysis)



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Schwinger Boson Mean-Field Theory of Hida Model

Schwinger boson representation

$$S_i^+ = a_i^\dagger b_i\,,$$

$$S_i^- = b_i^\dagger a_i\,,$$

$$S_i^z = \frac{1}{2}(a_i^\dagger a_i - b_i^\dagger b_i)$$

$$a_i^\dagger a_i + b_i^\dagger b_i = 2S$$ (constraint)

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Heisenberg exchange operator

$$\vec{S}_i \cdot \vec{S}_j =: F_{ij}^\dagger F_{ij} : - A_{ij}^\dagger A_{ij},$$
$$A_{ij} = \frac{1}{\sqrt{2}}(a_i b_j - b_i a_j)$$
$$F_{ij} = \frac{1}{\sqrt{2}}(a_i^\dagger a_j + b_i^\dagger b_j)$$

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Mean-field approximation for Hida model:

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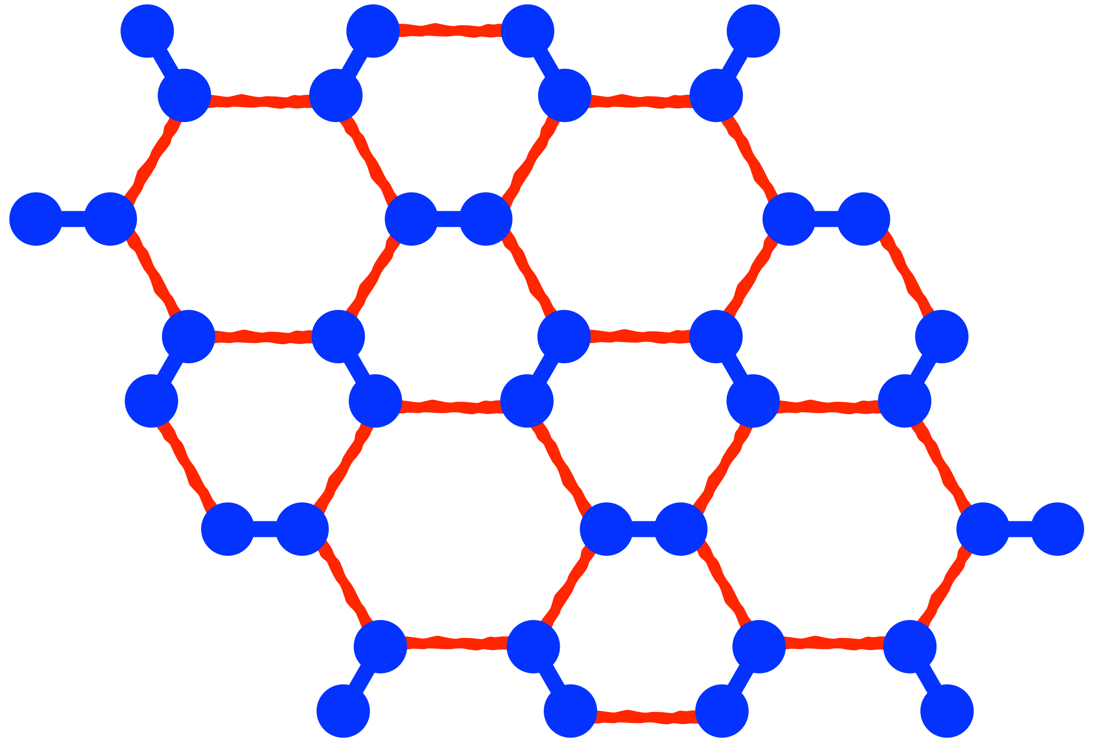

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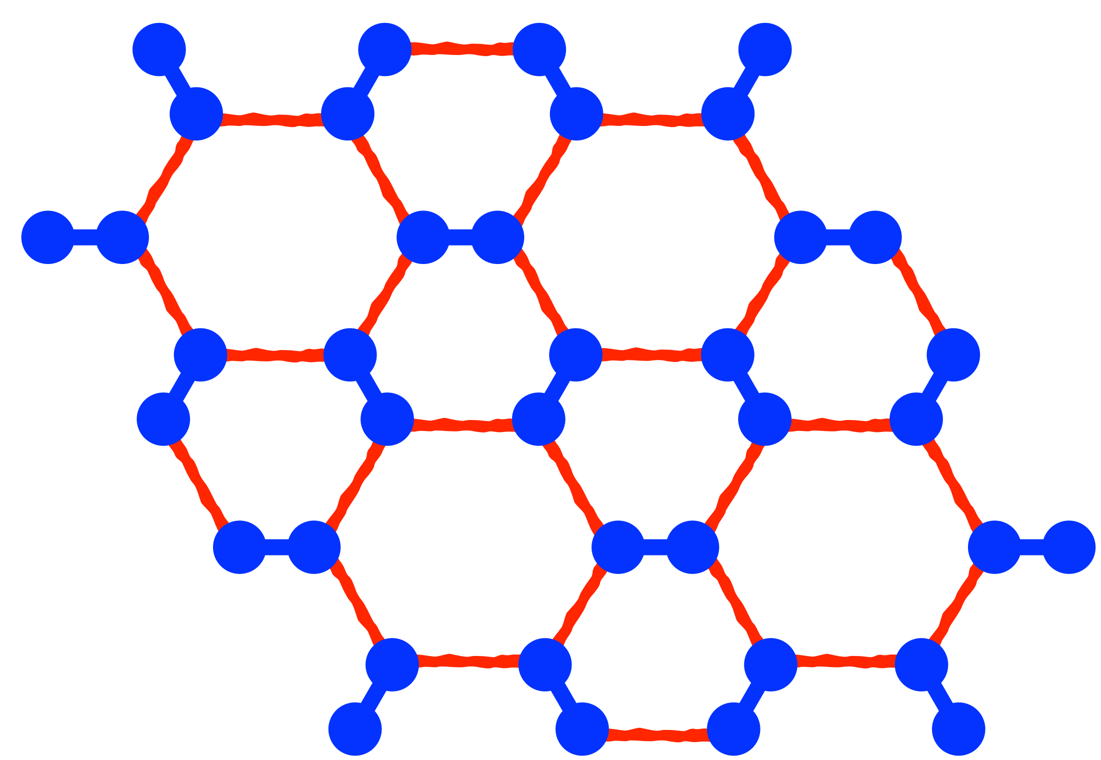
$$\alpha_F = \langle A_{ij} \rangle \text{ and } \phi_F = \langle F_{ij} \rangle$$ (FM bonds)

$$\left.\begin{array}{l} \alpha_A = \langle A_{ij} \rangle \text{ and } \phi_A = \langle F_{ij} \rangle \\ \alpha'_A = \langle A_{ij} \rangle \text{ and } \phi'_A = \langle F_{ij} \rangle \end{array}\right\}$$ (AFM bonds)



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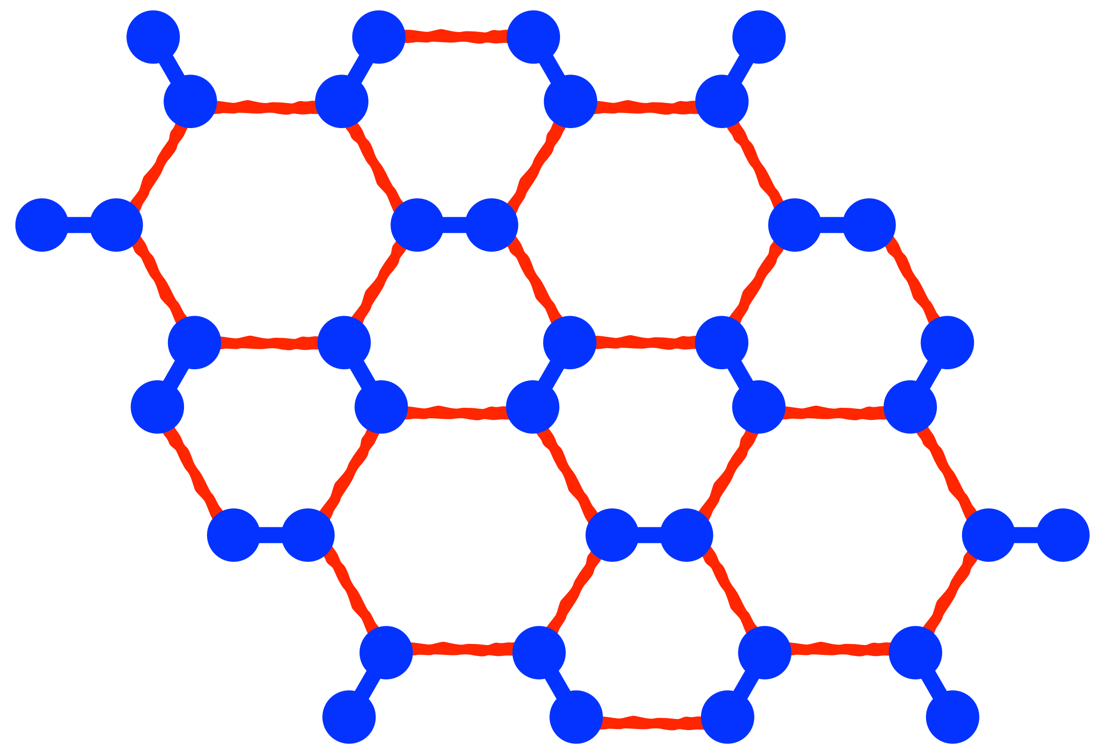

determine these mean-field parameters self-consistently.

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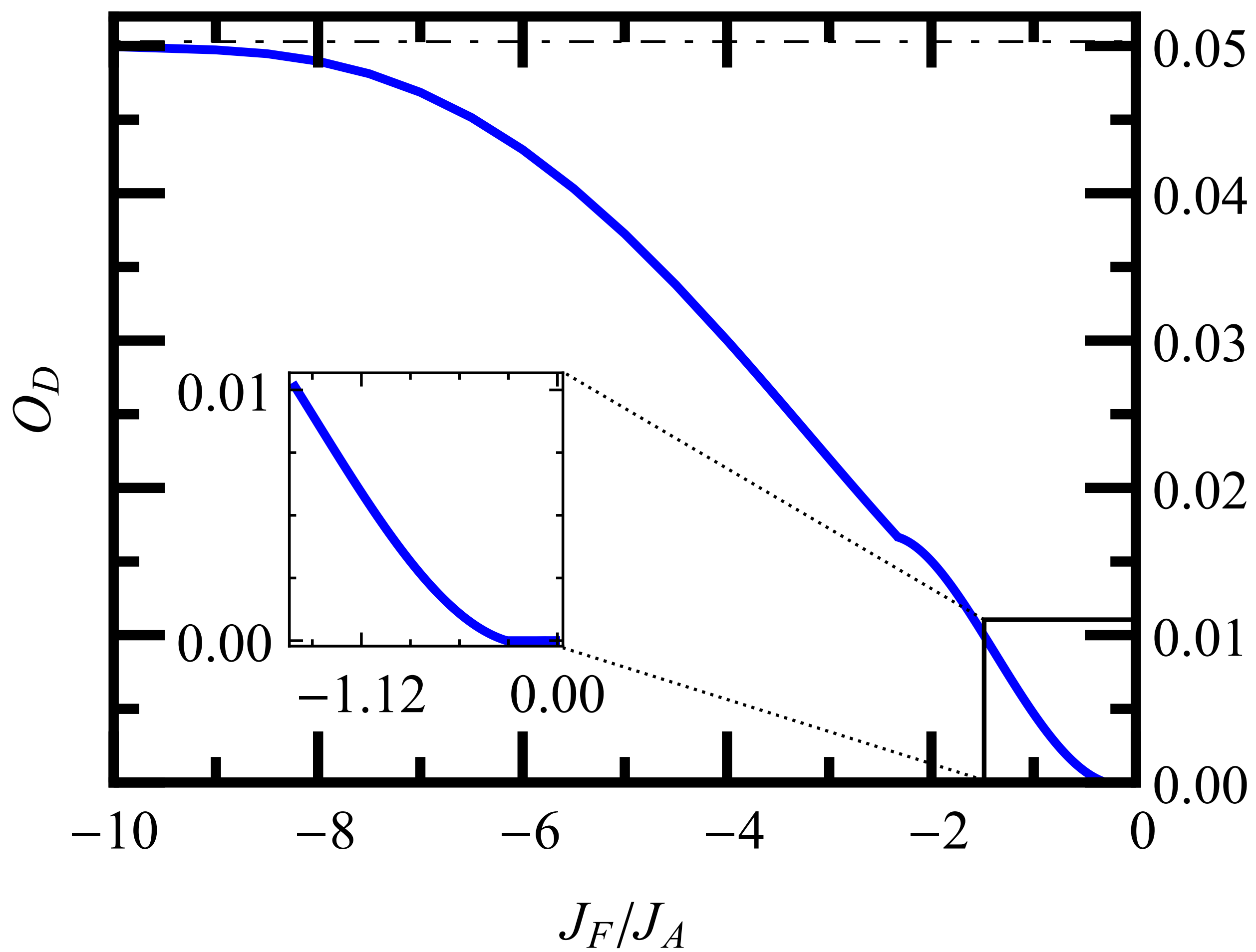
Schwinger Boson Mean-Field Theory of Hida Model

Two Quantum Phase Transitions



spontaneous dimerisation

$J_F/J_A \sim -0.28$

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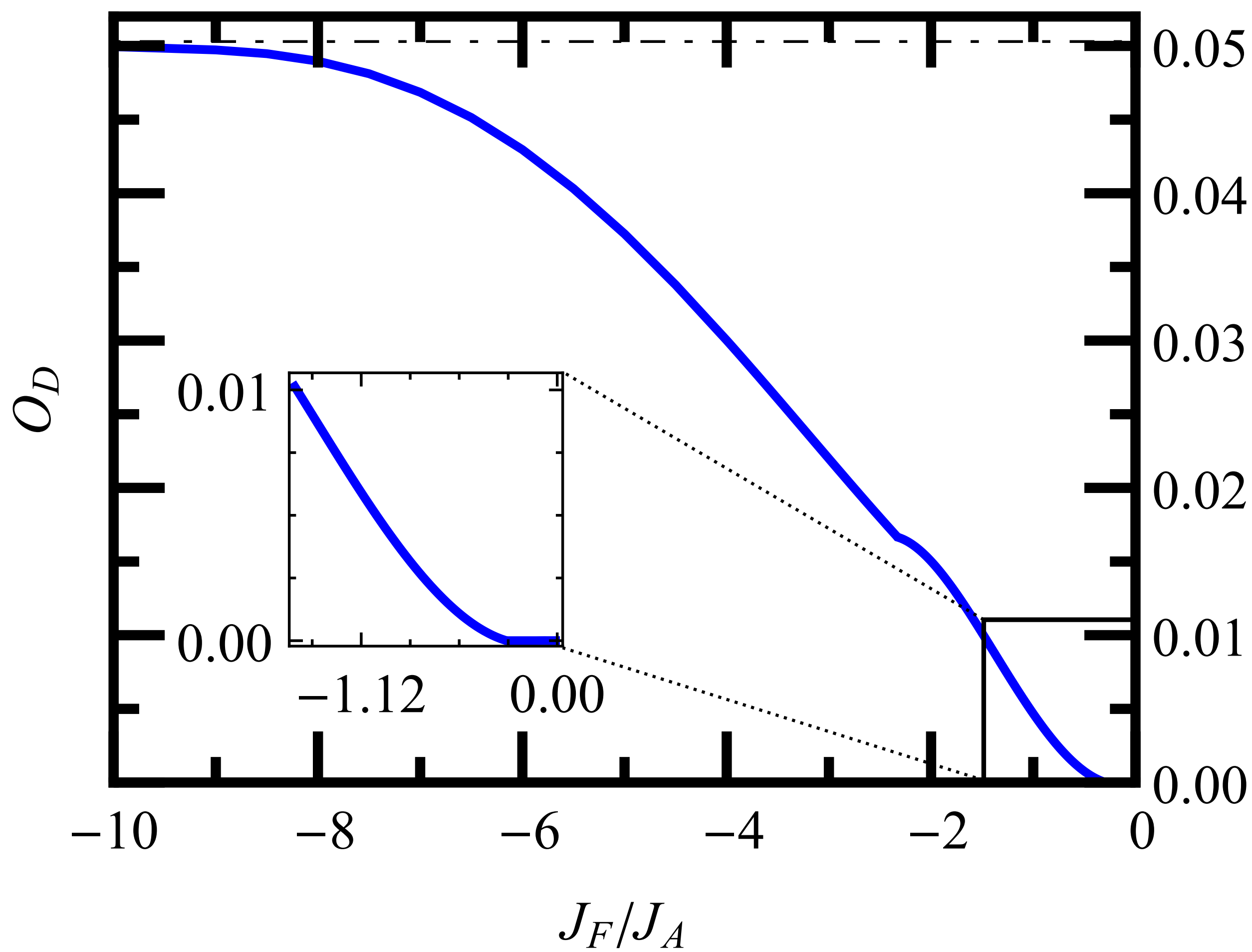

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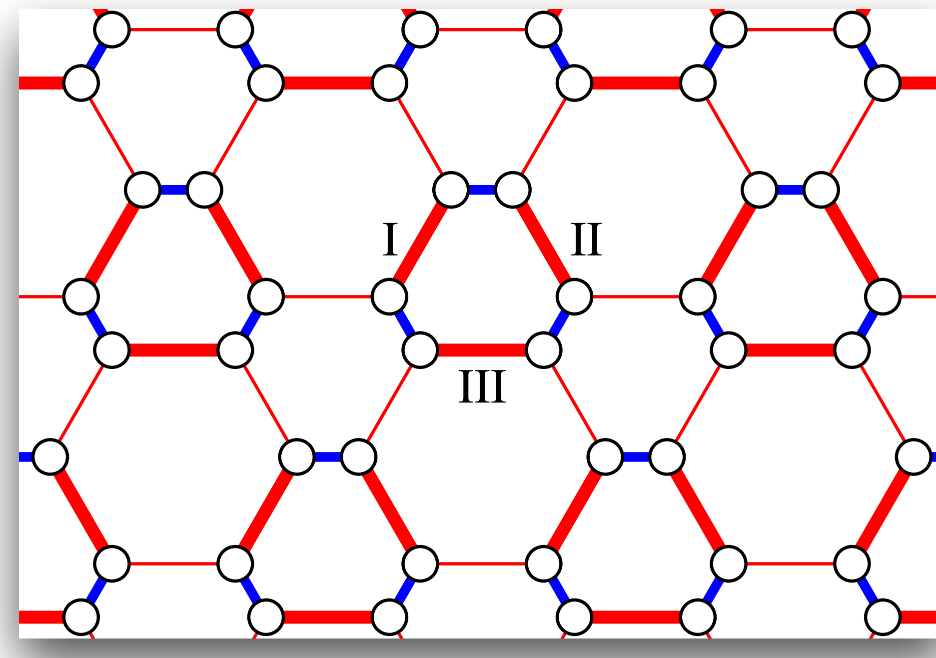

$$O_D = \frac{1}{3N_{\text{uc}}}\left|\sum_{\langle i,j\rangle}\langle \vec{S}_i \cdot \vec{S}_j\rangle - \sum_{\langle i,j\rangle}\langle \vec{S}_i \cdot \vec{S}_j\rangle\right|$$

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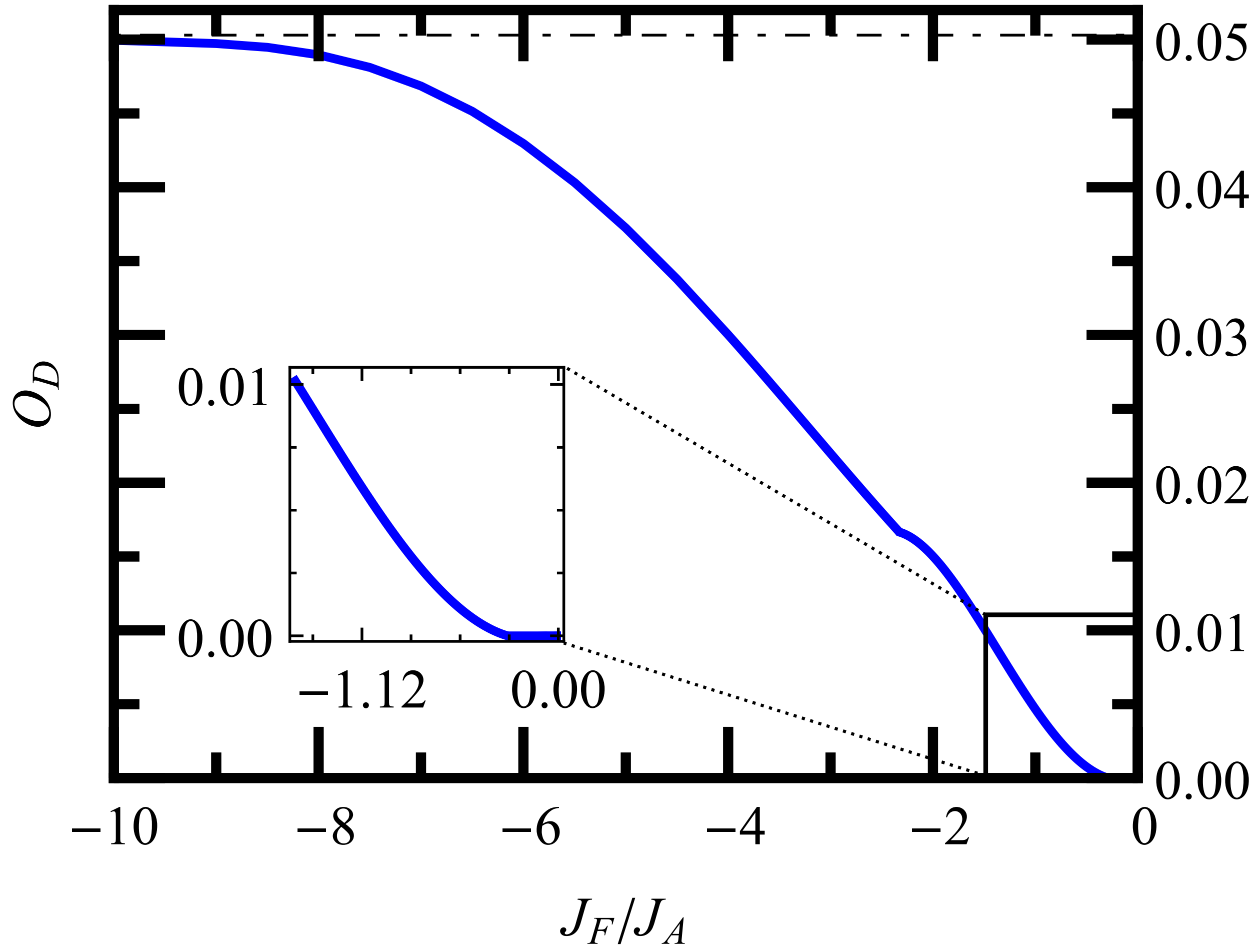

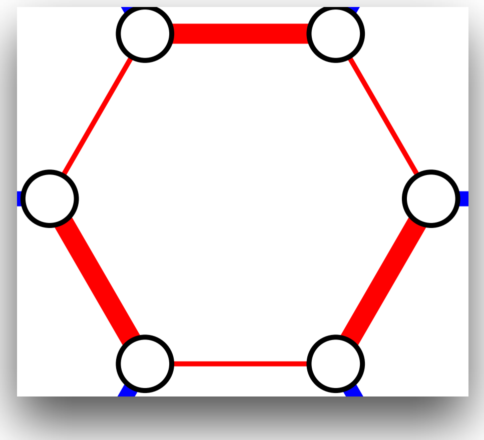

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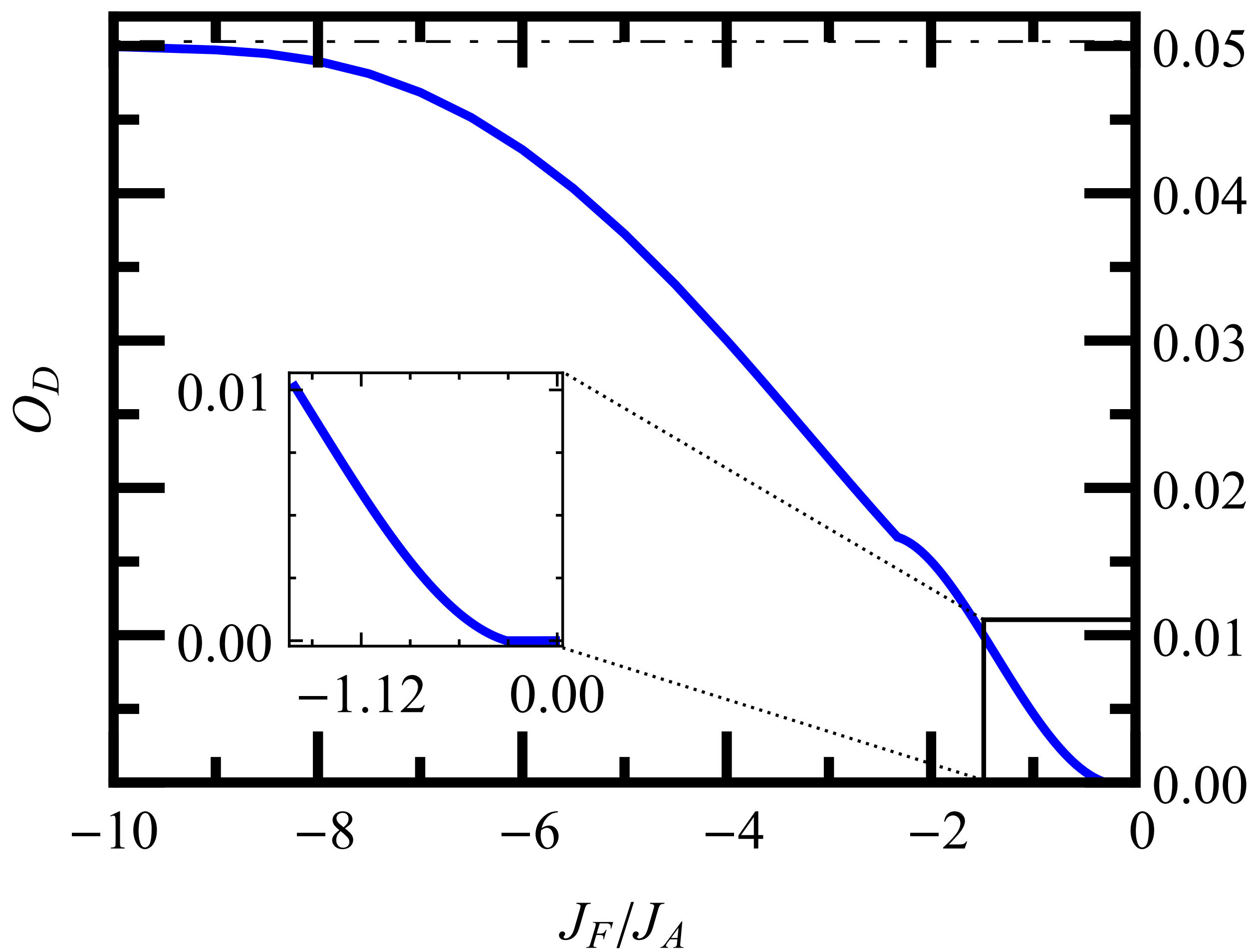

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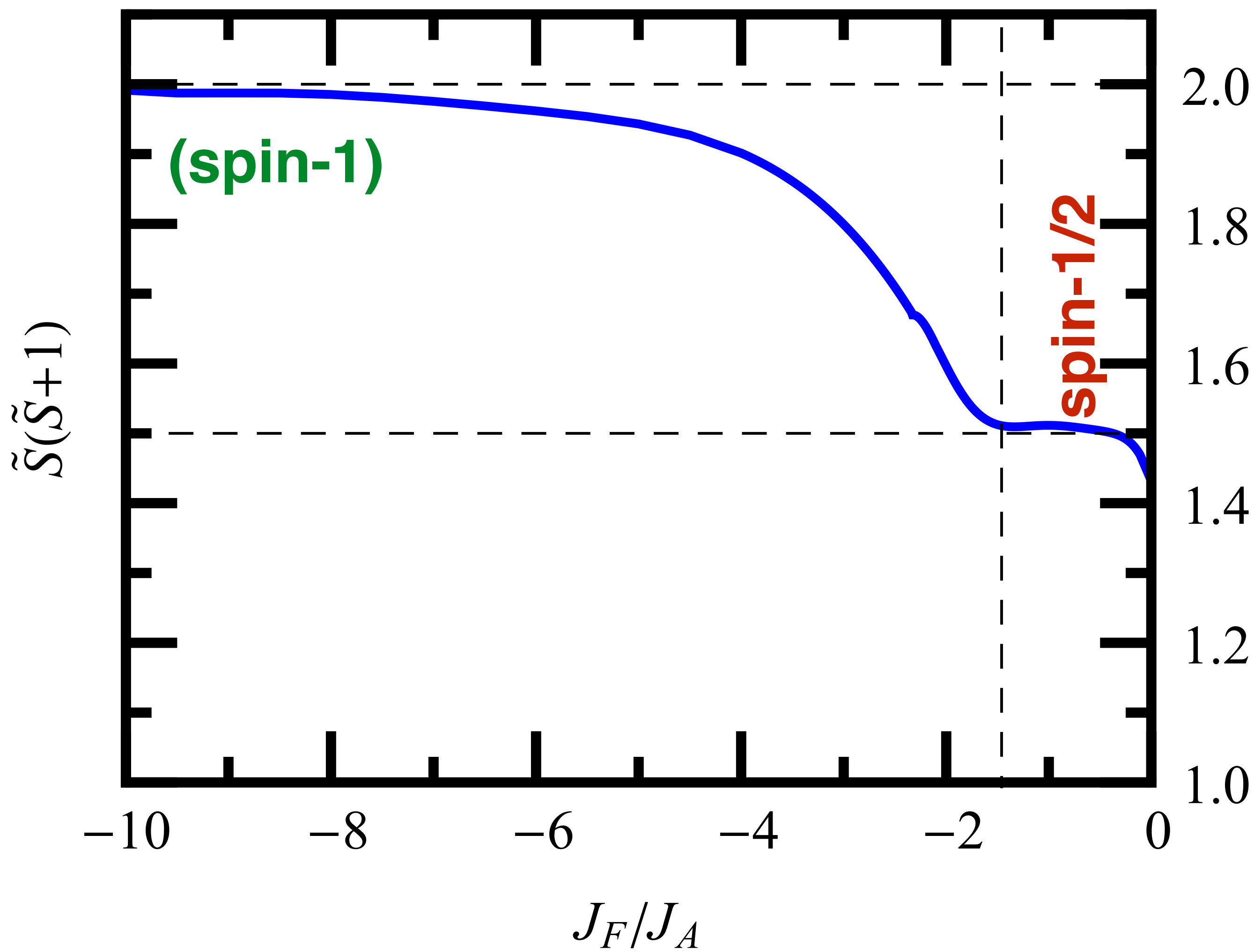

moment formation

$J_F/J_A \sim -1.46$

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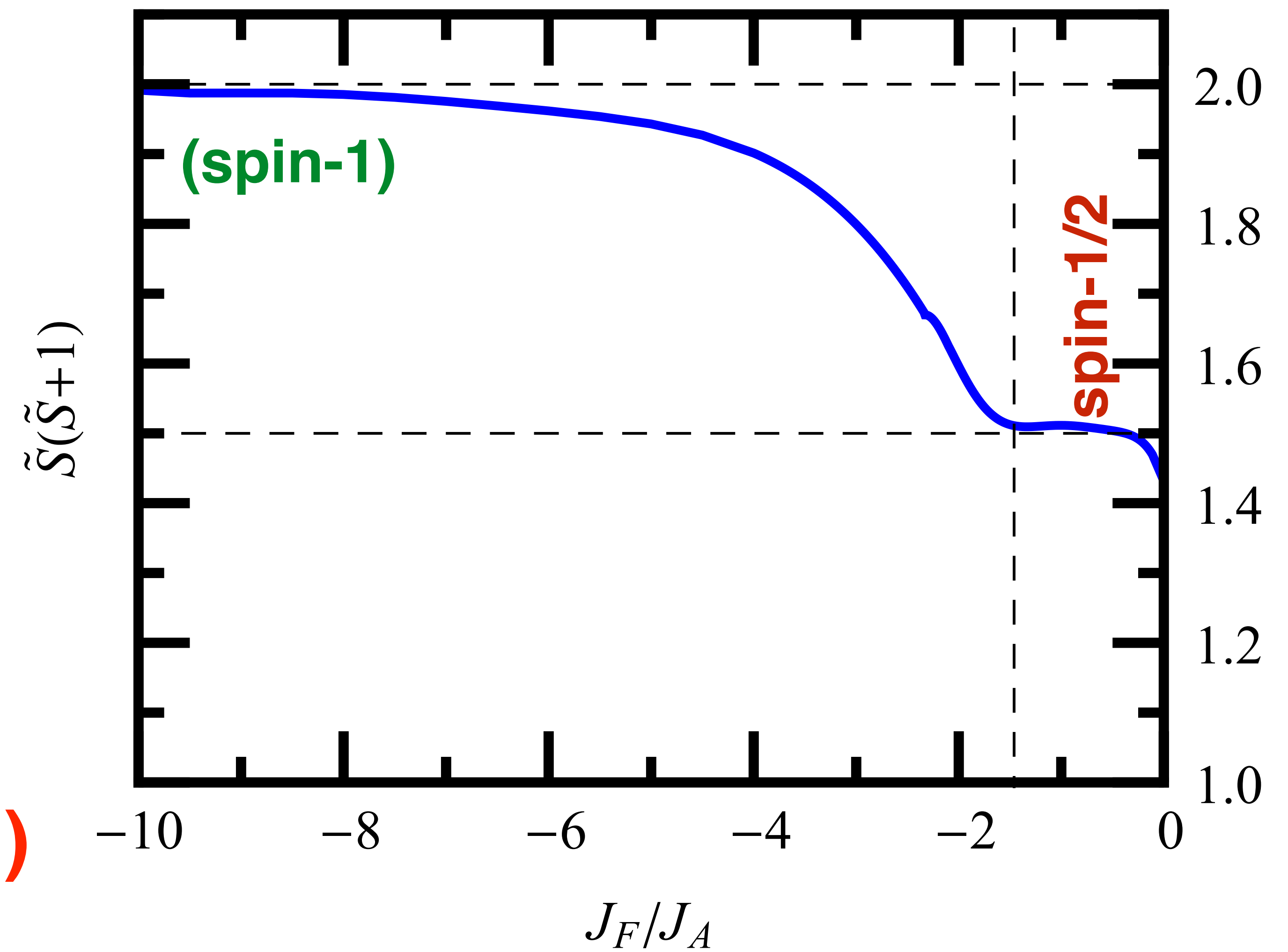
Schwinger Boson Mean-Field Theory of Hida Model

Two Quantum Phase Transitions

$$\widetilde{S}(\widetilde{S}+1) = \frac{1}{3N_{\rm uc}} \sum_{\langle i,j \rangle} \langle (\vec{S}_i + \vec{S}_j)^2 \rangle$$

$$= \frac{1}{3N_{\rm uc}} \sum_{\langle i,j \rangle} \left(\langle \vec{S}_i^2 \rangle + \langle \vec{S}_j^2 \rangle + 2 \langle \vec{S}_i \cdot \vec{S}_j \rangle \right)$$

(average total spin per FM bond)



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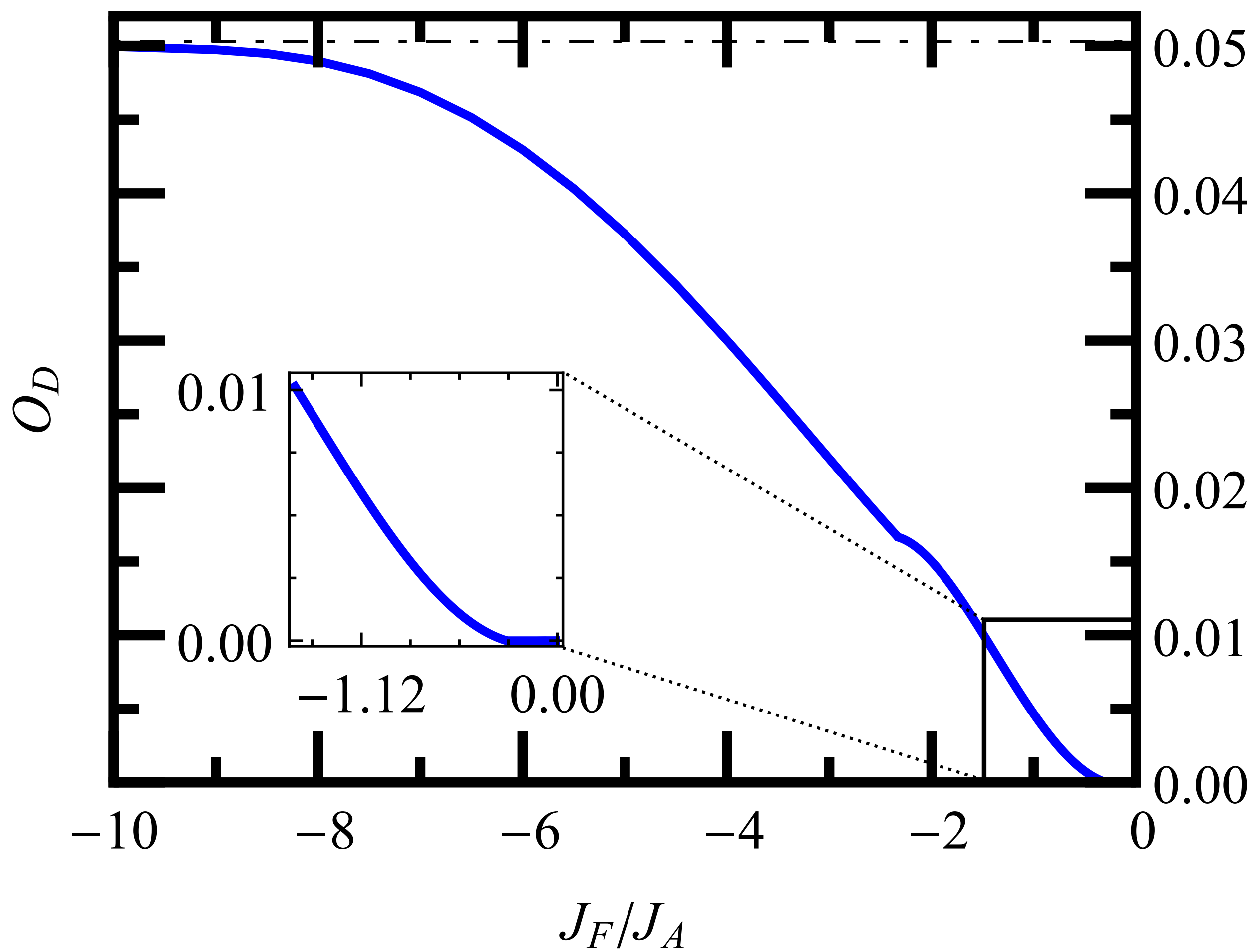

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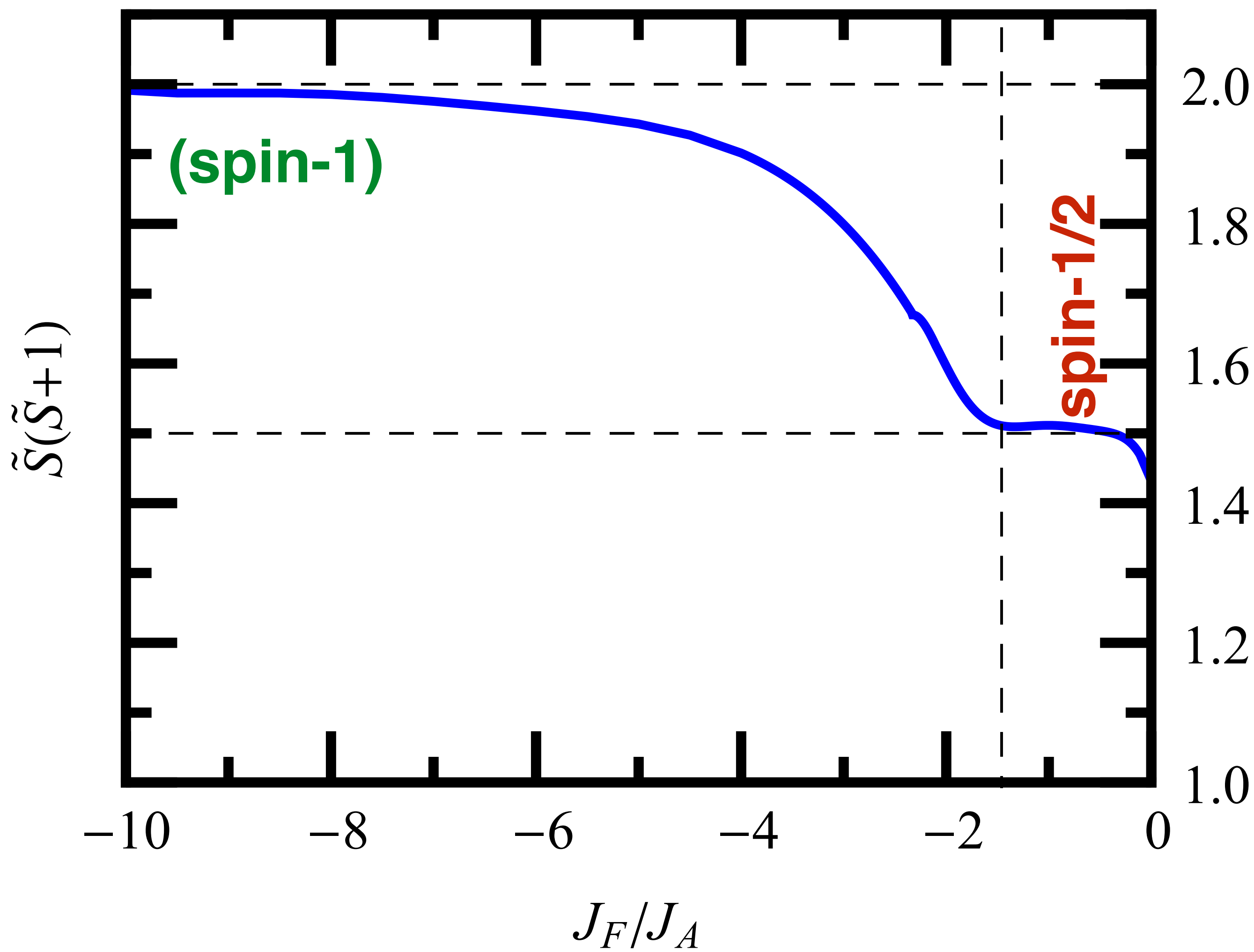

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Summary

The spin-1/2 Hida model, applicable to a family of spin-gapped organic salts, exhibits two transition in the spin-gapped, singlet ground with respect to J_F/J_A.

It first undergoes **spontaneous dimerisation**" at $J_F/J_A \sim -0.3$

For $J_F/J_A \sim -1.46$, pair of spin-1/2 moments on every FM bond begin to behave as "bound" moment.

The spontaneously trimerised singlet phase of the spin-1 KHA is same as the dimerised-HS phase of the Hida model for strong J_F/J_A.

The m-MPYNN.X family of organic salts realise the D-HS (TS) phase at low temperatures.

Thank you.