MAGNETIC ORDER AND ITS LOSS ON FRUSTRATED HONEYCOMB MONOLAYERS AND BILAYERS:

An Illustrative Use of the Coupled Cluster Method

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1. INTRODUCTION
   - Example: J_1–J_2–J_3 Model on a Honeycomb Monolayer
   - The Coupled Cluster Method
2. RESULTS
   - Results on the Honeycomb Monolayer
     - The spin-1/2 J_1–J_2–J_3 Heisenberg model
   - Results on the Honeycomb Bilayer
     - The spin-1/2 J_1–J_2–J_3–$J_1^{\perp}$ Heisenberg model
3. SUMMARY

References

D.J.J. Farnell, R.F. Bishop, P.H.Y. Li *et al.*, PRB **84**, 012403 (2011)

R.F. Bishop and P.H.Y. Li, PRB **85**, 155135 (2012)

P.H.Y. Li, R.F. Bishop *et al.*, PRB **86**, 144404 (2012)

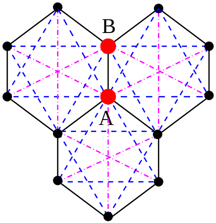
R.F. Bishop, P.H.Y. Li *et al.*, PRB **92**, 224434 (2015)

R.F. Bishop and P.H.Y. Li, eprint arXiv:1611.03287 (2016); unpublished (2017)

J_1–J_2–J_3 Model on the Honeycomb Monolayer Lattice

- J_1–J_2–J_3 model on the 2D honeycomb lattice (i.e., all bonds of Heisenberg type)
- We'll look at the case with $s = \frac{1}{2}$ spins (viz., the most quantum case)
- $H = J_1 \sum_{\langle i,j \rangle} \mathbf{s}_i \cdot \mathbf{s}_j + J_2 \sum_{\langle\langle i,k \rangle\rangle} \mathbf{s}_i \cdot \mathbf{s}_k + J_3 \sum_{\langle\langle\langle i,l \rangle\rangle\rangle} \mathbf{s}_i \cdot \mathbf{s}_l$

  (and set $J_1 \equiv 1$) where, on the honeycomb lattice:
  - $\langle i,j \rangle$ bonds $J_1 \equiv$ ——— all NN bonds
  - $\langle\langle i,k \rangle\rangle$ bonds $J_2 \equiv$ - - - - - all NNN bonds
  - $\langle\langle\langle i,l \rangle\rangle\rangle$ bonds $J_3 \equiv$ - · - · - all NNNN bonds

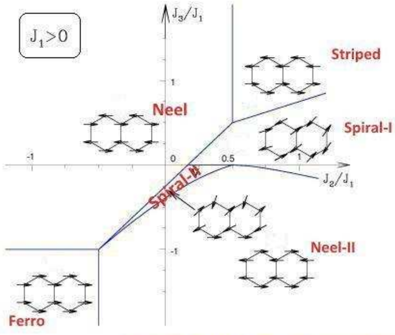


NOTE: The honeycomb lattice is bipartite but non-Bravais (– two sites per unit cell: *A, B*)

Limiting Cases

- limiting bond cases
  - $J_2 = J_3 = 0$: isotropic HAF on 2D honeycomb lattice
  - $J_1 = J_3 = 0$: two uncoupled isotropic HAFs on 2D triangular lattice
  - $J_1 = J_2 = 0$: four uncoupled isotropic HAFS on 2D honeycomb lattice
- classical limit ($s \to \infty$)
  - for $J_1 > 0$: ground-state (GS) phase diagram is complex, containing 6 different ordered phases -
    - Néel
    - Striped
    - Néel-II
    - Spiral-I
    - Spiral-II
    - Ferromagnetic
  - for $J_1 < 0$: also 6 phases, related to those above by simple symmetries (i.e., $J_1 \rightleftharpoons -J_1$; $J_3 \rightleftharpoons -J_3$; $\mathbf{s}_i{}^{\mathrm{B}} \rightleftharpoons -\mathbf{s}_i{}^{\mathrm{B}}$)

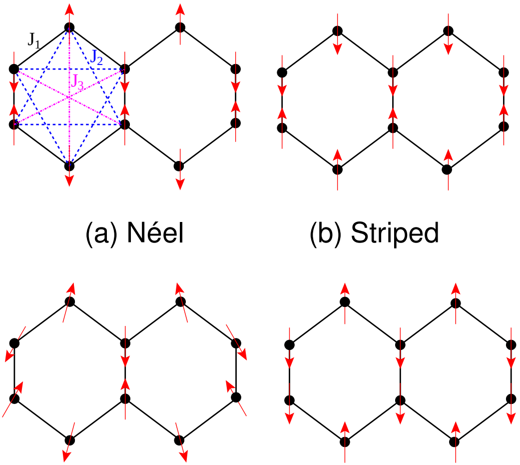
Classical ($s \to \infty$) Phase Diagram ($J_1 > 0$)



Classical J1-J2-J3 Model on the Honeycomb Lattice

- Both the Striped and Néel-II regions actually have an infinitely degenerate family of non-coplanar ground states, from which the collinear states shown are selected by thermal or quantum fluctuations
- The most highly frustrated point at $J_2/J_1 = \frac{1}{2}$, $J_3/J_1 = \frac{1}{2}$ (i.e., a classical triple point) lies along the line $J_3 = J_2$

Néel, Striped, Spiral-I, and Néel-II Model States



(a) Néel (b) Striped

(c) Spiral-I (d) Néel-II

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3. SUMMARY

Elements of the CCM

We use the coupled cluster method (CCM)

- ground-state (GS) wavefunction:
  $$|\Psi\rangle = \mathrm{e}^{S}|\Phi\rangle; \quad \langle\tilde{\Psi}| = \langle\Phi|\tilde{S}\mathrm{e}^{-S}; \quad \langle\tilde{\Psi}|\Psi\rangle = \langle\Phi|\Psi\rangle = \langle\Phi|\Phi\rangle \equiv 1$$
  $$S = \sum_{I\neq 0} \mathcal{S}_I C_I^+; \qquad \tilde{S} = 1 + \sum_{I\neq 0} \tilde{\mathcal{S}}_I C_I^-$$
  $$C_0^+ \equiv 1; \qquad C_I^- \equiv (C_I^+)^\dagger; \qquad C_I^-|\Phi\rangle = 0, \ \forall I \neq 0$$
- $C_I^+|\Phi\rangle$ are a complete set of wf's; $[C_I^+, C_J^+] = 0$
- choose model state $|\Phi\rangle$ to be, e.g., a classical GS (i.e., Néel, Striped, Spiral-I, and Néel-II)
- choose spin axes on each site so that $|\Phi\rangle = |\downarrow\downarrow\cdots\downarrow\rangle$ in these local axes
- $\Rightarrow C_I^+ \rightarrow s_{i_1}^+ s_{i_2}^+ \cdots s_{i_k}^+; \qquad s_j^+ \equiv s_j^x + i s_j^y$, in local axes

Elements of the CCM

- each s_i^+ in C_I^+ can appear at most once for $s = \frac{1}{2}$, twice for $s = 1, \cdots$, and $2s$ times for general spin-s case, on a given lattice site i
- solve for $\{\mathcal{S}_I, \tilde{\mathcal{S}}_I\}$ from GS Schrödinger eqs. for $|\Psi\rangle$, $\langle\tilde{\Psi}| \Longrightarrow$ equivalently, minimize $\bar{H} = \bar{H}(\mathcal{S}_I, \tilde{\mathcal{S}}_I) \equiv \langle\Phi|\tilde{S}\mathrm{e}^{-S}H\mathrm{e}^{S}|\Phi\rangle$ with respect to all parameters $\{\mathcal{S}_I, \tilde{\mathcal{S}}_I;\ \forall I \neq 0\}$

$$\longrightarrow \quad \frac{\delta \bar{H}}{\delta \tilde{\mathcal{S}}_I} = 0 \quad \Longrightarrow \quad \langle\Phi|C_I^- \mathrm{e}^{-S}H\mathrm{e}^{S}|\Phi\rangle = 0\,, \quad \forall I \neq 0$$

– a coupled set of nonlinear equations for $\{\mathcal{S}_I\}$

$$\Longrightarrow E = \langle\Phi|\mathrm{e}^{-S}H\mathrm{e}^{S}|\Phi\rangle = \langle\Phi|H\mathrm{e}^{S}|\Phi\rangle \qquad (1)$$

$$\longrightarrow \quad \frac{\delta \bar{H}}{\delta \mathcal{S}_I} = 0 \quad \Longrightarrow \quad \langle\Phi|\tilde{S}\mathrm{e}^{-S}[H, C_I^+]\mathrm{e}^{S}|\Phi\rangle = 0\,, \quad \forall I \neq 0$$

$$\Longrightarrow \quad \langle\Phi|\tilde{S}(\mathrm{e}^{-S}H\mathrm{e}^{S} - E)C_I^+|\Phi\rangle = 0\,, \quad \forall I \neq 0$$

– a coupled set of linear generalized eigenvalue equations for $\{\tilde{\mathcal{S}}_I)\}$ with $\{\mathcal{S}_I\}$ as input

Elements of the CCM

- Note that the nonlinear exponentiated terms only ever appear in the form of the similarity transform of the Hamiltonian: $\mathrm{e}^{-S}H\mathrm{e}^{S}$
  $\Longrightarrow$ use the nested commutator expansion
  $\mathrm{e}^{-S}H\mathrm{e}^{S} = H + [H,S] + \frac{1}{2!}[[H,S],S] + \cdots$
  NOTE: This series will terminate exactly after the term bilinear in S for our Heisenberg Hamiltonians $\Longrightarrow$
- CCM satisfies the Goldstone linked cluster theorem and
- satisfies the Hellmann-Feynman theorem, for all truncations on complete set $\{I\}$
- we use the natural lattice geometry to define the approximation schemes and we retain all distinct fundamental configurations (fc) in the set $\{I\}$ with respect to space- and point-group symmetries of both the Hamiltonian and the model state $|\Phi\rangle$
- A similar CCM parametrization exists for excited states too

CCM Truncation Schemes

- only approximation is to truncate set $\{I\}$
  - for $s = \frac{1}{2}$ case we typically use the LSUBm scheme in which we retain all possible multispin-flip correlations over different locales on the lattice defined by m or fewer contiguous lattice sites
  - for $s \geq 1$ cases we often use the alternative SUBn–m scheme in which we retain all multispin-flip correlations involving up to n spin flips spanning a range of no more than m adjacent (or contiguous) lattice sites. We then set $m = n$ and employ the so-called SUBm–m scheme
    NOTE: LSUB$m \equiv$ SUB2sm–m for general spin-s case, (i.e., LSUB$m \equiv$ SUBm–m only for $s = \frac{1}{2}$ case)

Number of CCM Fundamental Configurations, N_f

- For the spin-1/2 J_1–J_2–J_3 model on the honeycomb lattice:

Method	N_f			
	Néel	striped	Néel-II	spiral
LSUB4	5	9	9	66
LSUB6	40	113	85	1080
LSUB8	427	1750	1101	18986
LSUB10	6237	28805	17207	347287

NOTE: To obtain a single data point (i.e., for given values of J_2 and J_3, with $J_1 = 1$) for the spiral-I phase at the LSUB10 level we typically require about 6 h computing time using 2000 processors simultaneously.

CCM Extrapolations to Exact ($m \to \infty$) Limit

- at each LSUBm or SUBm–m level the CCM operates at the $N \to \infty$ limit from the outset
- calculate E/N and magnetic order parameter (i.e., local average onsite magnetization) $M \equiv -\frac{1}{N}\sum_N \langle\tilde{\Psi}|s_i^z|\Psi\rangle$ in the local rotated axes
- extrapolate to the exact $m \to \infty$ limit, using well-tested empirical scaling laws
  - $E/N = a_0 + a_1 m^{-2} + a_2 m^{-4}$
  - $M = b_0 + b_1 m^{-1} + b_2 m^{-2}$ for unfrustrated models
  - $M = b_0 + b_1 m^{-0.5} + b_2 m^{-1.5}$ for highly frustrated models

J_1–J_2–J_3 Model on the Honeycomb Monolayer ($s = \frac{1}{2}$)

- We have done a large study of this model
- Results include:
  - The case when $J_3 = J_2$ for which we have investigated the full phase diagram for both signs of the bonds
    References
    D.J.J. Farnell *et al.*, PRB **84**, 012403 (2011)
    P.H.Y. Li *et al.*, PRB **85**, 085115 (2012)
    R.F. Bishop and P.H.Y. Li, PRB **85**, 155135 (2012)
    R.F. Bishop, P.H.Y. Li *et al.*, PRB **92**, 224434 (2015)
  - The case when $J_3 = 0$ (i.e., the J_1–J_2 model); $J_1 > 0, J_2 > 0$
    References
    R.F. Bishop *et al.*, J. Phys.: Condens. Matter **24**, 236002 (2012)
    R.F. Bishop *et al.*, J. Phys.: Condens. Matter **25**, 306002 (2013)
  - The full J_1–J_2–J_3 model; $J_1 > 0, J_2 > 0, J_3 > 0$
    Reference
    P.H.Y. Li *et al.*, PRB **86**, 144404 (2012)

J_1–J_2–J_3 Model on the Honeycomb Monolayer ($s = \frac{1}{2}$)

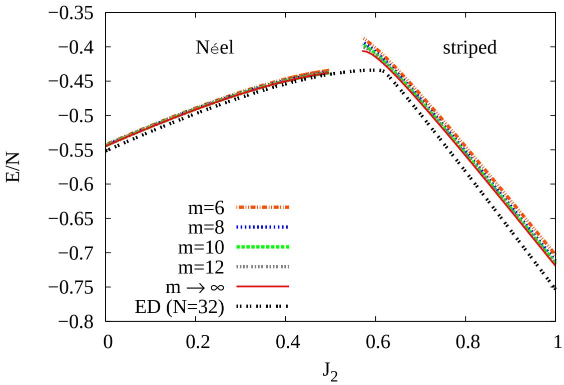
- the classical ($s \to \infty$) J_1–J_2–J_3 model on the monolayer honeycomb lattice is most frustrated at the classical tricritical point ($J_2/J_1 = \frac{1}{2}, J_3/J_1 = \frac{1}{2}$) at which three phases (Néel, striped and spiral-I) meet $\Longrightarrow$
- let us restrict ourselves initially, for illustrative reasons, to study the model along the line $J_3 = J_2 \equiv \alpha J_1$
- for $J_1 > 0$, at the point $\alpha = \frac{1}{2}$ there is a classical phase transition from a non-degenerate Néel phase to an infinitely degenerate family of GS phases (from which the striped phase is selected by quantum or thermal fluctuation) $\Longrightarrow$
- this region should be a fertile hunting-ground for novel phases for the $s = \frac{1}{2}$ quantum case

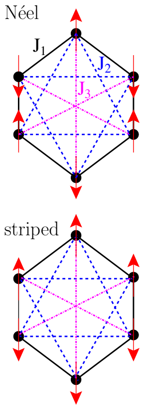
RESULTS I: Monolayer with $J_1 \equiv +1$; $J_3 = J_2$

- We study the case $J_1 \equiv +1$; $0 \leq J_3 = J_2 \equiv \alpha J_1 \leq 1$
- Notice how we obtain (real) solutions, for a given model state, only for certain ranges of $\alpha \equiv J_2/J_1$, with termination points shown
- The energy and magnetic order parameter results clearly show the existence of a GS phase intermediate between the Néel and striped phases
- We can test for other orderings by measuring the response to a field operator $F \equiv \delta \hat{O}_F$ added to H, and calculating $e(\delta) \equiv E(\delta)/N$ for the perturbed Hamiltonian $H + F$. We then measure the response by the susceptibility :
  $\chi_F \equiv -\left.[\partial^2 e(\delta)]/(\partial\delta^2)\right|_{\delta=0}$

$s = \frac{1}{2}$ J_1–J_2–J_3 Model with $J_3 = J_2$: GS Energy ($J_1 \equiv 1$) for the Néel and Striped States

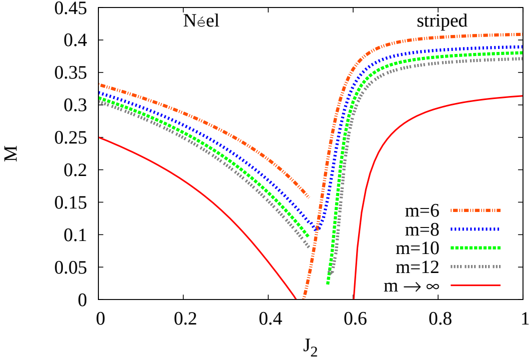
DJJF, RFB, PHYL, JR, CEC / PRB **84**, 012403 (2011)





$s = \frac{1}{2}$ J_1–J_2–J_3 Model with $J_3 = J_2$ ($J_1 \equiv 1$): Order Parameter for the Néel and Striped States

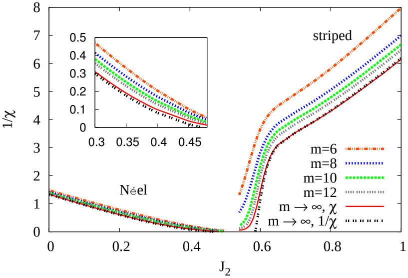
DJJF, RFB, PHYL, JR, CEC / PRB **84**, 012403 (2011)

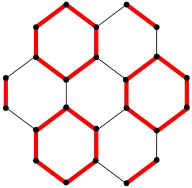


- Let us now test for PVBC order in the intermediate regime →

$s = \frac{1}{2}$ J_1–J_2–J_3 Model with $J_3 = J_2$: $1/\chi_p$ versus J_2 ($J_1 \equiv 1$) for the Néel and Striped States

DJJF, RFB, PHYL, JR, CEC / PRB **84**, 012403 (2011)





- Right: The perturbations (fields) $F = \delta\, \hat{O}_p$ for the plaquette susceptibility χ_p. Thick (red) and thin (black) lines correspond respectively to strengthened and weakened NN exchange couplings, where $\hat{O}_p = \sum_{\langle i,j \rangle} a_{ij} \mathbf{s}_i \cdot \mathbf{s}_j$, and the sum runs over all NN bonds, with $a_{ij} = +1$ and -1 for thick (red) and thin (black) lines respectively.
- LSUB∞ uses: $\chi_p^{-1}(m) = x_0 + x_1 m^{-2} + x_2 m^{-4}$ (to extrapolate LSUBm)

Intermediate Discussion

- The energy and order parameter results clearly show:
  - Néel ordering persists for $\frac{J_2}{J_1} \equiv \alpha < \alpha_{c_1} \approx 0.47$
  - Striped ordering exists only for $\alpha > \alpha_{c_2} \approx 0.60$
  - PVBC ordering appears to exist for $\alpha_{c_1} < \alpha < \alpha_{c_2}$

  compared to the direct classical phase transition between the Néel and striped AFM phases at $\alpha = 0.5$
- These results are confirmed from calculations of
  - Δ, triplet spin gap
  - ρ_s, spin stiffness coefficient
  - χ, zero-field, uniform transverse magnetic susceptibility

Reference

R.F. Bishop, P.H.Y. Li *et al.*, PRB **92**, 224434 (2015)

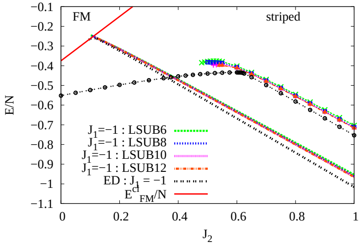
– and see Appendix for details

Completion of Phase Diagram

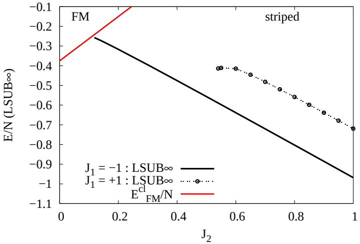
- We can also investigate the case $J_1 \equiv -1$ to examine the other boundary of the striped AFM phase
- Finally, we can also investigate the case $J_1 \equiv 1$ but with $J_2 < 0$ to examine the other boundary of the Néel AFM phase
- The classical FM state is also an eigenstate of the quantum Hamiltonian. Its GS energy is given by $\frac{E_{\mathrm{FM}}^{\mathrm{cl}}}{N} = s^2 \left(\frac{3}{2}J_1 + \frac{9}{2}J_2\right)$

$s = \frac{1}{2}$ J_1–J_2–J_3 Model with $J_3 = J_2$: GS energy ($J_1 \equiv -1$) vs J_2 for the Striped and FM States

PHYL, RFB, DJJF, JR, CEC / PRB **85**, 085115 (2012)



(a) LSUBm; $m = \{6, 8, 10, 12\}$ & ED



(b) LSUB∞

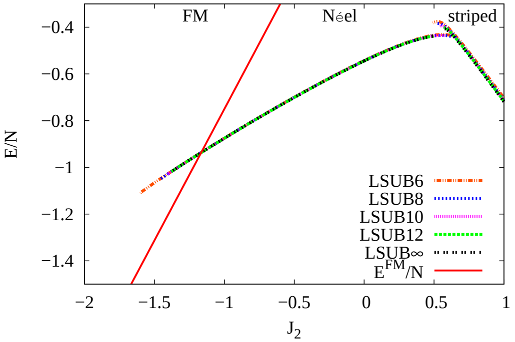
NOTE: Curves with symbols refer to the case $J_1 \equiv +1$, for comparison

There is clear evidence for either

- a direct first-order transition between the striped and FM phases at $\alpha \approx -0.10$, or
- an intervening phase in the very narrow range $-0.12 \lesssim \alpha \lesssim -0.10$ (c.f., the classical case of an intervening spiral phase in the larger range $-\frac{1}{5} < \alpha < -\frac{1}{10}$)

$s = \frac{1}{2}$ J_1–J_2–J_3 Model with $J_3 = J_2$: GS Energy ($J_1 \equiv 1$; $J_2 < 0$) for the Néel and Striped States

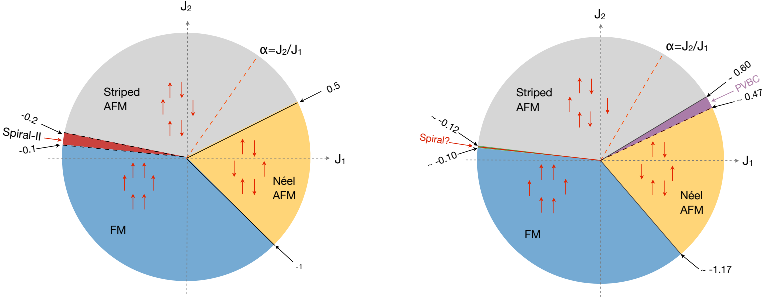
RFB, PHYL / PRB **85**, 155135 (2012)



- There is clear evidence for a direct first-order phase transition between the Néel and FM phases at $\alpha = -1.17 \pm 0.01$ (c.f., the classical value $\alpha = -1$)

$s = \frac{1}{2}$ J_1–J_2–J_3 Model ($J_3 = J_2$): Full Phase Diagram

RFB, PHYL / PRB **85**, 155135 (2012)



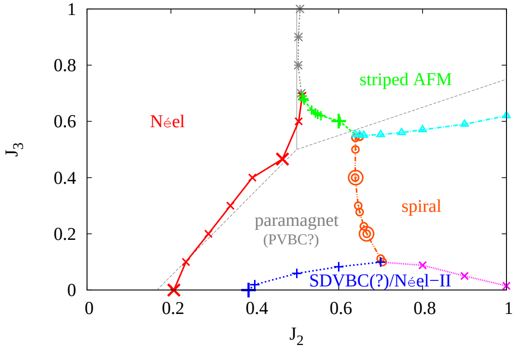
(a) Classical ($s \to \infty$)

(b) $s = \frac{1}{2}$

- The transition from Néel to PVBC order is a continuous (and hence deconfined) one
- The transition from PVBC to striped order is a first-order one
- The transitions from striped and Néel AFM order to FM order are both first-order ones

$s = \frac{1}{2}$ J_1–J_2–J_3 Model: Phase Diagram ($J_1 \equiv 1; 0 \leq J_2 \leq 1, 0 \leq J_3 \leq 1$)

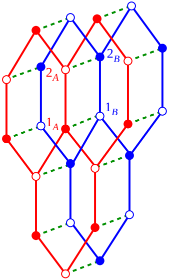
PHYL, RFB, DJJF, CEC / PRB **86**, 144404 (2012)

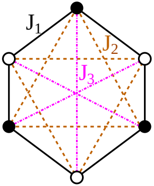


NOTE: c.f., the classical ($s \to \infty$) model has Néel, striped and spiral phases only, with phase boundaries shown by the light grey lines (dashed for continuous transitions and solid for first-order transition)

J_1–J_2–J_3–$J_1^\perp$ Model on the Honeycomb Bilayer Lattice

- J_1–J_2–J_3–$J_1^\perp$ model on the honeycomb bilayer lattice (i.e., all bonds of Heisenberg type) – now 4 sites per unit cell: 1_A, 2_A, 1_B, 2_B as shown
- We'll look at the case with $s = \frac{1}{2}$ spins (viz., the most quantum case)
- $H = J_1 \sum_{\langle i,j \rangle, \alpha} \mathbf{s}_{i,\alpha} \cdot \mathbf{s}_{j,\alpha} + J_2 \sum_{\langle\langle i,k \rangle\rangle, \alpha} \mathbf{s}_{i,\alpha} \cdot \mathbf{s}_{k,\alpha} + J_3 \sum_{\langle\langle\langle i,l \rangle\rangle\rangle, \alpha} \mathbf{s}_{i,\alpha} \cdot \mathbf{s}_{l,\alpha} + J_1^\perp \sum_i \mathbf{s}_{i,A} \cdot \mathbf{s}_{i,B}$
  (where $\alpha = A, B$ labels the two layers, and set $J_1 \equiv 1$)





- - - - = $J_1^\perp$: NN interlayer bond

on both layers $\alpha = A, B$

J_1–J_2–J_3–$J_1^{\perp}$ Model on the Honeycomb Bilayer ($s = \frac{1}{2}$)

- We have investigated several special cases for this model
- Results include
  - The case when $J_3 = J_2 \equiv \alpha J_1 > 0$; $J_1 > 0$, $J_1^{\perp} \equiv \delta J_1 > 0$, for which we have investigated the stability of the Néel and striped phases in the α–δ plane

    Reference

    R.F. Bishop and P.H.Y. Li, unpublished (2017)
  - The case when $J_3 = 0$ (i.e., the J_1–J_2–$J_1^{\perp}$ model); $J_1 > 0$, $J_2 \equiv \kappa J_1 > 0$, $J_1^{\perp} \equiv \delta J_1 > 0$, for which we have investigated the stability of the Néel phase in the κ–δ plane

    Reference

    R.F. Bishop and P.H.Y. Li, eprint arXiv:1611.03287 (2016)

Limiting Cases

- limiting bond cases
  - $J_1^{\perp} = 0$: two uncoupled honeycomb monolayers
  - $J_1^{\perp} \to \infty$: with finite J_1, J_2, J_3; NN interlayer pairs form spin-singlet dimers $\Longrightarrow$
    GS is a nonclassical interlayer dimer valence-bond crystal (IDVBC),

$$\frac{E}{N} \xrightarrow[J_1^{\perp} \to \infty]{} \frac{E^{\mathrm{IDVBC}}}{N} = -\frac{1}{2}s(s+1)J_1^{\perp}$$

(s = spin quantum number)

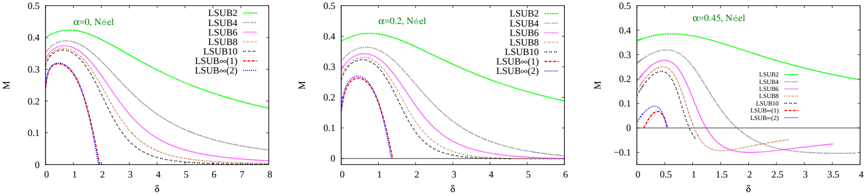
RESULTS II: Bilayer with $J_1 \equiv +1$; $J_3 = J_2$

- We study the case $J_1 \equiv +1$; $0 \leq J_3 = J_2 \equiv \alpha J_1 \leq 1$; $J_1^{\perp} \equiv \delta J_1 \geq 0$
- As before for the monolayer we obtain real solutions, for a given model state (i.e., Néel or striped), only for certain regions in the α–δ phase space
- We have calculated E/N, M as before
- We have also calculated
  - the triplet spin gap Δ (i.e., the excitation energy from the GS to the lowest-lying $s = 1$ excited state)
  - the zero-field uniform transverse magnetic susceptibility, χ [i.e., put system in a transverse magnetic field h, in units where $g\mu_B/\hbar = 1$, and calculate $\chi(h) = -\frac{1}{N}\mathrm{d}^2E/\mathrm{d}h^2$; $\quad \chi \equiv \chi(0)$]

$s = \frac{1}{2}$ J_1–J_2–J_3–$J_1^{\perp}$ Honeycomb Bilayer Model with $J_3 = J_2$ ($J_1 \equiv 1$): Order Parameter for the Néel State

RFB, PHYL / unpublished (2017)

- $\delta \equiv J_1^{\perp}/J_1;\quad \alpha \equiv J_3/J_1 (= J_2/J_1)$



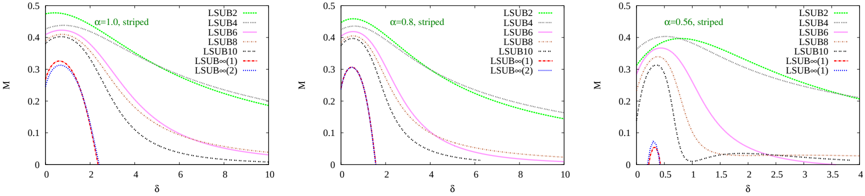
NOTE: LSUB$\infty(i)$ extrapolations are based on LSUBm data sets with

- $m = \{2, 6, 10\}$ for $i = 1$
- $m = \{4, 6, 8, 10\}$ for $i = 2$

$s=\frac{1}{2}$ J_1–J_2–J_3–$J_1^{\perp}$ Honeycomb Bilayer Model with $J_3=J_2$ ($J_1\equiv 1$): Order Parameter for the Striped State

RFB, PHYL / unpublished (2017)

- $\delta \equiv J_1^{\perp}/J_1$; $\alpha \equiv J_3/J_1 (= J_2/J_1)$



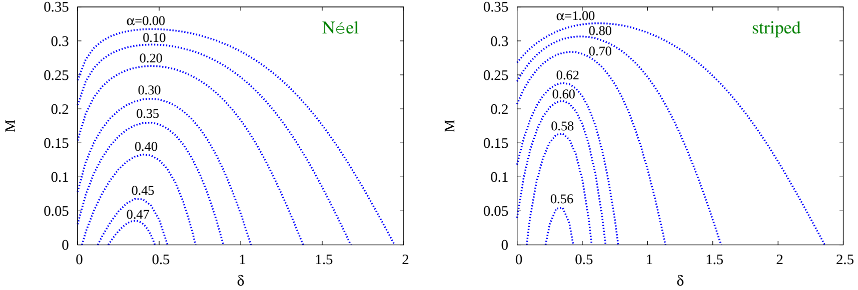
NOTE: LSUB∞(i) extrapolations are based on LSUBm data sets with

- $m=\{2,6,10\}$ for $i=1$
- $m=\{4,6,8,10\}$ for $i=2$

$s = \frac{1}{2}$ J_1–J_2–J_3–$J_1^{\perp}$ Honeycomb Bilayer Model with $J_3 = J_2$ ($J_1 \equiv 1$): Extrapolated Order Parameter for the Néel and Striped States

RFB, PHYL / unpublished (2017)

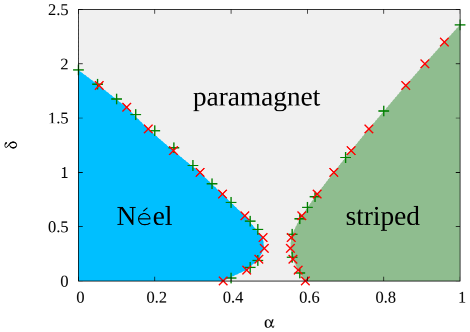
- $\delta \equiv J_1^{\perp}/J_1$; $\alpha \equiv J_3/J_1 (= J_2/J_1)$



NOTE: LSUB∞ extrapolations are based on LSUBm data sets with $m = \{2, 6, 10\}$

$s = \frac{1}{2}$ J_1–J_2–J_3–$J_1^{\perp}$ Model: Phase Diagram ($J_3 = J_2 \equiv \alpha J_1 > 0$; $J_1^{\perp} \equiv \delta J_1 > 0$; $J_1 \equiv 1$)

RFB, PHYL / unpublished (2017)



NOTE:

- LSUB∞ extrapolations are based on LSUBm data sets with $m = \{2, 6, 10\}$
- The red cross ($\times$) symbols and the green plus ($+$) symbols are points at which the extrapolated GS magnetic order parameter M for the Néel and striped phases vanishes, for specified values of δ and α, respectively

Discussion

- Both the Néel and striped AFM phases exhibit reentrant regimes
- The phase boundaries of the two quasiclassical AFM phases exhibit a prototypical avoided crossing behaviour
- The paramagnetic regime is likely to contain a mixture (at least) of phases with IDVBC order and PVBC order in both layers separately

Summary

- In conclusion, we know of no more powerful nor more accurate method than the CCM for dealing with these strongly correlated and highly frustrated 2D spin-lattice models of quantum magnets, such as the honeycomb examples used here for an illustration
- By now, we have used the CCM for many other spin-lattice models. Some other typical examples are:
  - the J_1–J_2 model on the Union Jack lattice
  - the J_1–J_2 model on the checkerboard lattice
  - other similar depleted J_1–J_2 models on the square lattice
  - other models that interpolate between various lattices, e.g.,

    (a) kagome-triangle; (b) kagome-square;
    (c) square-triangle; (d) hexagon-square
- There are now $\gtrsim$ 125 papers using the CCM for spin lattices

Acknowledgements

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- Minnesota Supercomputing Institute — for a generous grant of supercomputing facilities
- The Leverhulme Trust — for supporting RFB with a Leverhulme Emeritus Fellowship

THANK YOU FOR YOUR ATTENTION!

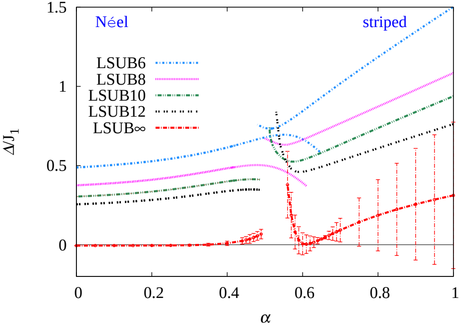
For Further Reading

Some references for the CCM methodology and applications

- R. F. Bishop and H. G. Kümmel, Phys. Today **40**(3), 52 (1987)
- R. F. Bishop, Theor. Chim. Acta **80**, 95 (1991)
- R. F. Bishop, in *Microscopic Quantum Many-Body Theories and Their Applications*, (eds., J. Navarro and A. Polls), Lecture Notes in Physics Vol. **510**, Springer-Verlag, Berlin (1998), 1
- D. J. J. Farnell and R. F. Bishop, in *Quantum Magnetism*, (eds., U. Schollwöck, J. Richter, D. J. J. Farnell and R. F. Bishop), Lecture Notes in Physics Vol. **645**, Springer-Verlag, Berlin (2004), 307

$s = \frac{1}{2}$ J_1–J_2–J_3 Model with $J_3 = J_2 \equiv \alpha J_1$ ($J_1 > 0$): Triplet Spin Gap

RFB, PHYL, OG, JR, CEC / PRB **92**, 224434 (2015)

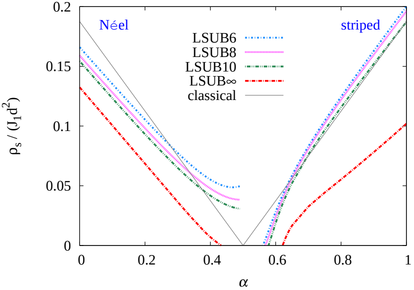


- LSUB∞ uses: $\Delta(m) = d_0 + d_1 m^{-1} + d_2 m^{-2}$ (to extrapolate LSUBm)

$s = \frac{1}{2}$ J_1–J_2–J_3 Model with $J_3 = J_2 \equiv \alpha J_1$ $(J_1 > 0)$: Spin Stiffness Coefficient

RFB, PHYL, OG, JR, CEC / PRB **92**, 224434 (2015)

- Impose a twist θ per unit length ($d \equiv$ honeycomb lattice spacing) to a quasiclassical state
  $\frac{E(\theta)}{N} = \frac{E(\theta=0)}{N} + \frac{1}{2}\rho_s\theta^2 + O(\theta^4)$
  $\rho_s =$ spin stiffness coefficient

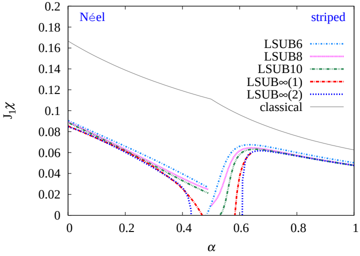


- LSUB∞ uses: $\rho_s(m) = s_0 + s_1 m^{-1} + s_2 m^{-2}$ (to extrapolate LSUBm)

$s = \frac{1}{2}$ J_1–J_2–J_3 Model with $J_3 = J_2 \equiv \alpha J_1$ $(J_1 > 0)$: Zero-Field Transverse Magnetic Susceptibility

RFB, PHYL, OG, JR, CEC / PRB **92**, 224434 (2015)

- Put z_s-aligned system in a transverse magnetic field $\mathbf{h} = h\hat{x}_s$ (in units where $g\mu_B/\hbar = 1$): $H \rightarrow H(h) = H(0) - h\sum_i s_i^x$
  $\frac{E(h)}{N} = \frac{E(h{=}0)}{N} - \frac{1}{2}\chi h^2 + O(h^4)$
  $\chi =$ zero-field, uniform, transverse magnetic susceptibility



- LSUB∞(1) uses: $\chi(m) = x_0 + s_1 m^{-1} + x_2 m^{-2}$ (to extrapolate LSUBm)
- LSUB∞(2) uses: $\chi(m) = \bar{x}_0 + \bar{x}_1 m^{-\nu}$ (to extrapolate LSUBm)

$s = \frac{1}{2}$ J_1–J_2–J_3 Model with $J_3 = J_2 \equiv \alpha J_1$ ($J_1 > 0$): Discussion

- The extrapolated curves for Δ show clear evidence of a gapped state between the Néel and striped phases (i.e., consistent with our previous identification of a PVBC intermediate state)
- Points where $\rho_s \rightarrow 0$ are clear signals of a magnetic phase losing its stability
- Points where $\chi \rightarrow 0$ are clear signals of the opening up of a gapped state (c.f., the classical transition from Néel to striped)
- Each of the curves for Δ, ρ_s and χ yields corresponding QCPs to those found from the previous curves for M