HIGHLY FRUSTRATED SPIN-LATTICE MODELS OF MAGNETISM AND THEIR QUANTUM PHASE TRANSITIONS:

A Microscopic Treatment Via The Coupled Cluster Method

by

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OUTLINE

- An Illustrative Model: J_1–J_2–J_3 model on the honeycomb lattice
- The Coupled Cluster Method
- Results on the Honeycomb Lattice:
  - The spin-1/2 J_1–J_2–J_3 Heisenberg model
  - The spin-1/2 J_1^{XX}–J_2^{XX} model (i.e., isotropic J_1–J_2 XY model)
  - The spin-1/2 J_1^{XXZ}–J_2^{XXZ} model

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References

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

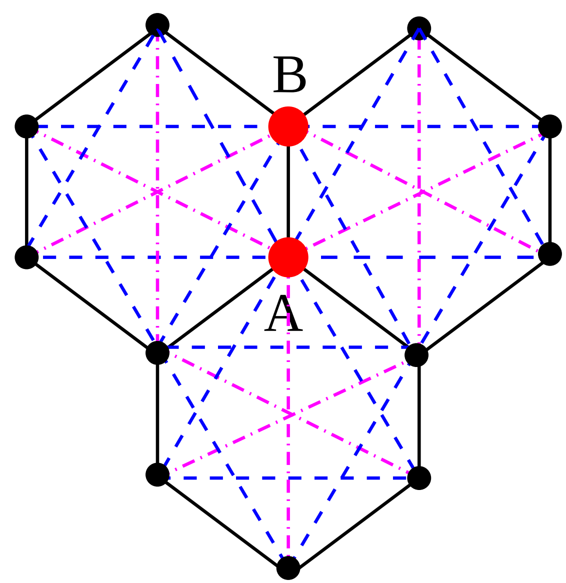
R.F. Bishop, P.H.Y. Li and C.E. Campbell, PRB **89**, 214413 (2014)

P.H.Y. Li, R.F. Bishop and C.E. Campbell, PRB **89**, 220408(R) (2014)

AN ILLUSTRATIVE MODEL: J_1–J_2–J_3 Model on the Honeycomb 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 $J_1 \equiv 1$)

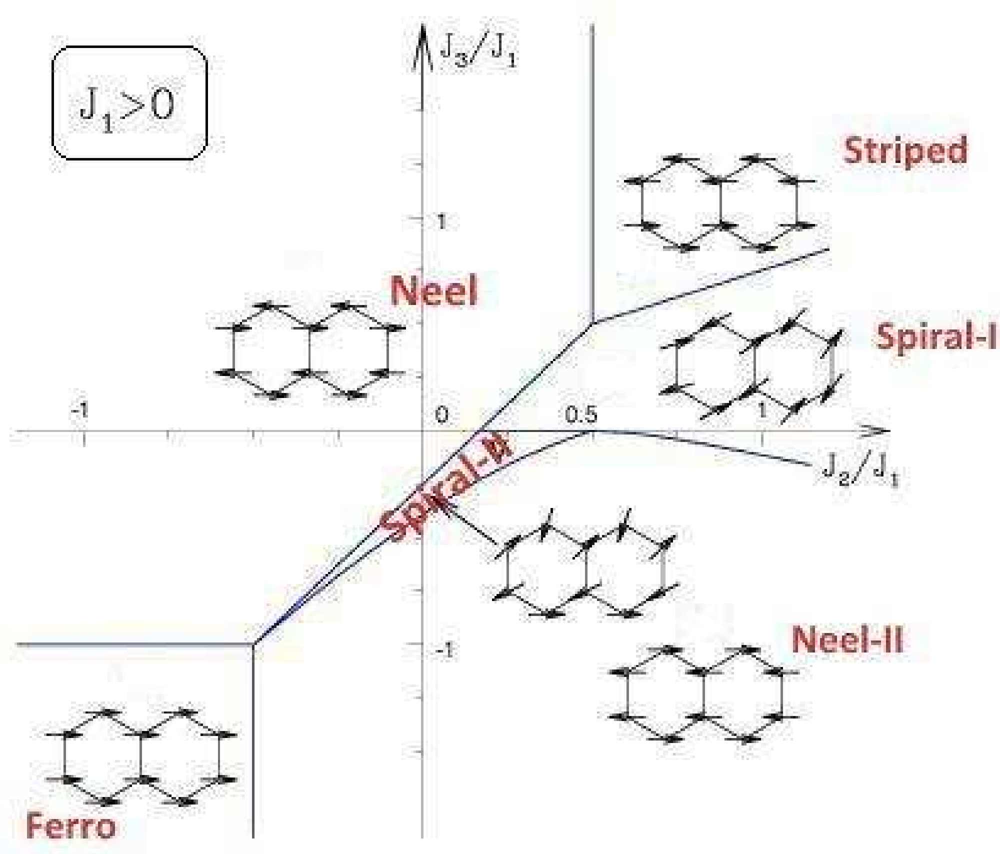
  where, on the honeycomb lattice:
  - $\langle i,j \rangle$ bonds $J_1 \equiv$ ——— all NN bonds
  - $\langle\langle i,k \rangle\rangle$ bonds $J_2 \equiv$ - - - - - all NNN bonds
  - $\langle\langle\langle i,l \rangle\rangle\rangle$ bonds $J_3 \equiv$ - · - · - all NNNN bonds



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 ($s \rightarrow \infty$)
  - 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., $J_1 \rightleftharpoons -J_1$; $J_3 \rightleftharpoons -J_3$; $\mathbf{s}_i{}^{\mathrm{B}} \rightleftharpoons -\mathbf{s}_i{}^{\mathrm{B}}$)

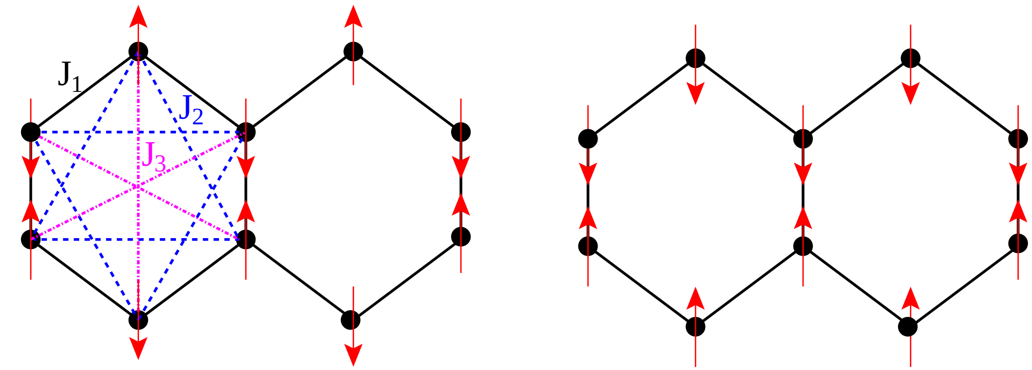
J_1–J_2–J_3 Honeycomb Model ($s \to \infty$): Classical Phase Diagram ($J_1 > 0$)



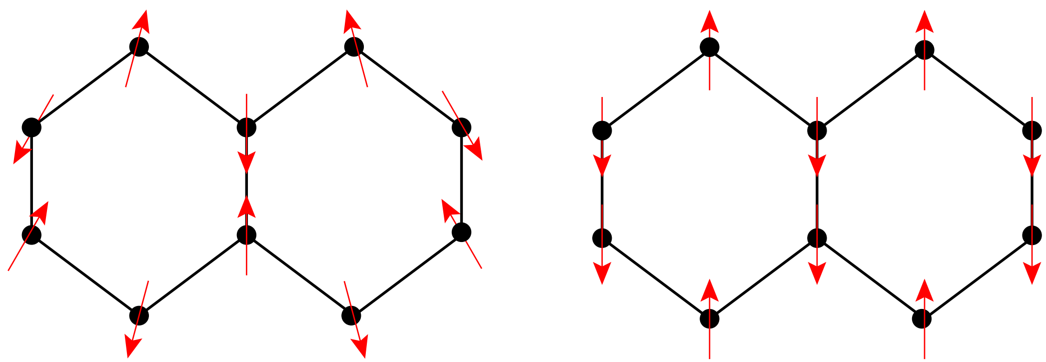
Classical J1-J2-J3 Model on the Honeycomb Lattice

NOTE: 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

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



(a) Néel (b) Striped



(c) Spiral-I (d) Néel-II

THE COUPLED CLUSTER METHOD

We use the coupled cluster method (CCM)

- ground-state (GS) wavefunction:

$$|\Psi\rangle = \mathrm{e}^{S}|\Phi\rangle; \;\; \langle\tilde{\Psi}| = \langle\Phi|\tilde{S}\mathrm{e}^{-S}; \;\; \langle\tilde{\Psi}|\Psi\rangle = \langle\Phi|\Psi\rangle = \langle\Phi|\Phi\rangle \equiv 1$$

$$S = \sum_{I\neq 0}\mathcal{S}_I C_I^{+}; \qquad \tilde{S} = 1 + \sum_{I\neq 0}\tilde{\mathcal{S}}_I C_I^{-}$$

$$C_0^{+} \equiv 0; \qquad C_I^{-} \equiv (C_I^{+})^{\dagger}; \qquad C_I^{-}|\Phi\rangle = 0, \; \forall I \neq 0$$

- $C_I^{+}|\Phi\rangle$ 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
- $\Rightarrow C_I^{+} \rightarrow s_{i_1}^{+}s_{i_2}^{+}\cdots s_{i_k}^{+}; \qquad s_j^{+} \equiv s_j^{x} + is_j^{y},$ in local axes

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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
- CCM satisfies the Goldstone linked cluster theorem and
- satisfies the Hellmann-Feynman theorem, for all truncations on complete set $\{I\}$
- solve for $\{\mathcal{S}_I, \tilde{\mathcal{S}}_I\}$ from GS Schrödinger eqs. for $|\Psi\rangle$, $\langle\tilde{\Psi}|$
- 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 $|\Phi\rangle$

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CCM Truncation Schemes

- only approximation is to truncate set $\{I\}$
  - for $s = \frac{1}{2}$ case we 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 $s = 1$ case we use the 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$m \equiv$ SUB$2sm$–m for general spin-s case, e.g., 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

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RESULTS I

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

- We have done a large study of this model
- Results include:
  - The case when $J_3 = J_2$ for which we investigate 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)
  - The case when $J_3 = 0$ (i.e., the J_1–J_2 model); $J_1 > 0, J_2 > 0$

    Reference

    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

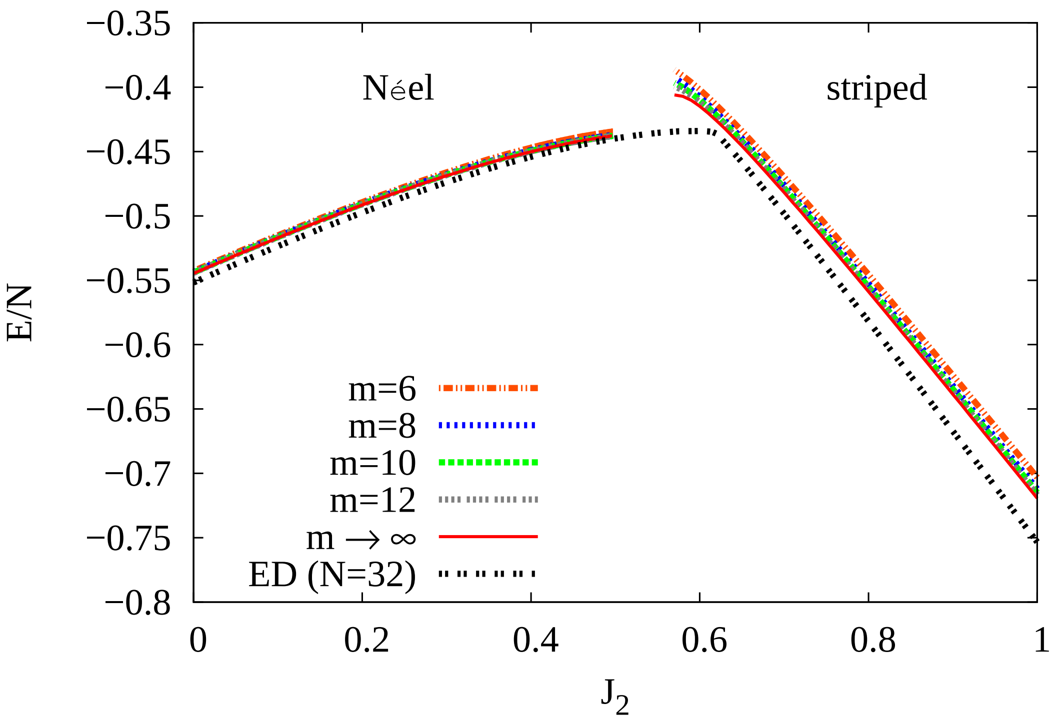
    P.H.Y. Li *et al.*, PRB **86**, 144404 (2012)

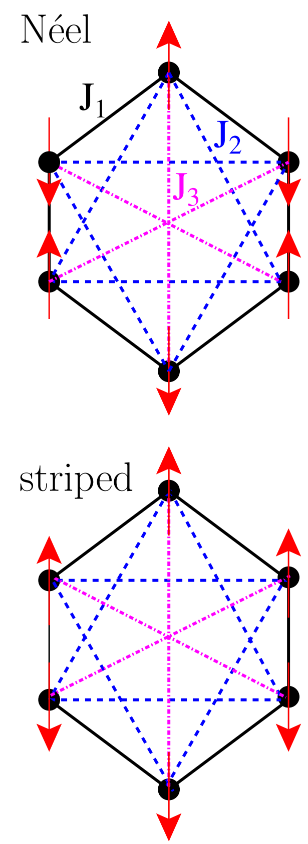
RESULTS I: The Case when $J_1 \equiv +1$; $J_3 = J_2$

- The $s = \frac{1}{2}$ J_1–J_2–J_3 Model on the Honeycomb Lattice (with $J_3 = J_2$)
  - 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

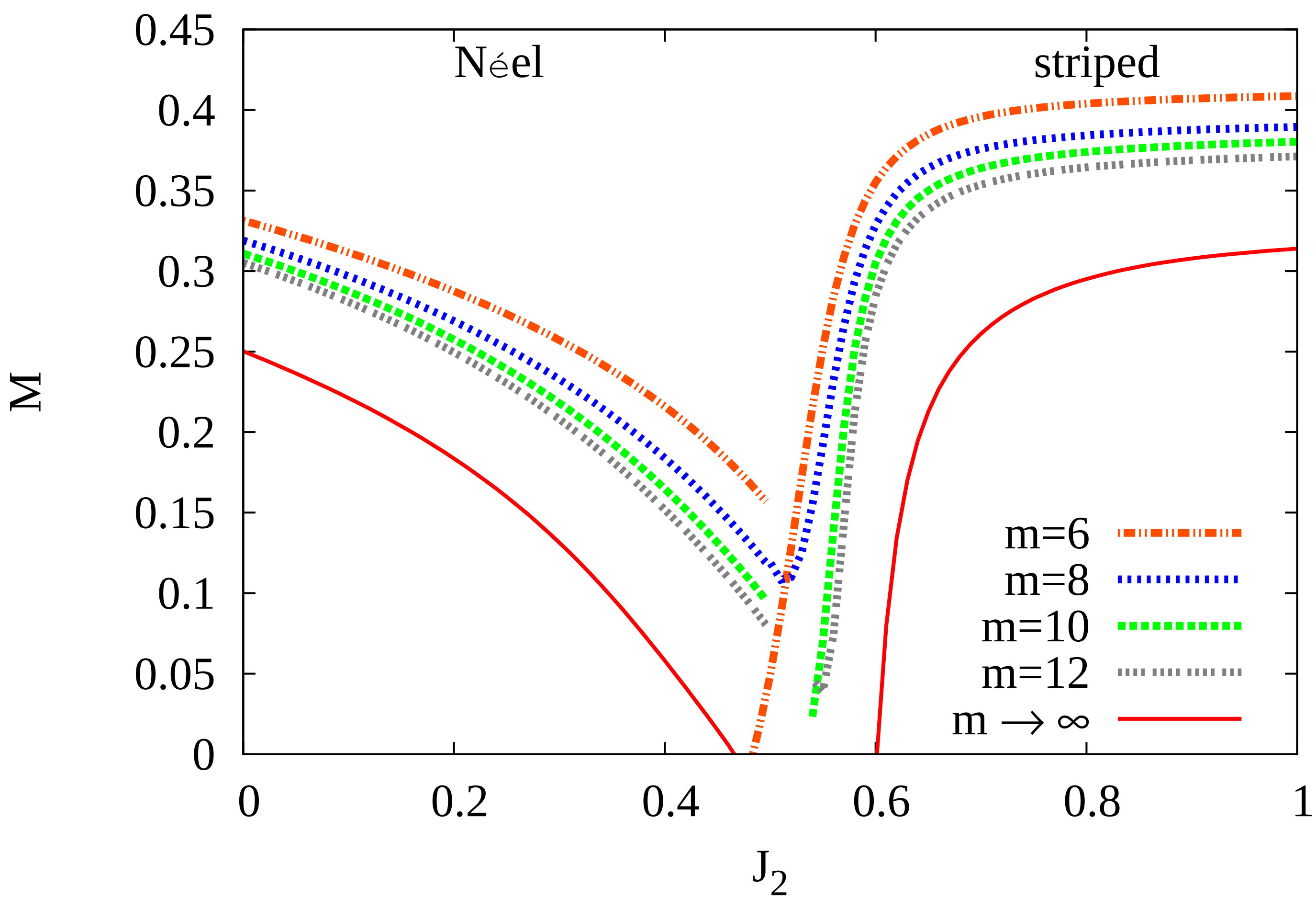
DJJF, RFB, PHYL, JR, CEC / PRB **84**, 012403 (2011)





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

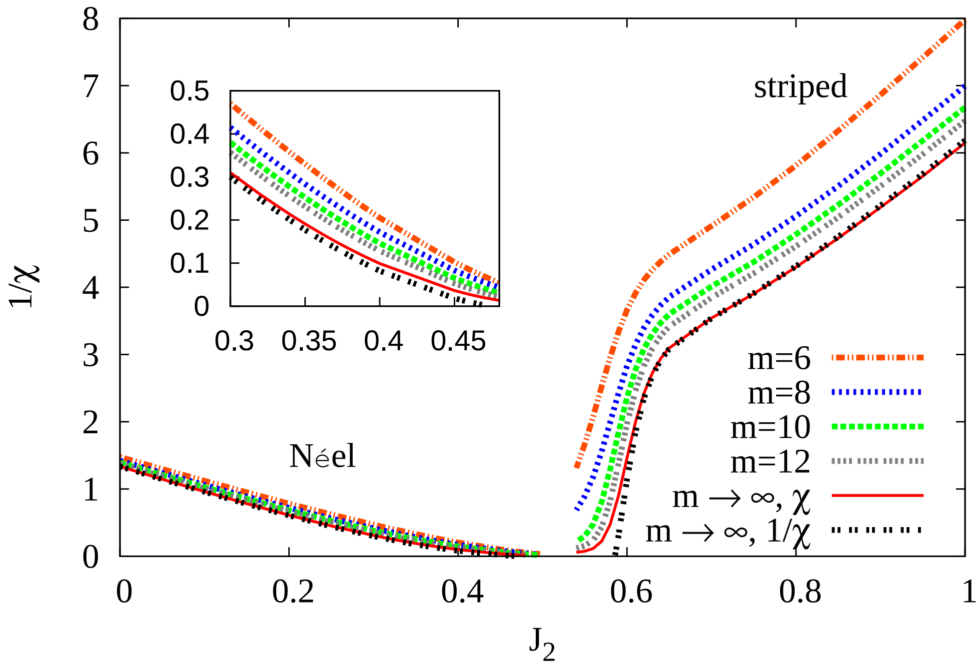
DJJF, RFB, PHYL, JR, CEC / PRB **84**, 012403 (2011)

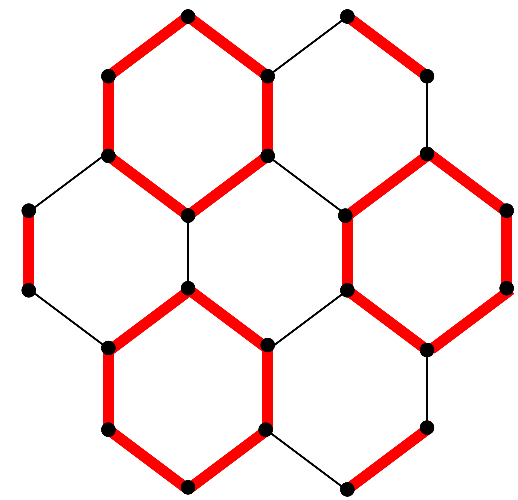


- Let us now test for PVBC order in the intermediate regime →

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

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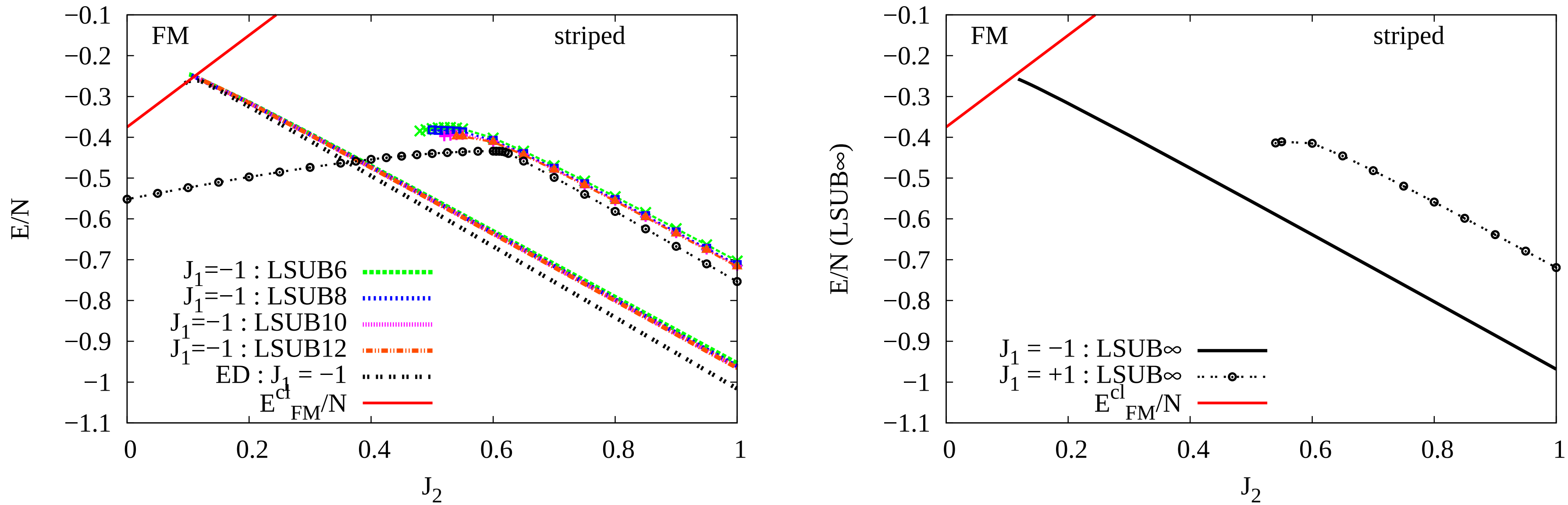
Intermediate Results

- 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 $\alpha = 0.5$
- 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 $\frac{E^{\text{cl}}_{\text{FM}}}{N} = s^2 \left(\frac{3}{2}J_1 + \frac{9}{2}J_2\right)$

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



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

(b) LSUB∞

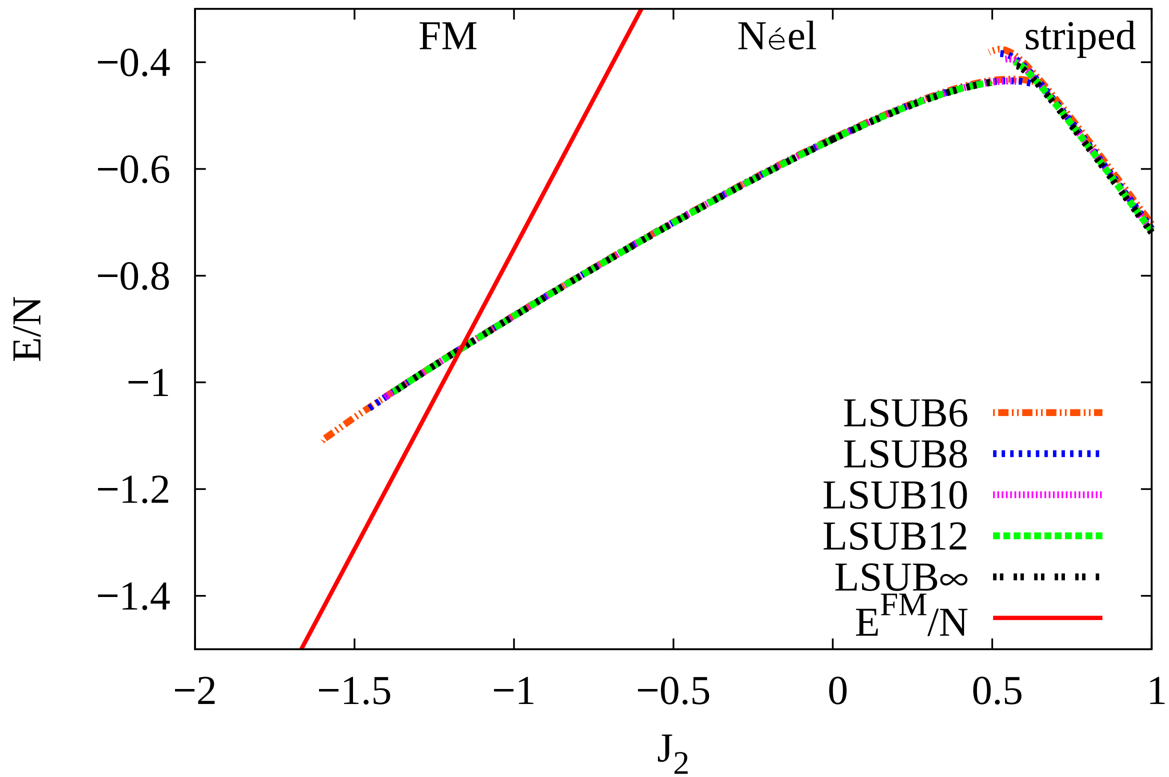
NOTE: Curves with symbols refer to the case $J_1 \equiv +1$, for comparison

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 $-\frac{1}{5} < \alpha < -\frac{1}{10}$

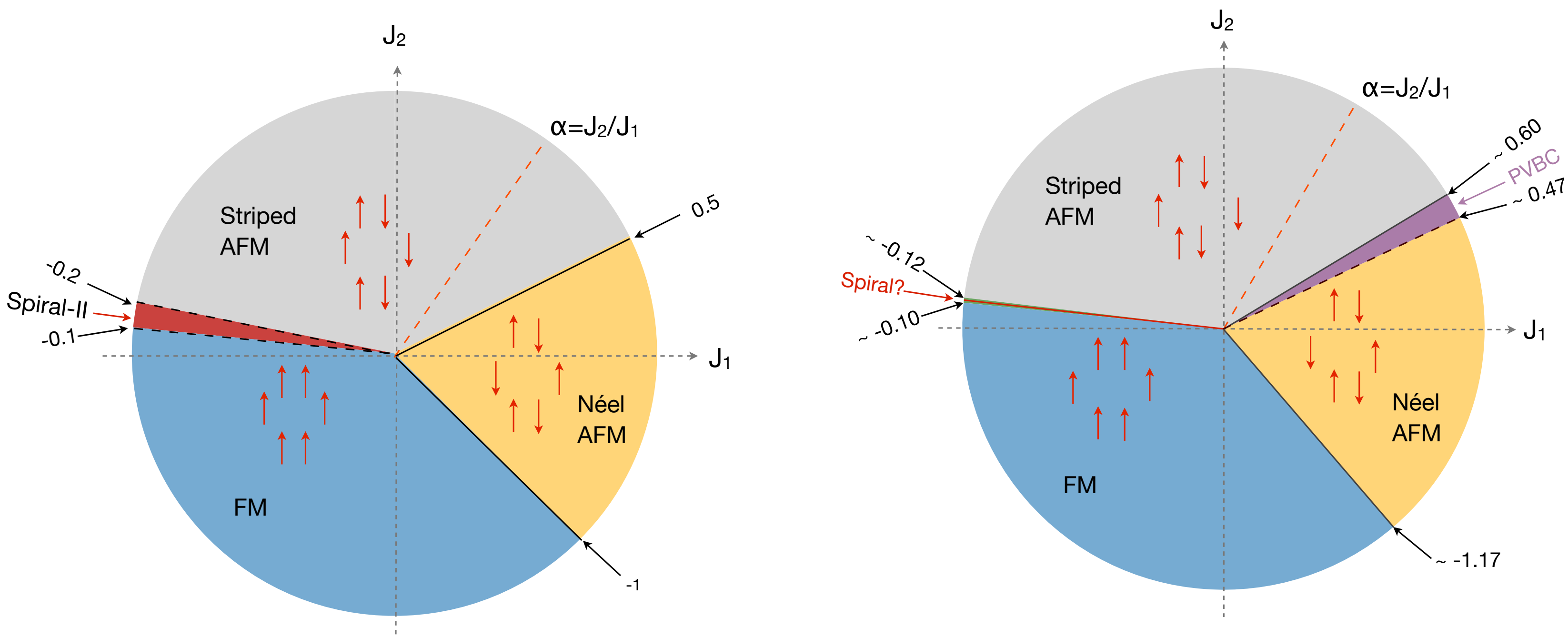
RFB, PHYL / PRB **85**, 155135 (2012)



- 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 with $J_3 = J_2$: 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

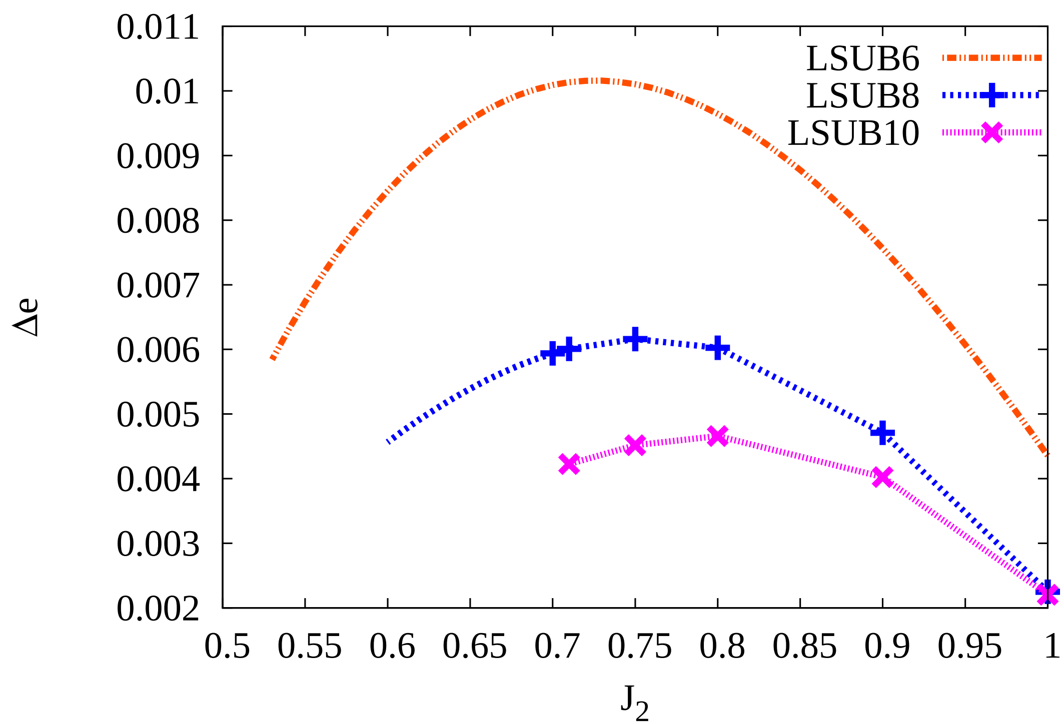
RESULTS I: The Case $J_3 = 0$ (i.e., the J_1–J_2 Model); $J_1 > 0$, $0 \leq x \equiv J_2/J_1 \leq 1$

▶ The $s = \frac{1}{2}$ J_1–J_2 Model on the Honeycomb Lattice (i.e., $J_3 = 0$)

- We now use the classical Néel, spiral-I and Néel-II states as our CCM model states
- for $|\Phi\rangle = |\Phi_{\text{spiral}}\rangle$ we treat pitch angle ϕ as a variable and choose ϕ such that $E_{\text{LSUB}m}(\phi) =$ min at $\phi = \phi_{\text{LSUB}m}$
- The energy and magnetic order parameter results clearly show the existence of a GS phase intermediate between the Néel and Néel-II phases

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

RFB, PHYL, DJJF, CEC / JPCM **24**, 236002 (2012)



- We plot $\Delta e \equiv e^{\text{spiral}} - e^{\text{N-II}}$ where $e \equiv E/N$
- There is clear evidence that quantum fluctuations stabilize the collinear Néel-II order for a considerable range of $x \equiv J_2/J_1 \lesssim 1$
- c.f., the classical case where the spiral state is the GS phase for all $x \geq \frac{1}{6}$

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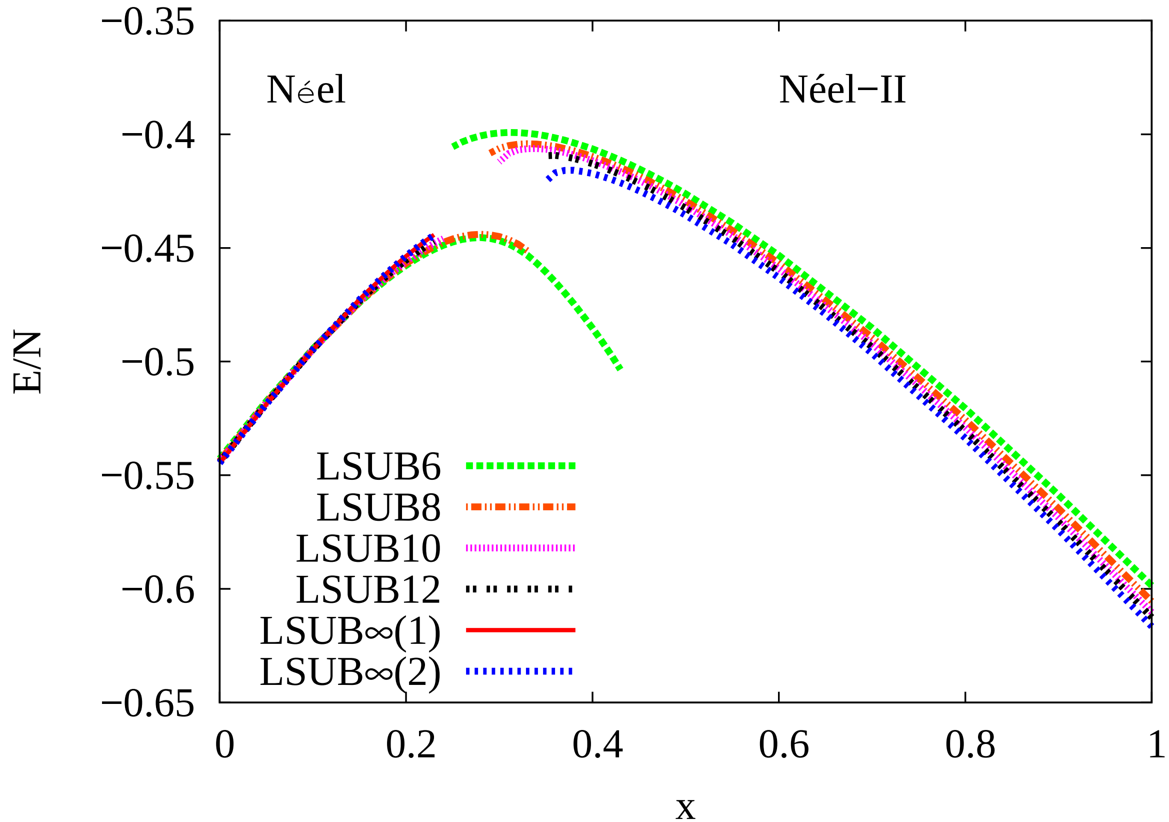
$s = \frac{1}{2}$ J_1–J_2 Model: GS Energy ($J_1 \equiv 1$) for the Néel and Néel-II States

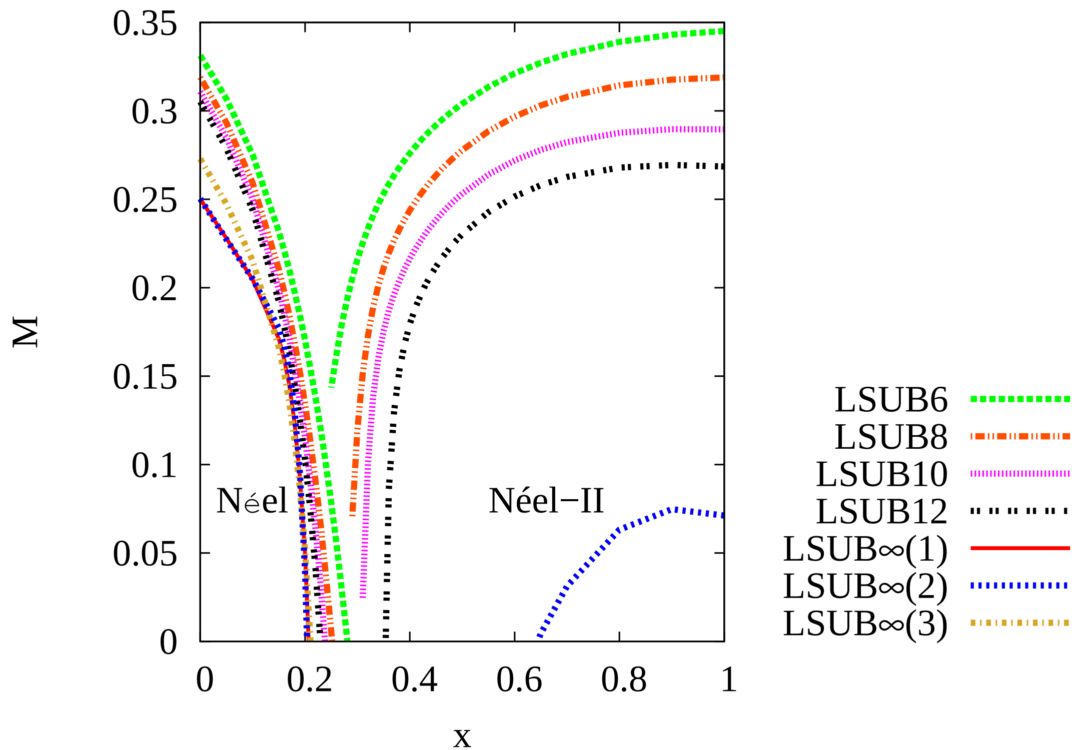
RFB, PHYL, CEC / JPCM **25**, 306002 (2013)



- LSUB∞(1) uses the data set $m = \{6, 8, 10, 12\}$
- LSUB∞(2) uses the data set $m = \{8, 10, 12\}$

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

RFB, PHYL, CEC / JPCM **25**, 306002 (2013)



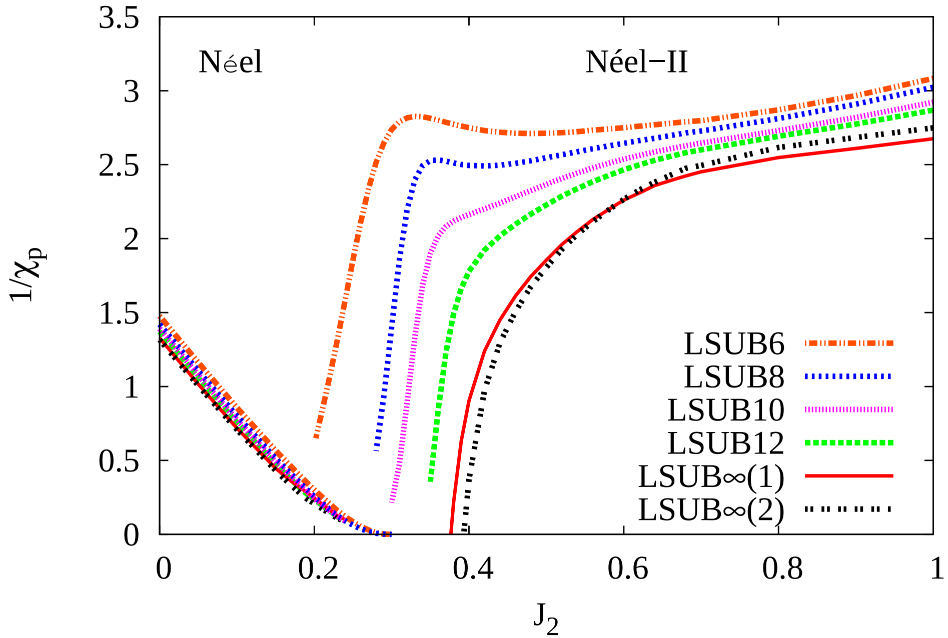
- LSUB∞(1) uses the data set $m = \{6, 8, 10, 12\}$ with $M = b_0 + b_1 m^{-0.5} + b_2 m^{-1.5}$
- LSUB∞(2) uses the data set $m = \{8, 10, 12\}$ with $M = b_0 + b_1 m^{-0.5} + b_2 m^{-1.5}$
- LSUB∞(3) uses the data set $m = \{6, 8, 10, 12\}$ with $M = b_0 + b_1 m^{-1} + b_2 m^{-2}$

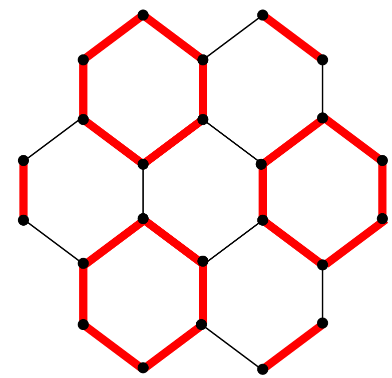
Intermediate Results

- The energy and order parameter results clearly show:
  - Néel ordering persists for $\frac{J_2}{J_1} \equiv x < x_{c_1} = 0.207 \pm 0.003$
  - Néel-II ordering exists only for $x > x_{c_2} = 0.385 \pm 0.010$
  - A phase intermediate between the Néel and Néel-II phases in the range $x_{c_1} < x < x_{c_2}$
- The Néel-II order parameter results give preliminary evidence that Néel-II order is unstable in the range $x_{c_2} < x < x_{c_3} \approx 0.65$
- Our previous results for the J_1–J_2–J_3 model suggest a PVBC-ordered GS as a candidate in the range $x_{c_1} < x < x_{c_2}$
- For the range $x_{c_2} < x < x_{c_3}$ the order parameter results suggest a GS phase that breaks the same symmetries as the Néel-II state: an obvious candidate is the SDVBC state
- We test the susceptibility of both phases to each of these VBC states

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

RFB, PHYL, DJJF, CEC / JPCM **24**, 236002 (2012)





- 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: $\chi_p^{-1}(m)=x_0+x_1m^{-2}+x_2m^{-4}$ (to extrapolate LSUBm)
- LSUB∞(1) uses the data set $m=\{6,8,10,12\}$ and LSUB∞(2) uses $m=\{8,10,12\}$

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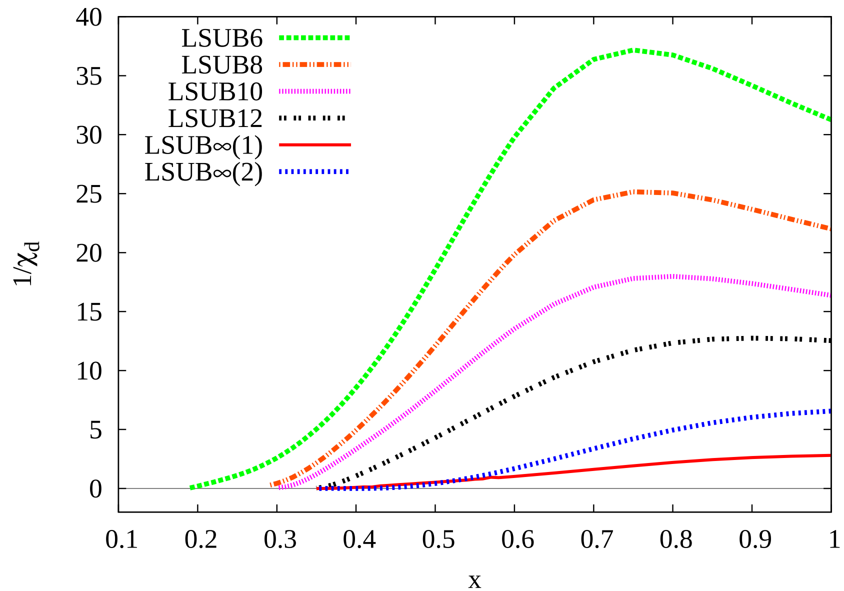
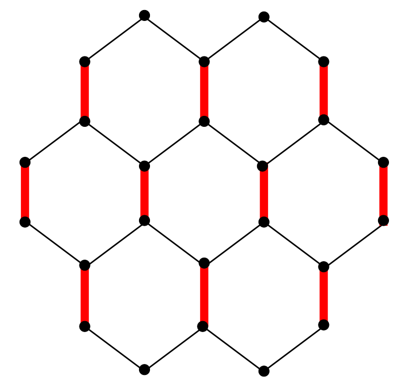
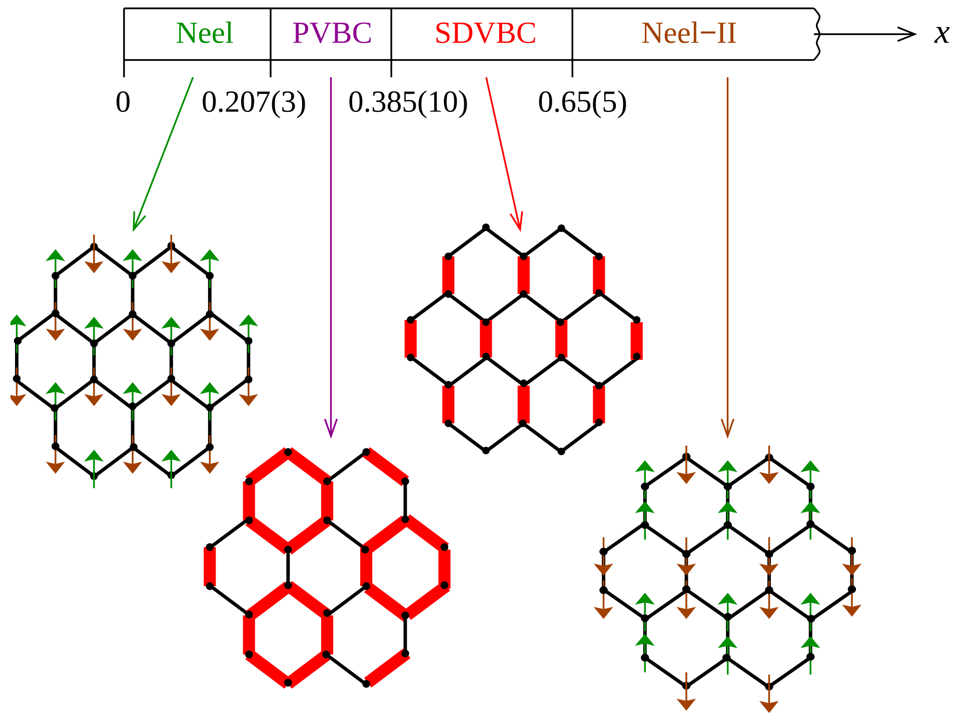




- Right: The perturbations (fields) $F = \delta\, \hat{O}_d$ for the staggered dimer susceptibility χ_d. Thick (red) and thin (black) lines correspond respectively to strengthened and unaltered NN exchange couplings, where $\hat{O}_d = \sum_{\langle i,j \rangle} a_{ij} \mathbf{s}_i \cdot \mathbf{s}_j$, and the sum runs over all NN bonds, with $a_{ij} = +1$ and 0 for thick (red) and thin (black) lines.
- LSUB∞ results for χ_d are based on fitting the LSUBm perturbed energies as $e^{(m)}(\delta) = e_0(\delta) + e_1(\delta) m^{-\nu}$
- LSUB∞(1) uses data set $m = \{6, 8, 10, 12\}$ and LSUB∞(2) uses $m = \{8, 10, 12\}$

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

RFB, PHYL, CEC / JPCM **25**, 306002 (2013)



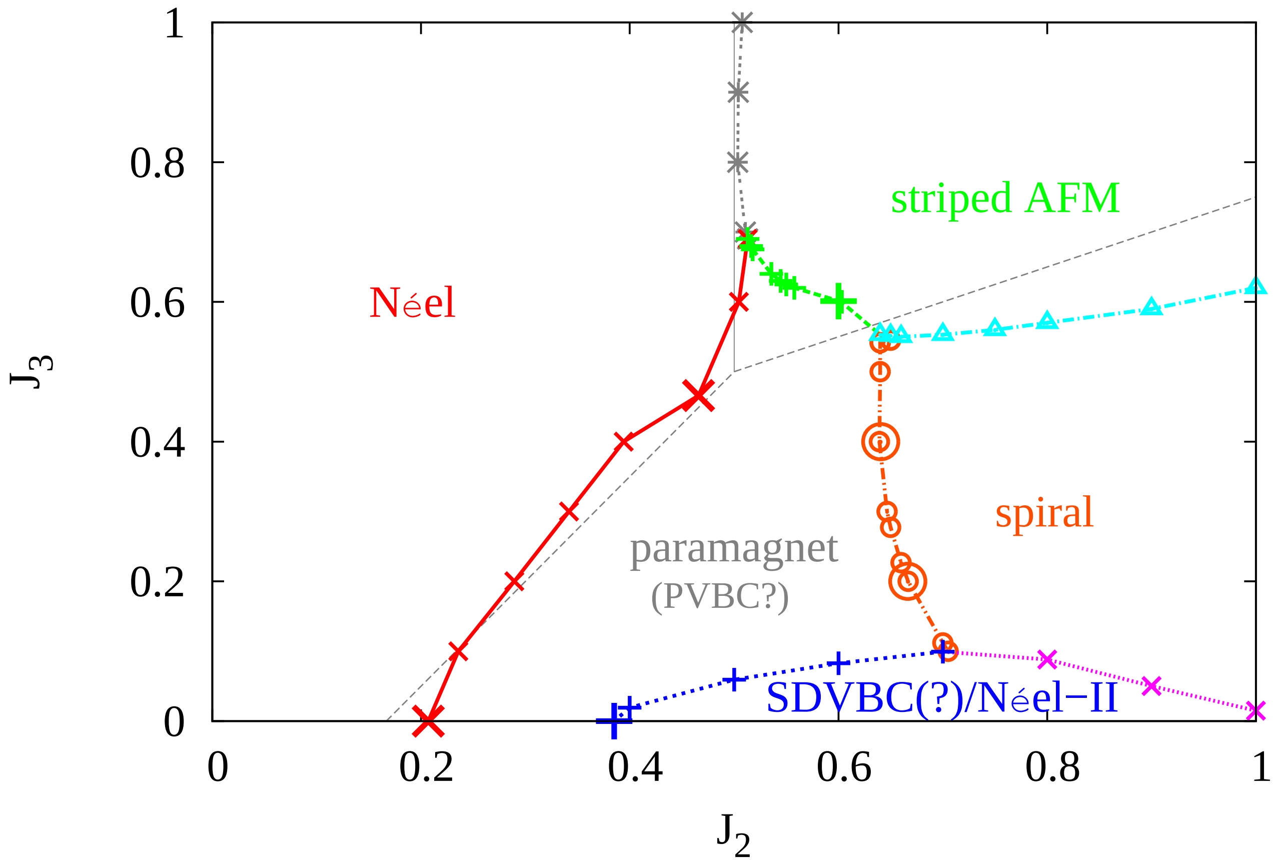
- The quantum critical points are at $x_{c_1} \approx 0.207(3)$, $x_{c_2} \approx 0.385(10)$, and $x_{c_3} \approx 0.65(5)$
- At some value $x_{c_4} > 1$ there will be a 4th QCP to a spiral phase
- c.f., the classical ($s \to \infty$) model with $J_1 > 0$ has a single QCP at $x_{\rm cl} = \frac{1}{6}$ from Néel order ($0 < x < \frac{1}{6}$) to spiral-I order (for all $x > \frac{1}{6}$)

▶ The Full J_1–J_2–J_3 Model on the Honeycomb Lattice

- We now use the classical Néel, striped, spiral-I and Néel-II states as our CCM model states
- for $|\Phi\rangle = |\Phi_{\rm spiral}\rangle$ we treat pitch angle ϕ as a variable and choose ϕ such that $E_{{\rm LSUB}m}(\phi) =$ min at $\phi = \phi_{{\rm LSUB}m}$
- The energy and magnetic order parameter results clearly show the existence of a paramagnetic phase intermediate between the Néel and spiral phases (tentatively identified as PVBC)
- Using similar techniques to those above we find the full phase diagram shown below

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

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RESULTS II

Isotropic J_1–J_2 XY Model on the Honeycomb Lattice ($s = \frac{1}{2}$)

- We now replace the isotropic Heisenberg ($\equiv XXX$) J_1 and J_2 bonds by isotropic XY ($\equiv XX$) bonds
- $$H_{XX} = J_1 \sum_{\langle i,j \rangle} (s_i^x s_j^x + s_i^y s_j^y) + J_2 \sum_{\langle\langle i,k \rangle\rangle} (s_i^x s_k^x + s_i^y s_k^y)$$
- Results include:
  - The case when $J_1 > 0$; $0 \leq J_2 \equiv \kappa J_1 \leq 1$

    Reference

    R.F. Bishop, P.H.Y. Li and C.E. Campbell, PRB **89**, 214413 (2014)
- In the classical case ($s \to \infty$) the J_1–$J_2 \equiv J_1^{XXX}$–J_2^{XXX} and J_1^{XX}–J_2^{XX} models on the honeycomb lattice share exactly the same $T = 0$ GS phase diagram
- c.f., for $s = \frac{1}{2}$, as we shall see, the two models have quite different GS phase diagrams
- We now use the classical Néel z-aligned [N(z)] state as a CCM model state, as well as the Néel planar [N(p)] and Néel planar [N-II(p)] states
- Amazingly, we find clear evience for a region in which the N(z) state is a GS phase

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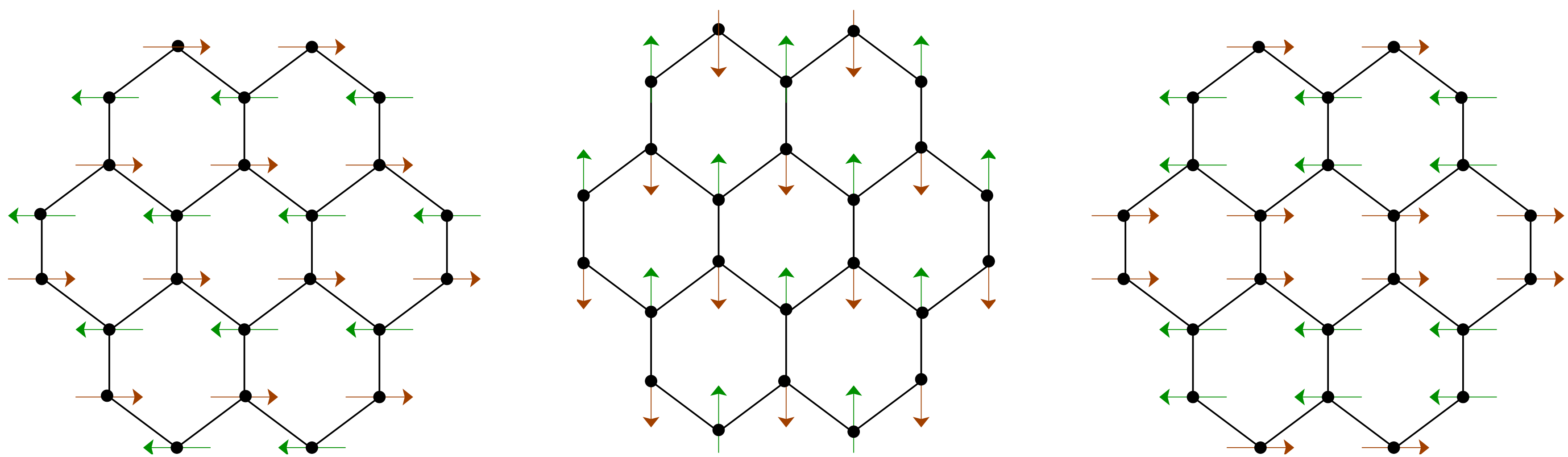
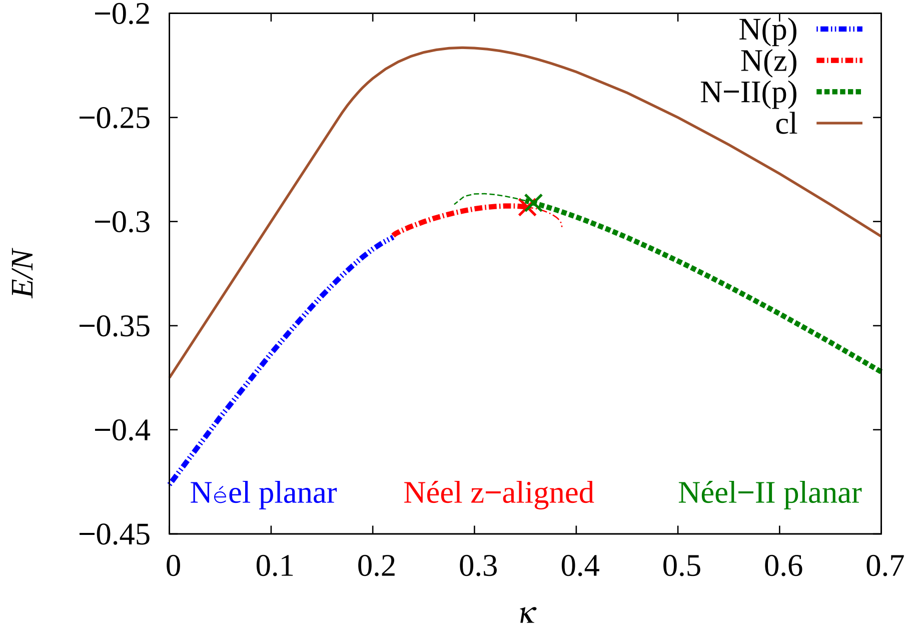
Néel planar, Néel z-aligned, and Néel-II planar Model States



(a) Néel planar, N(p) (b) Néel z-aligned, N(z) (c) Néel-II planar, N-II(p)

$s=\frac{1}{2}\ J_1^{XX}$–J_2^{XX} Model: GS Energy ($J_1 \equiv 1$) for N(p), N(z) and N-II(p) States

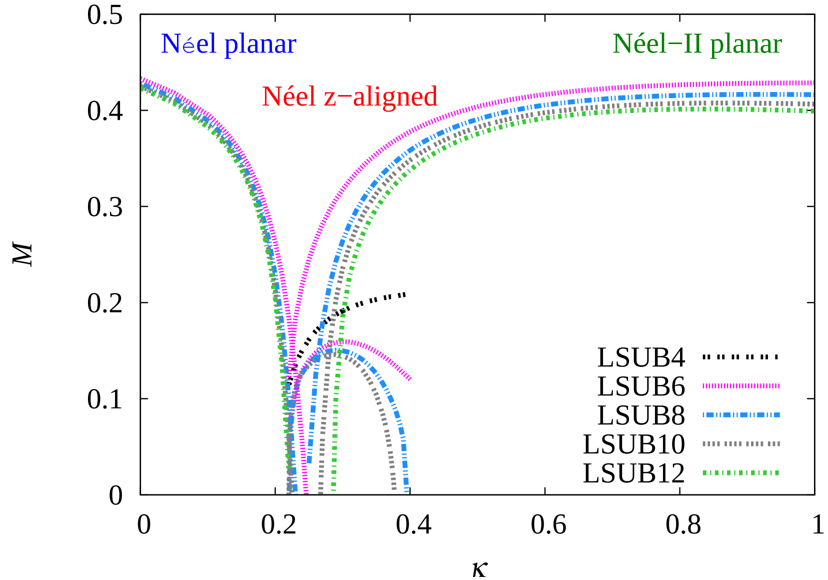
RFB, PHYL, CEC / PRB **89**, 214413 (2014)

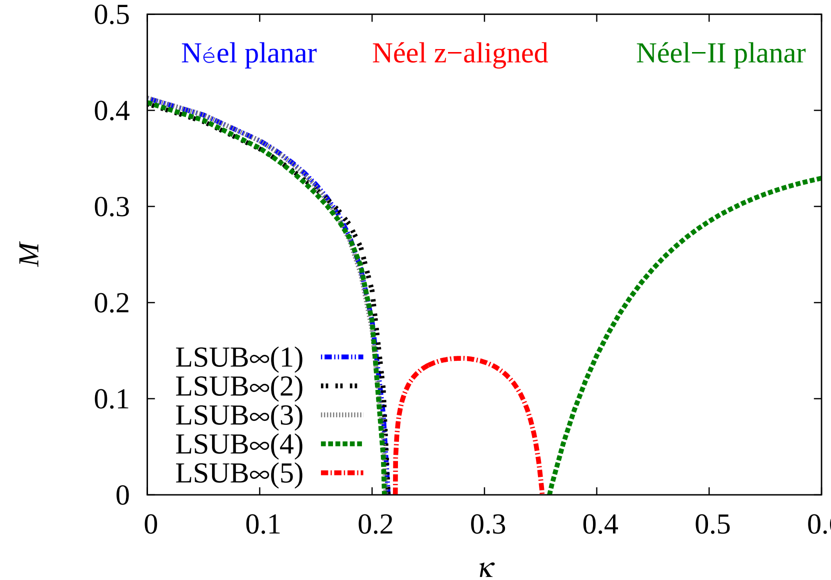


- Extrapolations: N(p) and N-II(p) use $m=\{6,8,10,12\}$; N(z) uses $m=\{4,6,8,10\}$
- The $\times$ symbols mark where the extrapolated values for $M \rightarrow 0$, and the thinner lines beyond $\times$ out to the termination points are unphysical regions (with $M<0$)
- We show the classical ($s \rightarrow \infty$; cl) results for comparison
- There is clear evidence of an intermediate phase between the N(z) and N-II(p) states for $x \gtrsim 0.35$, since the energy curves do not quite meet

$s = \frac{1}{2}$ J_1^{XX}–J_2^{XX} Model: GS Order Parameter ($J_1 \equiv 1$) for the N(p), N(z) and N-II(p) States

RFB, PHYL, CEC / PRB **89**, 214413 (2014)

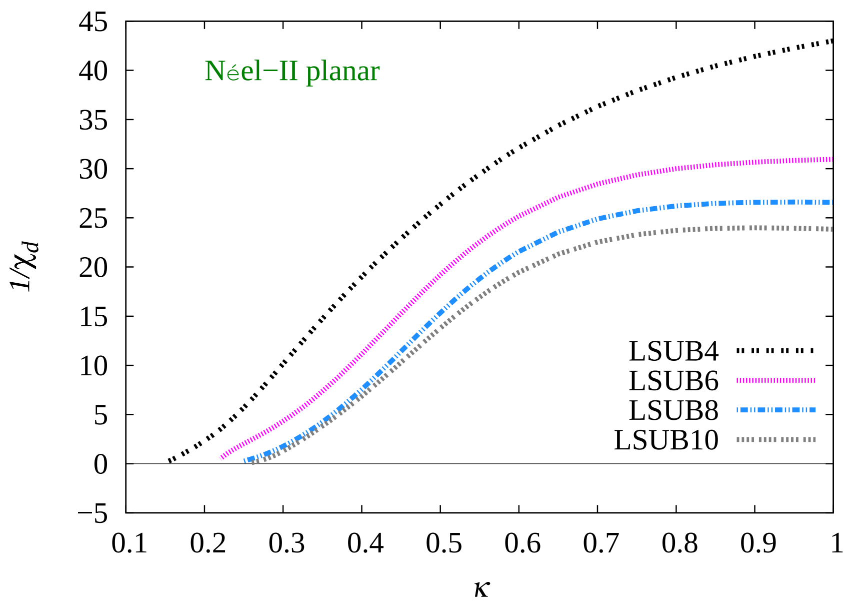


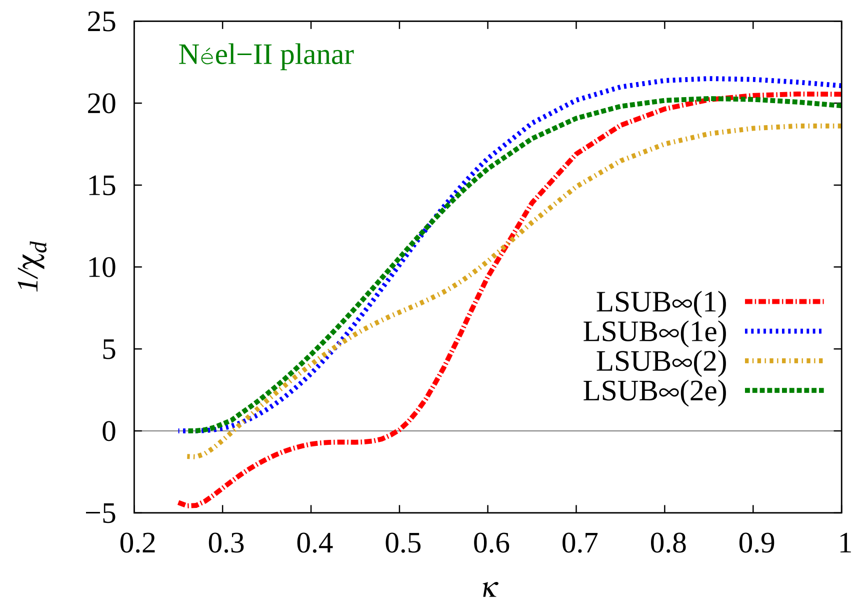


- LSUB∞(1) and LSUB∞(3): N(p) uses $M(m) = b_0 + b_1 m^{-1} + b_2 m^{-2}$, with LSUB∞(1) for $m = \{6, 8, 10, 12\}$ and LSUB∞(3) for $m = \{8, 10, 12\}$
- LSUB∞(2) and LSUB∞(4): N(p) uses $M(m) = c_0 + c_1 m^{-1/2} + c_2 m^{-3/2}$, with LSUB∞(2) for $m = \{6, 8, 10, 12\}$ and LSUB∞(4) for $m = \{8, 10, 12\}$
- LSUB$\infty(5)$: N(z) uses $M(m) = d_0 + d_1 m^{-\nu}$ with $m = \{4, 6, 8, 10\}$
- N-II(p): We only show LSUB∞(4); its shape compared to the raw LSUBm results also suggests an intermediate (SDVBC?) phase between the N(z) and N-II(p) states $\rightarrow$

$s = \frac{1}{2}\ J_1^{XX}$–$J_2^{XX}$ Model: $1/\chi_d$ versus J_2 ($J_1 \equiv 1$) for the N-II(p) State

RFB, PHYL, CEC / PRB **89**, 214413 (2014)

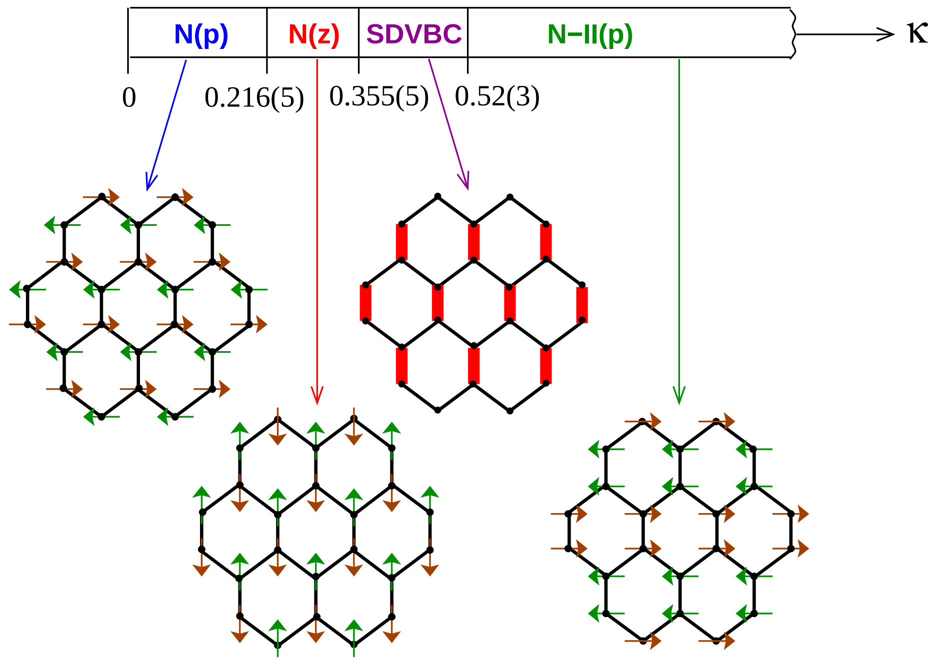




- LSUB$\infty(1e)$ uses $m = \{4, 6, 8\}$ and LSUB$\infty(2e)$ uses $m = \{4, 6, 8, 10\}$ for χ_d^{-1}, which are based on fitting the perturbed energies as $e^{(m)}(\delta) = e_0(\delta) + e_1(\delta)m^{-\nu}$
- LSUB$\infty(1)$ uses $m = \{4, 6, 8\}$ and LSUB$\infty(2)$ uses $m = \{4, 6, 8, 10\}$ for χ_d^{-1}, which are based on $\chi_d^{-1}(m) = y_0 + y_1 m^{-\nu}$
- The most reliable result, LSUB∞(1), shows clear evidence for SDVBC ordering in the range $0.36 \lesssim \kappa \lesssim 0.51$

$s = \frac{1}{2}\ J_1^{XX}$–$J_2^{XX}$ Model: Phase Diagram ($J_1 > 0$)

RFB, PHYL, CEC / PRB **89**, 214413 (2014)



- Combining all results gives the $T = 0$ GS phase diagram shown above
- The quantum critical points are at $x_{c_1} \approx 0.216(5)$, $x_{c_2} \approx 0.355(5)$, and $x_{c_3} \approx 0.52(3)$
- c.f., the classical ($s \to \infty$) model with $J_1 > 0$ has a single QCP at $\kappa_{\rm cl} = \frac{1}{6}$ from Néel order ($0 < \kappa < \frac{1}{6}$) to spiral-I order ($\forall\, \kappa > \frac{1}{6}$); identical to the classical J_1–J_2 model
- c.f., The two $s = \frac{1}{2}$ models (J_1^{XX}–J_2^{XX} and J_1–J_2) have different phase diagrams

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RESULTS III

J_1^{XXZ}–J_2^{XXZ} Model on the Honeycomb Lattice ($s = \frac{1}{2}$)

- Since the $s = \frac{1}{2}$ J_1^{XX}–J_2^{XX} and J_1–J_2 ($\equiv J_1^{XXX}$–J_2^{XXX}) models have such different phase diagrams, we also examine the interpolating J_1^{XXZ}–J_2^{XXZ} model:
- $$H_{XXZ} = J_1 \sum_{\langle i,j \rangle} (s_i^x s_j^x + s_i^y s_j^y + \Delta s_i^z s_j^z) + J_2 \sum_{\langle\langle i,k \rangle\rangle} (s_i^x s_k^x + s_i^y s_k^y + \Delta s_i^z s_k^z)$$
- Limiting cases:
  - $\Delta = 1:$ J_1^{XXX}–J_2^{XXZ} ($\equiv$ isotropic J_1–J_2 HAF)
  - $\Delta = 0:$ J_1^{XX}–J_2^{XX} ($\equiv$ isotropic J_1–J_2 XY model)
- Results include:
  - The case when $J_1 > 0; 0 \leq \kappa \equiv J_2/J_1 \leq 1$, $0 \leq \Delta \leq 1$

    Reference

    P.H.Y. Li, R.F. Bishop and C.E. Campbell, PRB **89**, 220408(R) (2014)

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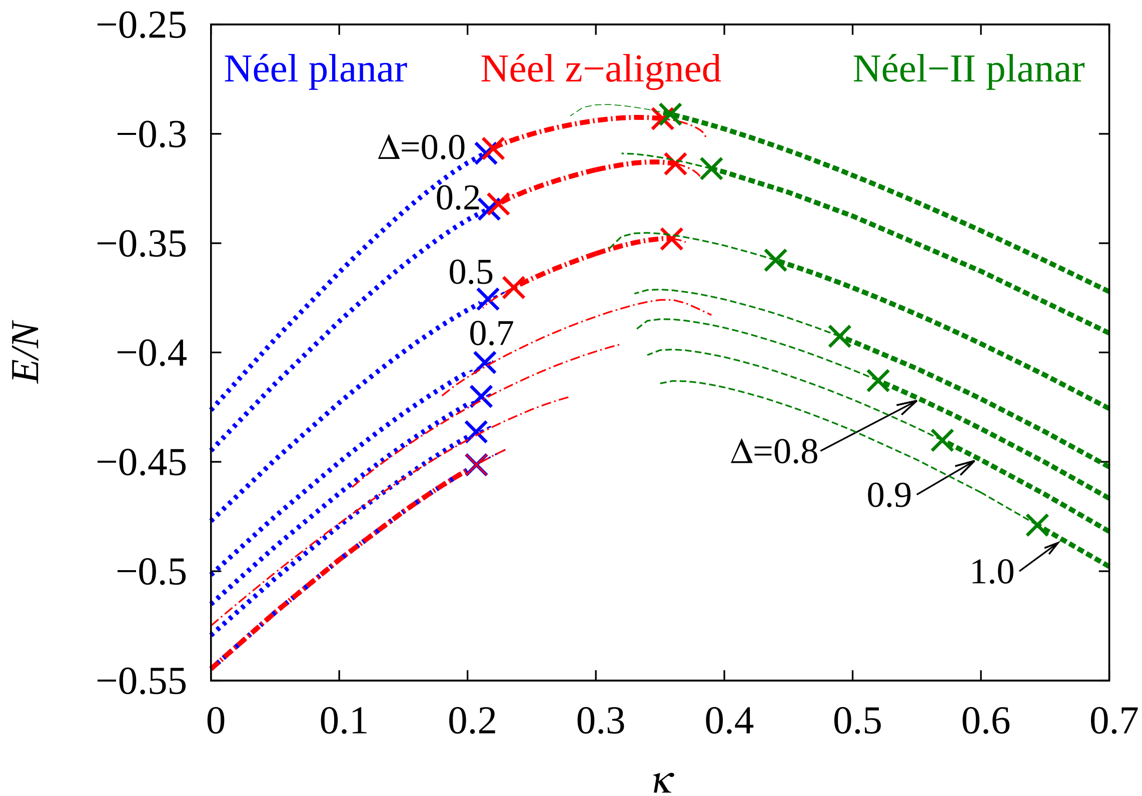
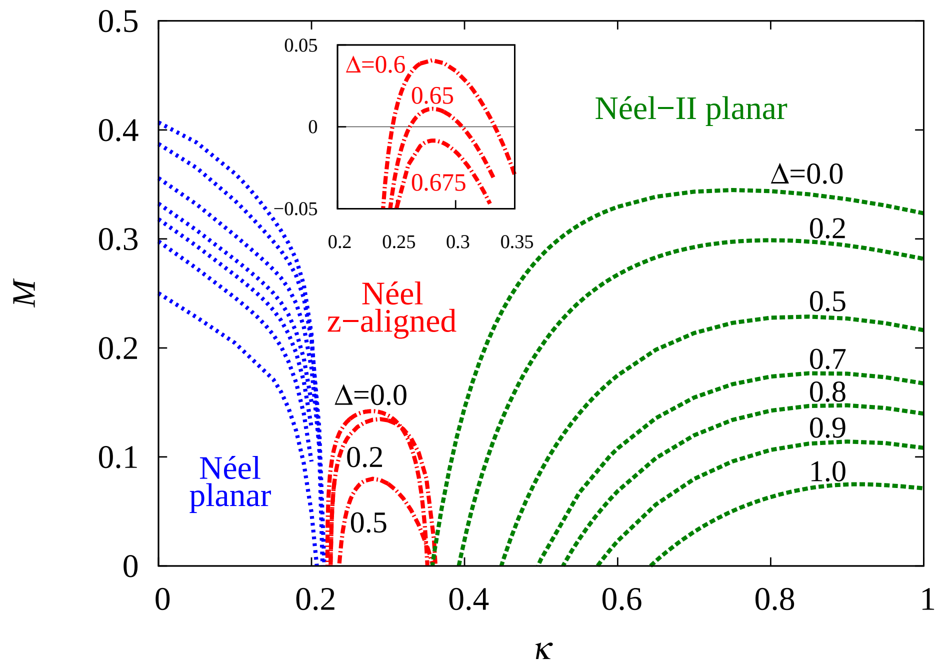
PHYL, RFB, CEC / PRB **89**, 220408(R) (2014)



- N(p) and N-II(p) extrapolations use the data set $m = \{6, 8, 10, 12\}$
- N(z) extrapolation uses the data set $m = \{4, 6, 8, 10\}$
- Clearly, the N(z) regime disappears for $\Delta > \Delta_c$

$s=\frac{1}{2}\ J_1^{XXZ}$–J_2^{XXZ} Model: Order Parameter ($J_1 \equiv 1$) for the N(p), N(z) and N-II(p) States

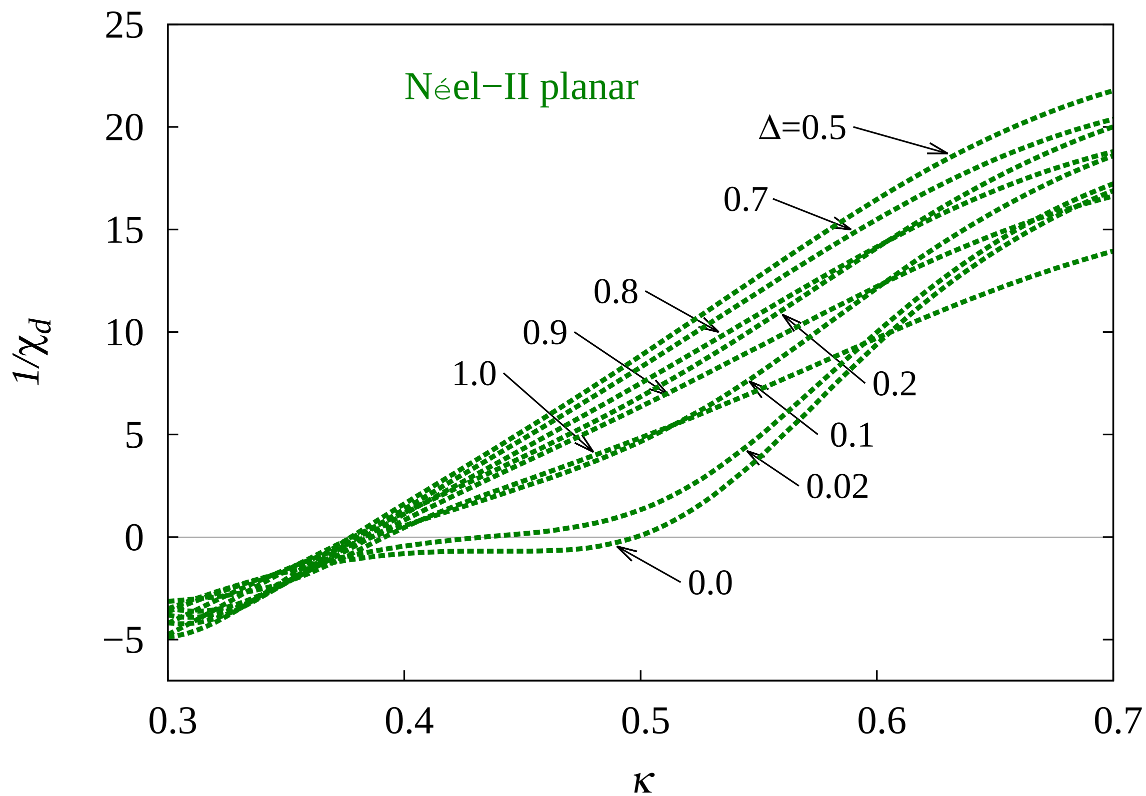
PHYL, RFB, CEC / PRB **89**, 220408(R) (2014)



- N(p) and N-II(p) extrapolations use the data set $m = \{6, 8, 10, 12\}$ with $M(m) = d_0 + d_1 m^{-1/2} + d_2 m^{-3/2}$
- N(z) extrapolation uses the data set $m = \{4, 6, 8, 10\}$ with $M(m) = c_0 + c_1(1/m)^{c_2}$
- Again, there is clear evidence that the N(z) regime disappears for $\Delta > \Delta_c$
- We can again now also test for SDVBC order $\longrightarrow$

$s = \frac{1}{2}$ J_1^{XXZ}–J_2^{XXZ} Model: $1/\chi_d$ versus J_2 ($J_1 \equiv 1$) for the N-II(p) State

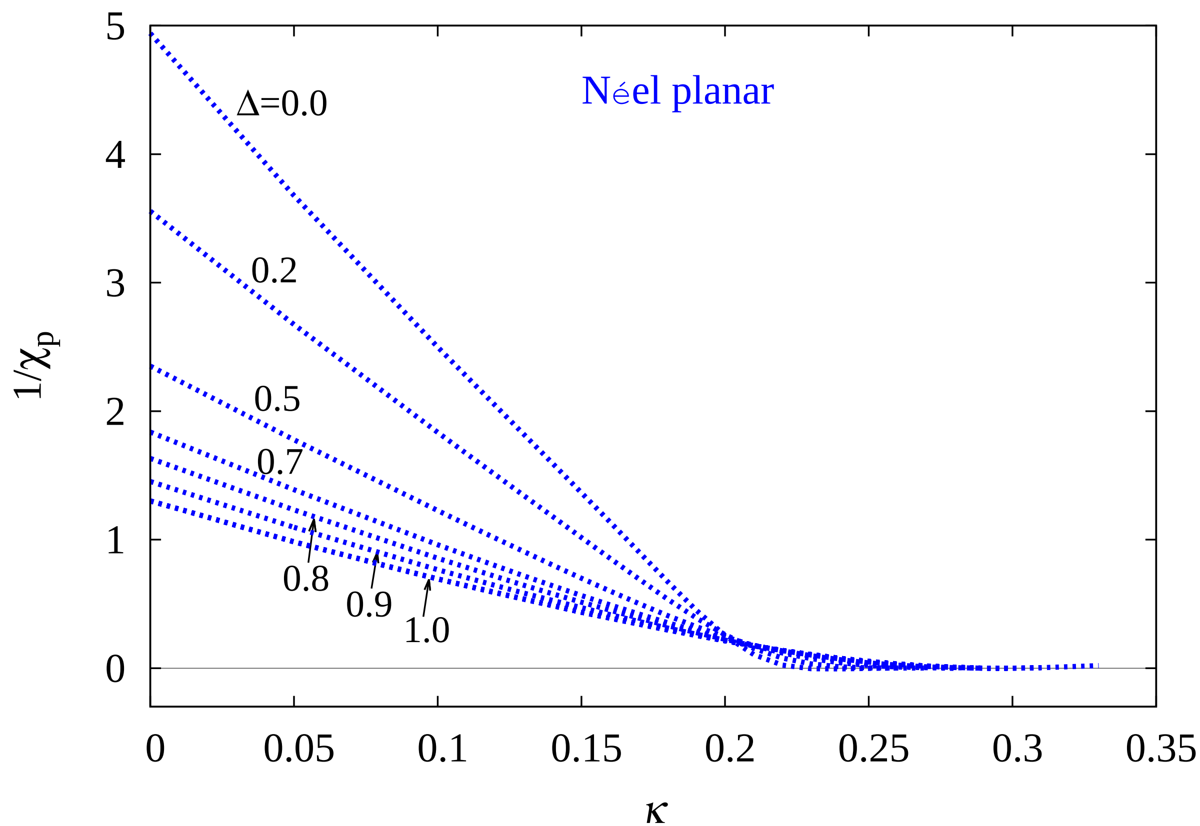
PHYL, RFB, CEC / PRB **89**, 220408(R) (2014)



- The LSUB∞ extrapolations are based on the "leading power-law" scheme, $\chi_d^{-1} \rightarrow x_0 + x_1 m^{-\nu}$ with LSUBm results $m = \{4, 6, 8\}$, for various values of Δ
- We can again similarly test for PVBC order $\rightarrow$

$s = \frac{1}{2}$ J_1^{XXZ}–J_2^{XXZ} Model: $1/\chi_p$ versus J_2 ($J_1 \equiv 1$) for the N(p) State

PHYL, RFB, CEC / PRB **89**, 220408(R) (2014)



- The LSUB∞ extrapolations are based on the "leading power-law" scheme, $\chi_p^{-1} \rightarrow x_0 + x_1 m^{-\nu}$ with LSUBm results $m = \{4, 6, 8\}$, for various values of Δ

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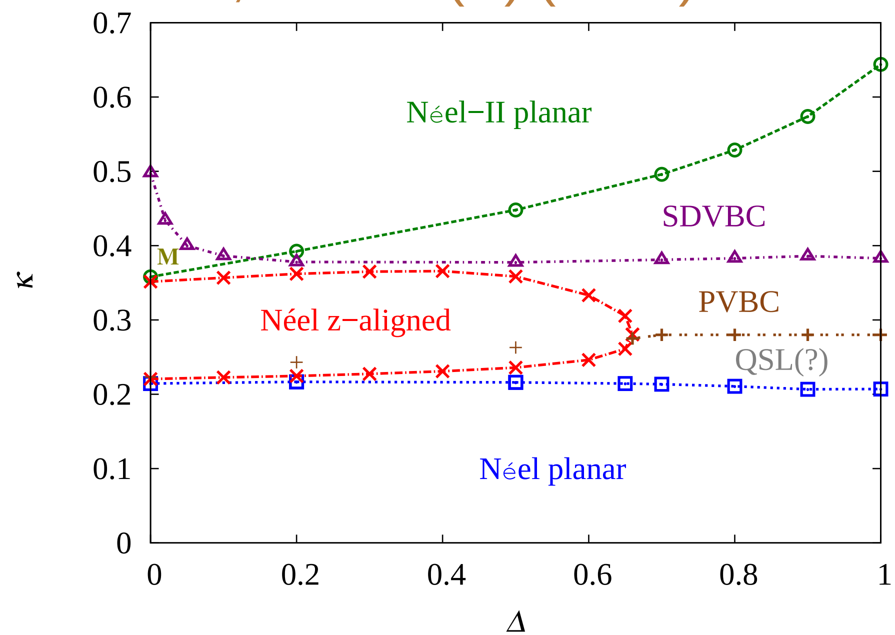
$s=\frac{1}{2}\ J_1^{XXZ}$–J_2^{XXZ} Model: Phase Diagram ($J_1 \equiv 1; 0 < J_2 < 1, 0 < \Delta < 1$)

PHYL, RFB, CEC / PRB **89**, 220408(R) (2014)



- Combining all our results give the $T = 0$ GS phase diagram shown above
- The triangle (△) symbols mark LSUB∞ points where $\chi_d^{-1} \rightarrow 0$ (SDVBC)
- The plus (+) symbols mark LSUB∞ points where $\chi_p^{-1} \rightarrow 0$ (PVBC)
- The phase marked “M” has mixed SDVBC and N-II(p) order
- The remaining region above the N(p) state but below the N(z) and PVBC states is a candidate quantum spin liquid (QSL) phase

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CONCLUSIONS

- 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]
- Probably by now there are > 100 papers using the CCM for spin lattices

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THANK YOU FOR YOUR ATTENTION!