MAGNETIC ORDERING OF ANTIFERROMAGNETS ON A SPATIALLY ANISOTROPIC TRIANGULAR LATTICE

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OUTLINE

- The Model
- The Method
- Results

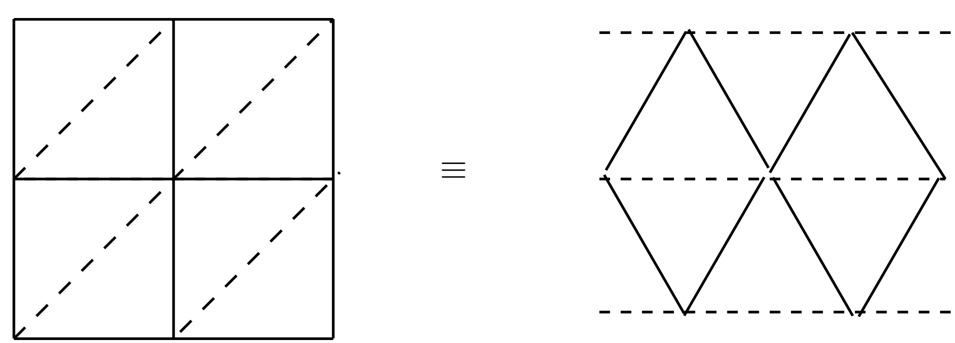
Reference

R.F. Bishop *et al.*, Phys. Rev. B 79, 174405 (2009)

THE MODEL

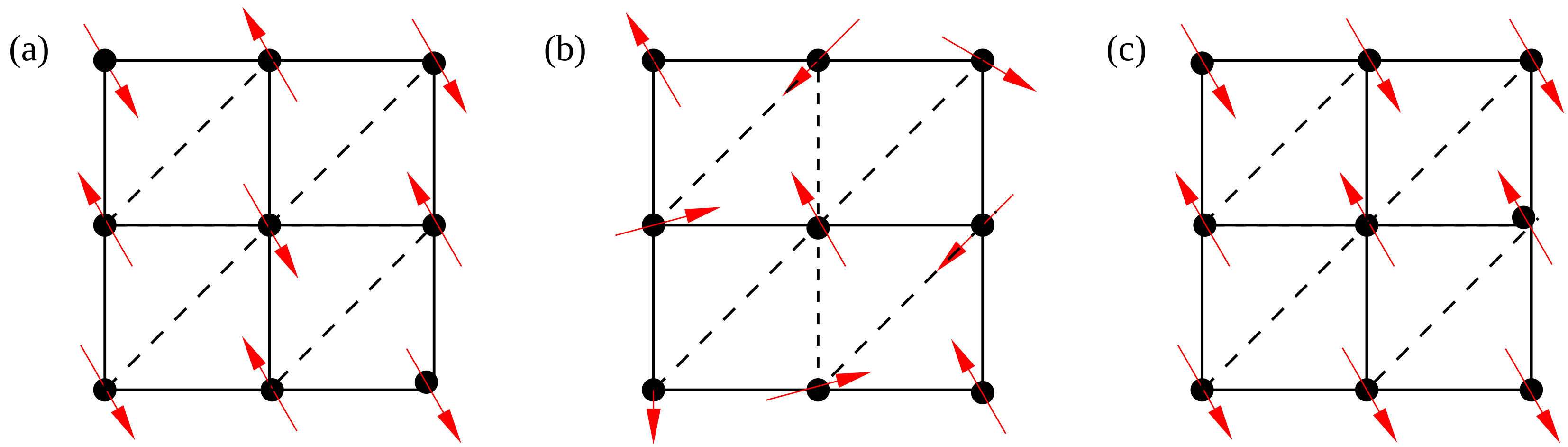
- spin-1/2 J_1–J_2' model on a 2D square (or triangular) lattice
- $H = J_1 \sum_{\langle i,j \rangle} \mathbf{s}_i \cdot \mathbf{s}_j + J_2' \sum_{[i,j]} \mathbf{s}_i \cdot \mathbf{s}_j$ (and set $J_1 \equiv 1$)

  where, on square lattice:
  - $\langle i, j \rangle$ bonds $J_1 \equiv$ — all NN bonds
  - $[i, j]$ bonds $J_2' \equiv$ - - - half NNN bonds



- limits
  - $J_2' = 0$: isotropic HAF on 2D square lattice
  - $J_2' = 1$: isotropic HAF on 2D triangular lattice
  - $J_2' \to \infty$: uncoupled HAF 1D chains
- classical limit ($s \to \infty$)
  - for $J_2' < \frac{1}{2}J_1$: gs is Néel ordered as in (a)
  - for $J_2' > \frac{1}{2}J_1$: gs is spiral ordered as in (b) with pitch angle at site (i, j)
    $\alpha_{ij} = \alpha_0 + (i+j)\alpha_{\rm cl}$,
    $\alpha_{\rm cl} = \cos^{-1}(-\frac{J_1}{2J_2'}) \equiv \pi - \phi_{\rm cl}$

Néel, Spiral, and Striped Model States



$\Rightarrow$ in limit $J_2' \to \infty$: uncoupled 1D HAF chains with relative spin orientation of 90° between neighbouring chains (although with complete degeneracy between states of arbitrary relative ordering between chains)
$\Rightarrow$ clearly, exact spin-1/2 limit should also be 1D uncoupled isotropic HAF chains **but**

question : might *order by disorder* phenomenon lift this degeneracy to give, e.g., a striped state as in (c) above?

THE METHOD

We use the coupled cluster method (CCM)

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

- 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 $|\Psi\rangle$, $\langle\tilde{\Psi}|$
- only approximation is to truncate set $\{I\}$
  $\rightarrow$ we use the LSUBm scheme in which we retain all possible multispin-flip correlations over different locales on lattice defined by m or fewer contiguous lattice sites
- we use triangular lattice geometry to define the LSUBm scheme and retain all distinct fundamental configurations (fc) with respect to space- and point-group symmetries of both the Hamiltonian and the model state $|\Phi\rangle$

Number of fundamental configurations

Method	♯ f.c.	
	stripe	spiral
LSUB2	2	3
LSUB3	4	14
LSUB4	27	67
LSUB5	95	370
LSUB6	519	2133
LSUB7	2617	12878
LSUB8	15337	79408

[NOTE: To obtain a single data point (i.e., for a given value of J_2', with $J_1 = 1$) for the spiral phase at the LSUB8 level we typically required about 0.3 h computing time using 600 processors simultaneously.]

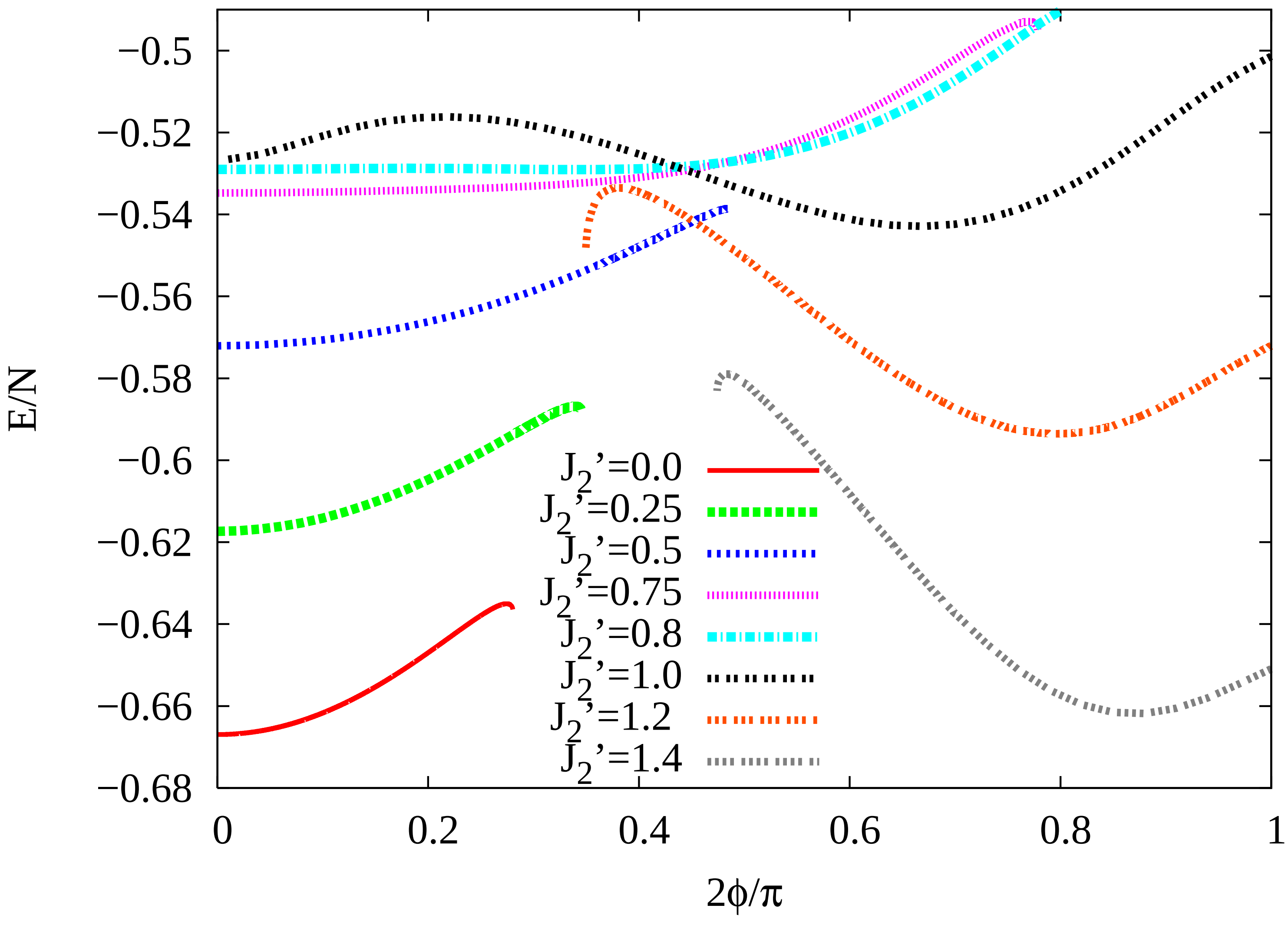
- at each LSUBm level the CCM operates at the $N \to \infty$ limit from the outset
- calculate E/N and onsite magnetization $M \equiv -\langle\tilde{\Psi}|s_i^z|\Psi\rangle$ in local axes
- extrapolate to the exact $m \to \infty$ limit, using well-tested empirical scaling laws
  - $E/N = a_0 + a_1 m^{-2} + a_2 m^{-4}$
  - $M = b_0 + b_1 m^{-1} + b_2 m^{-2}$

RESULTS

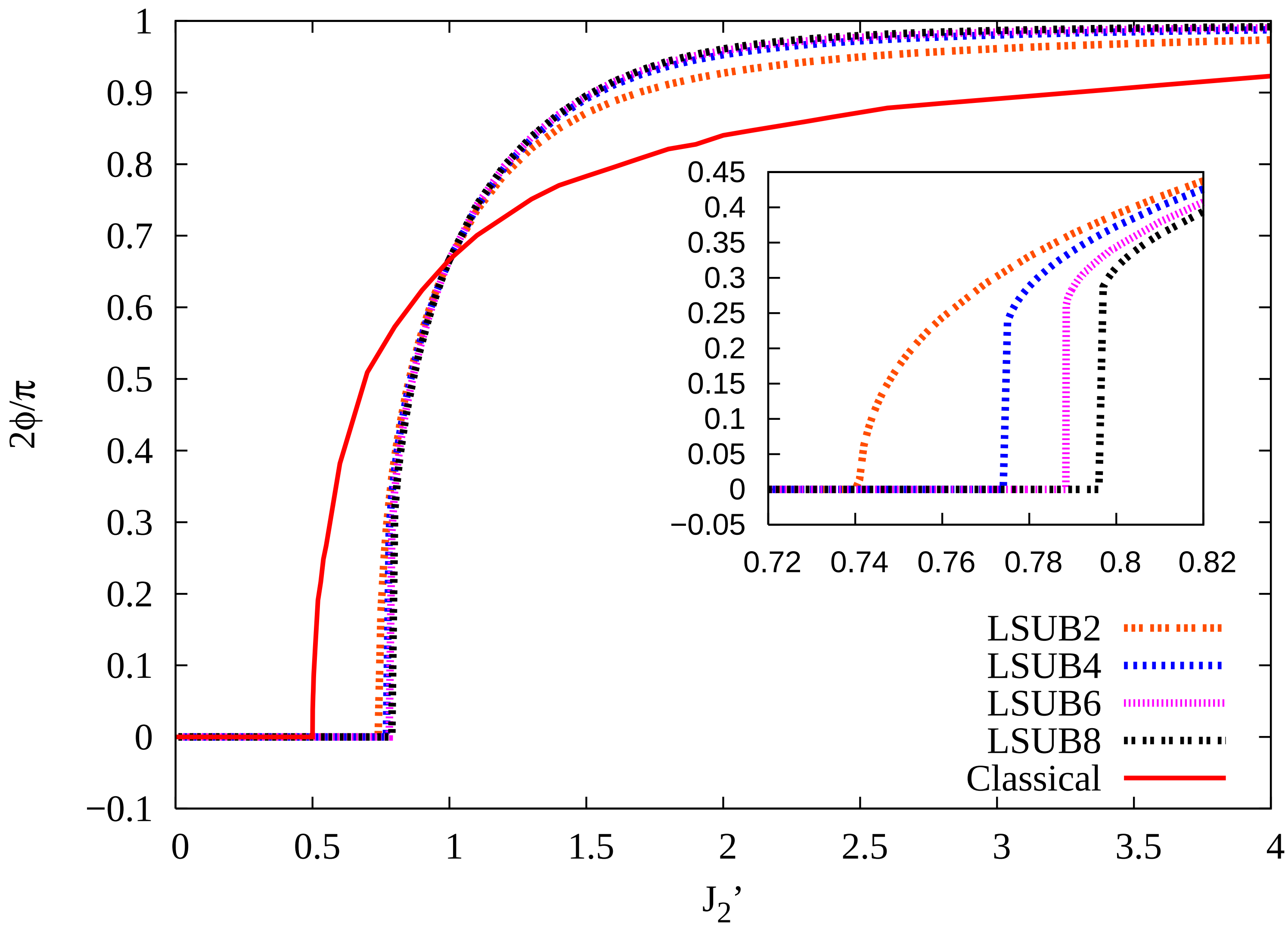
1. Néel and Spiral Phases

- 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 $\phi = \phi_{{\rm LSUB}_m}$
- we observe how $\phi \to \frac{1}{2}\pi$ as $J_2' \to \infty$ much faster than for classical counterpart ($\Rightarrow$ more rapid approach to collinearity on the uncoupled 1D chains)

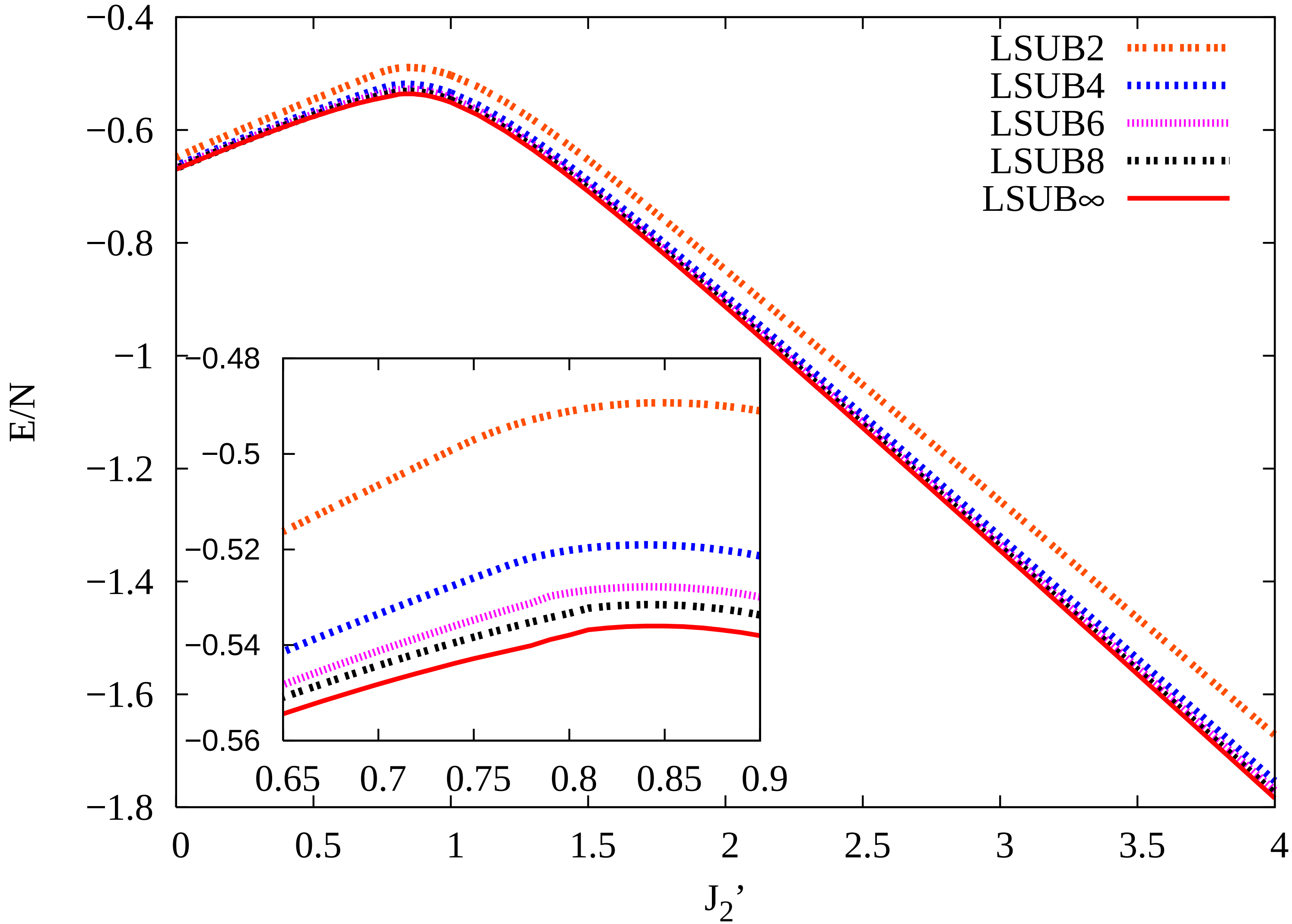
GS Energy versus Pitch Angle for Spiral Phase



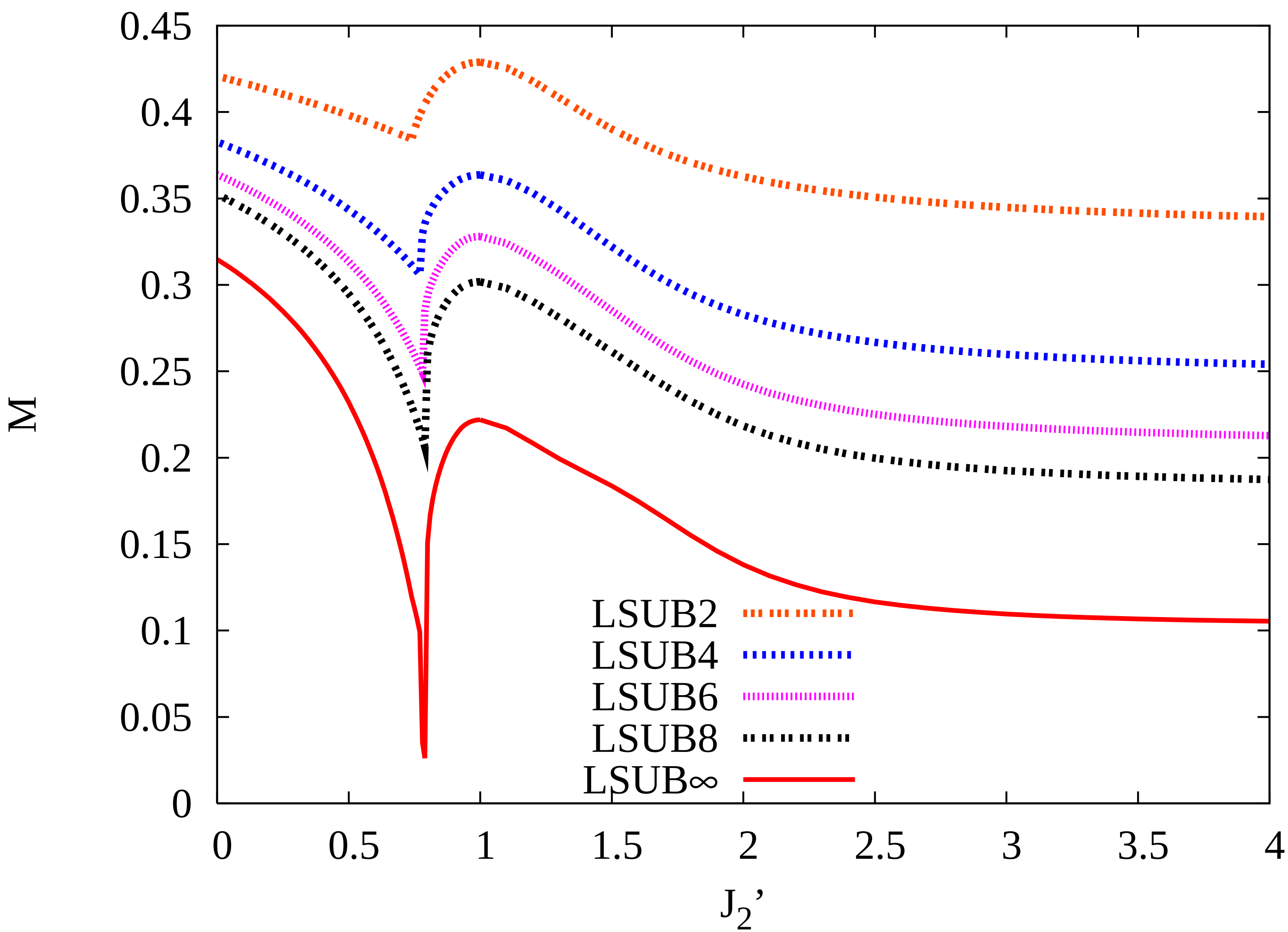
Pitch Angle of Spiral Phase versus J_2' ($\phi = 0 \Rightarrow$ Néel Phase)



GS Energy versus J_2' in Néel and Spiral Phases



Onsite Magnetization (Order Parameter) versus J_2' in Néel and Spiral Phases



Results for Isotropic HAF on Square and Triangular Lattices

Method	E/N	M	E/N	M
	square ($\kappa = 0$)		triangular ($\kappa = 1$)	
LSUB2	-0.64833	0.4207	-0.50290	0.4289
LSUB3	-0.64931	0.4182	-0.51911	0.4023
LSUB4	-0.66356	0.3827	-0.53427	0.3637
LSUB5	-0.66345	0.3827	-0.53869	0.3479
LSUB6	-0.66695	0.3638	-0.54290	0.3280
LSUB7	-0.66696	0.3635	-0.54502	0.3152
LSUB8	-0.66816	0.3524	-0.54679	0.3018
Extrapolations				
LSUB∞ [a]	-0.66974	0.3099	-0.55244	0.1893
LSUB∞ [b]	-0.67045	0.3048	-0.55205	0.2085
QMC	-0.669437(5)	0.3070(3)	-0.5458(1)	0.205(10)
SE	-0.6693(1)	0.307(1)	-0.5502(4)	0.19(2)

[a] Based on $n = \{4, 6, 8\}$

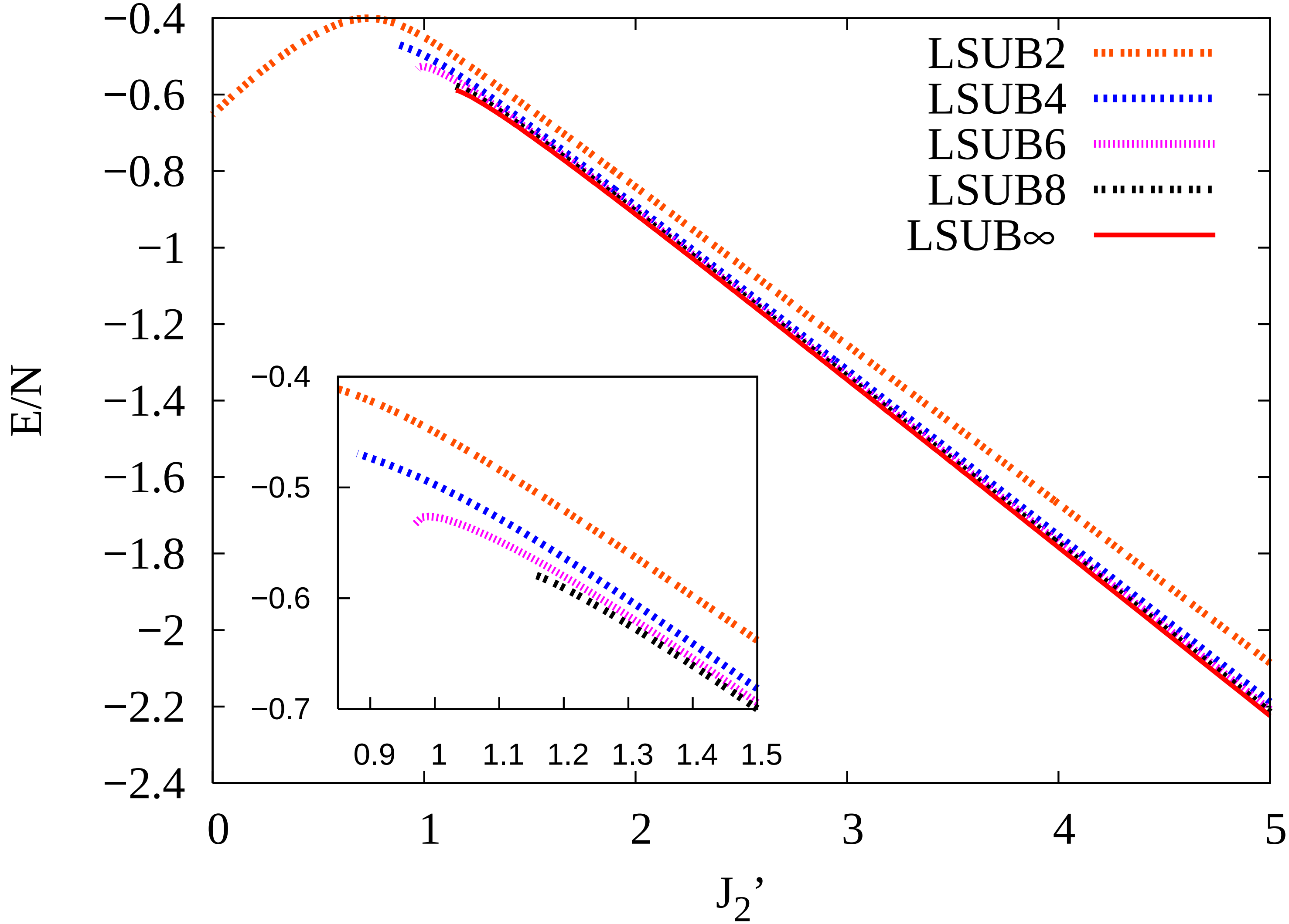
[b] Based on $n = \{3, 5, 7\}$

- we observe a weakly first-order (or possibly second-order) quantum phase transition at a *first critical point* $\kappa_{c_1} = 0.80 \pm 0.01$ ($\kappa \equiv J_2'/J_1$) [c.f. second-order classical transition at $\kappa_{\rm cl} = 0.5$]
  - and thus the collinear Néel order exists to larger frustration than in the classical counterpart
  - which is another example of the fact that quantum fluctuations favour collinearity

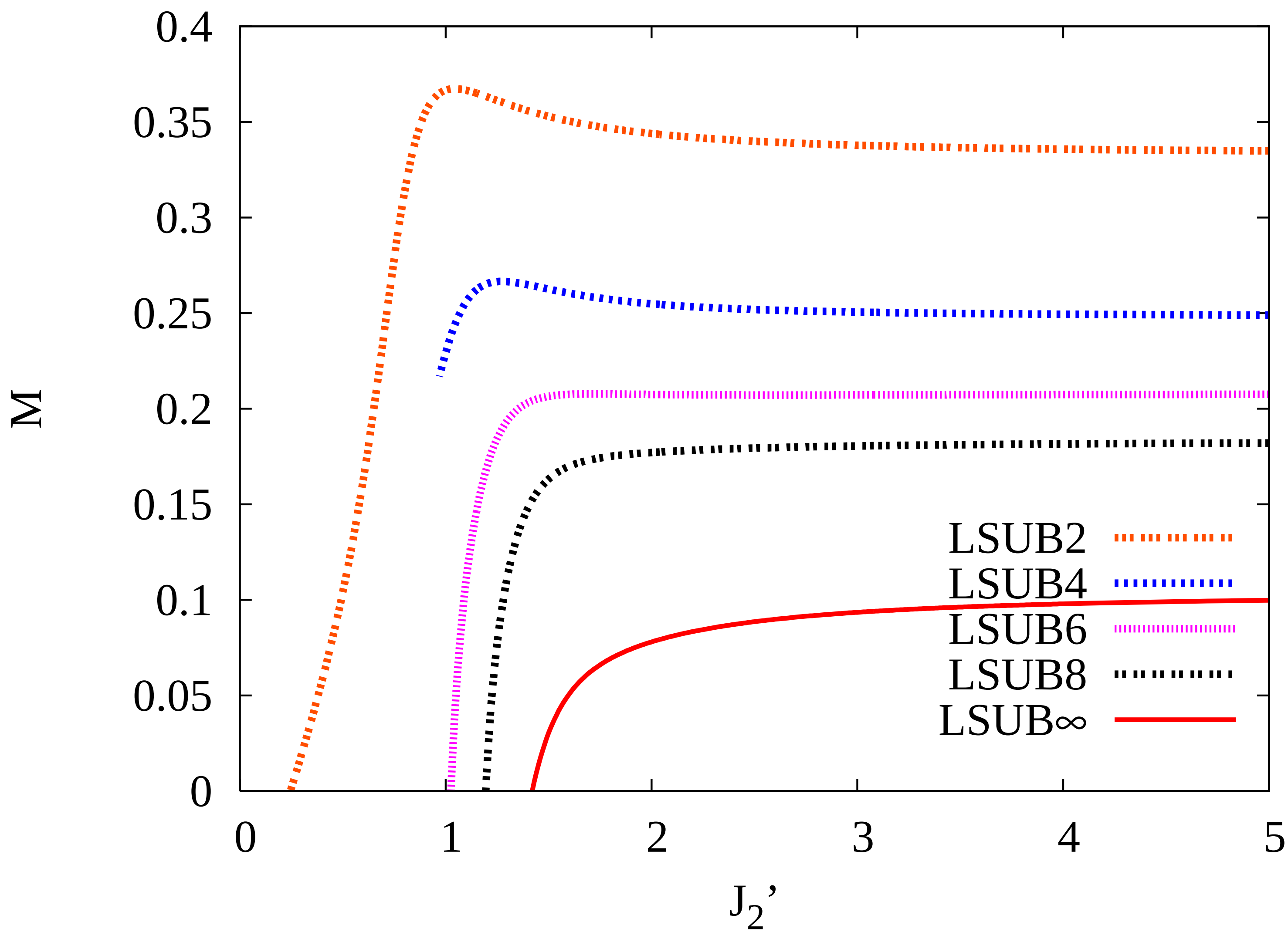
2. Spiral and Striped Phases

- we also use $|\Phi\rangle \rightarrow |\Phi_{\rm stripe}\rangle$ as CCM model state
- and recall again : the spiral phase approaches collinearity ($\phi = \frac{1}{2}\pi$) for the uncoupled 1D chain limit (as $J'_2 \rightarrow \infty$) much faster than in the corresponding classical model

GS Energy versus J_2' in Striped Phase

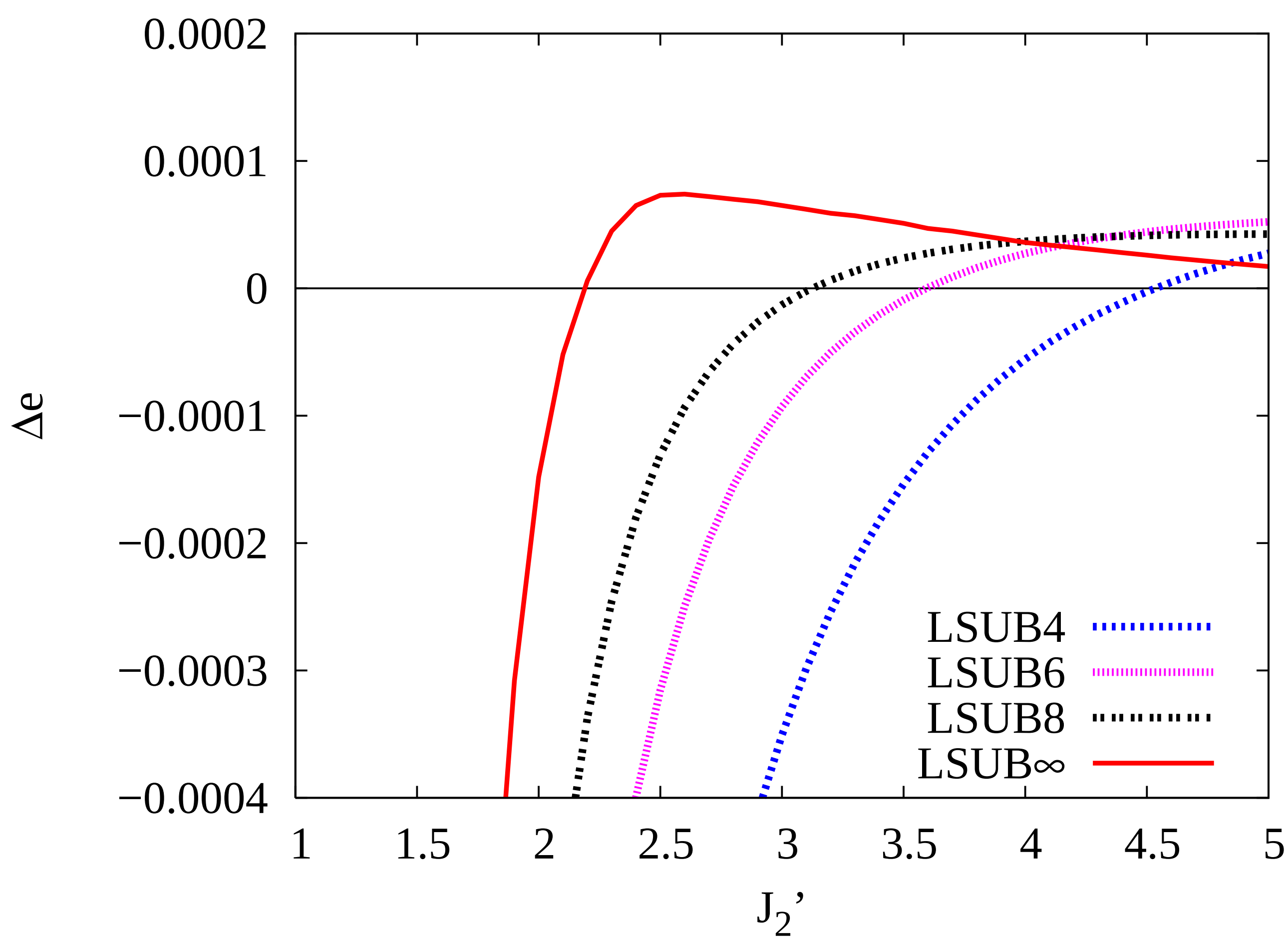


Onsite Magnetization (Order Parameter) versus J_2' in Striped Phases



Energy Difference Between Spiral and Striped Phases versus J_2'

- we calculate $\Delta e = e^{\text{spiral}} - e^{\text{stripe}}$, $e \equiv E/N$



- we observe a *second critical point* at $\kappa_{c_2} = 1.8 \pm 0.4$ where a first-order quantum phase transition occurs from the spiral phase to the striped phase
  - thereby providing quantitative verification of a recent qualitative prediction of Starykh and Balents using an RG analysis of this model, which did not, however, evaluate the actual critical point
  - thus providing yet another example of the fact that quantum fluctuations tend to preserve collinear order
  - and where, this time, the quantum phase transition is driven by the competition between different collinear structures on the chains connected by J_2' bonds
  - but where the striped phase is also completely collinear

THANK YOU FOR YOUR ATTENTION!