QUANTUM PHASE TRANSITIONS IN STRONGLY CORRELATED AND HIGHLY FRUSTRATED SPIN-LATTICE SYSTEMS :

An Ab Initio Quantum Many-Body Theory Formulation

by

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OUTLINE

- An Illustrative Model
- The Coupled Cluster Method
- Results
  - spin-1/2
  - spin-1

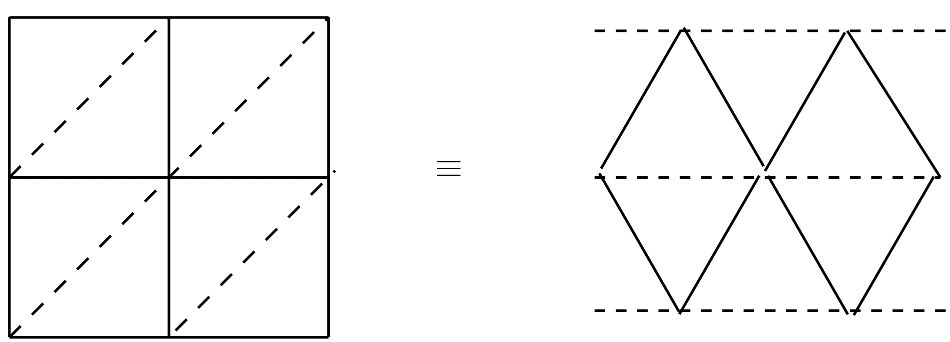
Reference ($s = 1/2$ only)

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

AN ILLUSTRATIVE MODEL

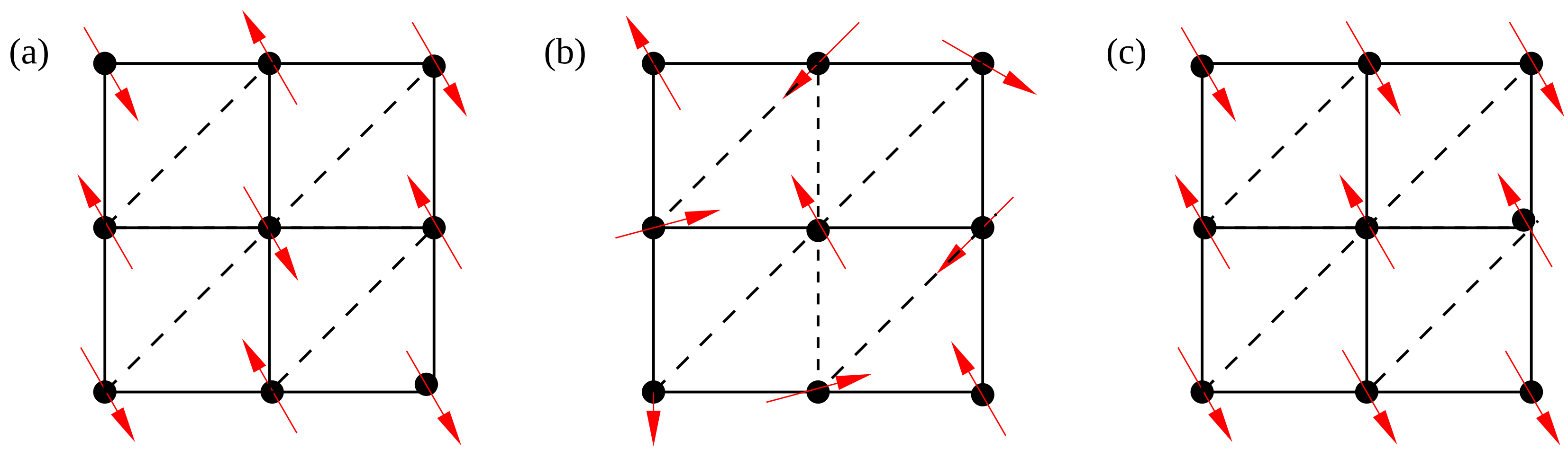
- J_1–J_2' model on a 2D square (or triangular) lattice
- We'll look at two cases : $s = 1/2$ spins and $s = 1$ spins
- $H = J_1 \sum_{\langle i,j \rangle} \mathbf{s}_i \cdot \mathbf{s}_j + J_2' \sum_{[i,j]} \mathbf{s}_i \cdot \mathbf{s}_j$ (and set $J_1 \equiv 1$)

  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) below
  - for $J_2' > \frac{1}{2}J_1$: gs is spiral ordered as in (b) below with pitch angle at site (i,j)
    $\alpha_{ij} = \alpha_0 + (i+j)\alpha_{\text{cl}}$,
    $\alpha_{\text{cl}} = \cos^{-1}(-\frac{J_1}{2J_2'}) \equiv \pi - \phi_{\text{cl}}$

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 limit for the spin-1/2 and spin-1 cases should also be 1D uncoupled isotropic HAF chains **but**

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

question : will the $s = 1/2$ and $s = 1$ cases be different?

THE COUPLED CLUSTER 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

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- each s_i^+ in C_I^+ can appear at most once for $s = 1/2$, 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 triangular 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 $|\Phi\rangle$

- only approximation is to truncate set $\{I\}$
  - for $s=1/2$ case 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
  - 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 $s=1/2$ case)

Number of fundamental configurations

$s=1/2$			$s=1$		
Method	♯ f.c.		Method	♯ f.c.	
	stripe	spiral		stripe	spiral
LSUB2	2	3	SUB2–2	2	4
LSUB3	4	14	SUB3–3	4	26
LSUB4	27	67	SUB4–4	60	189
LSUB5	95	370	SUB5–5	175	1578
LSUB6	519	2133	SUB6–6	2996	14084
LSUB7	2617	12878	SUB7–7	11778	131473
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 for the spin-1/2 case we typically required about 0.3 h computing time using 600 processors simultaneously.]

- at each LSUBm or SUBm–m level the CCM operates at the $N \rightarrow \infty$ 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 $m \rightarrow \infty$ 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

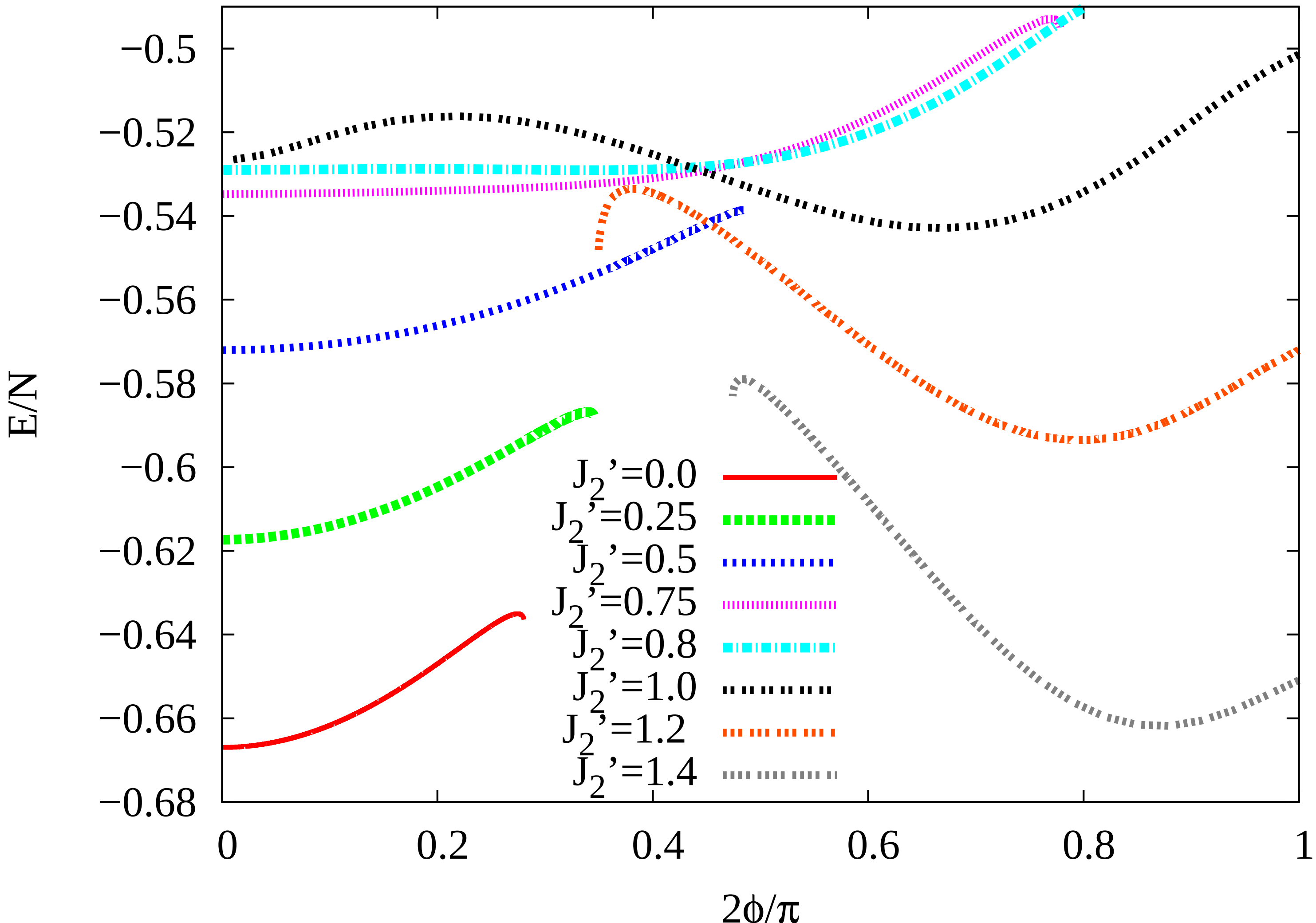
SPIN-1/2 CASE

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 $\phi \rightarrow \frac{1}{2}\pi$ as $J_2' \rightarrow \infty$ much faster than for classical counterpart ($\Rightarrow$ more rapid approach to collinearity on the uncoupled 1D chains)
- notice how we often obtain (real) solutions only for certain ranges of ϕ depending on the value of $\kappa \equiv J_2'/J_1$, with termination points shown

GS Energy versus Pitch Angle for Spiral Phase

($s = 1/2$ case; LSUB6 results shown)



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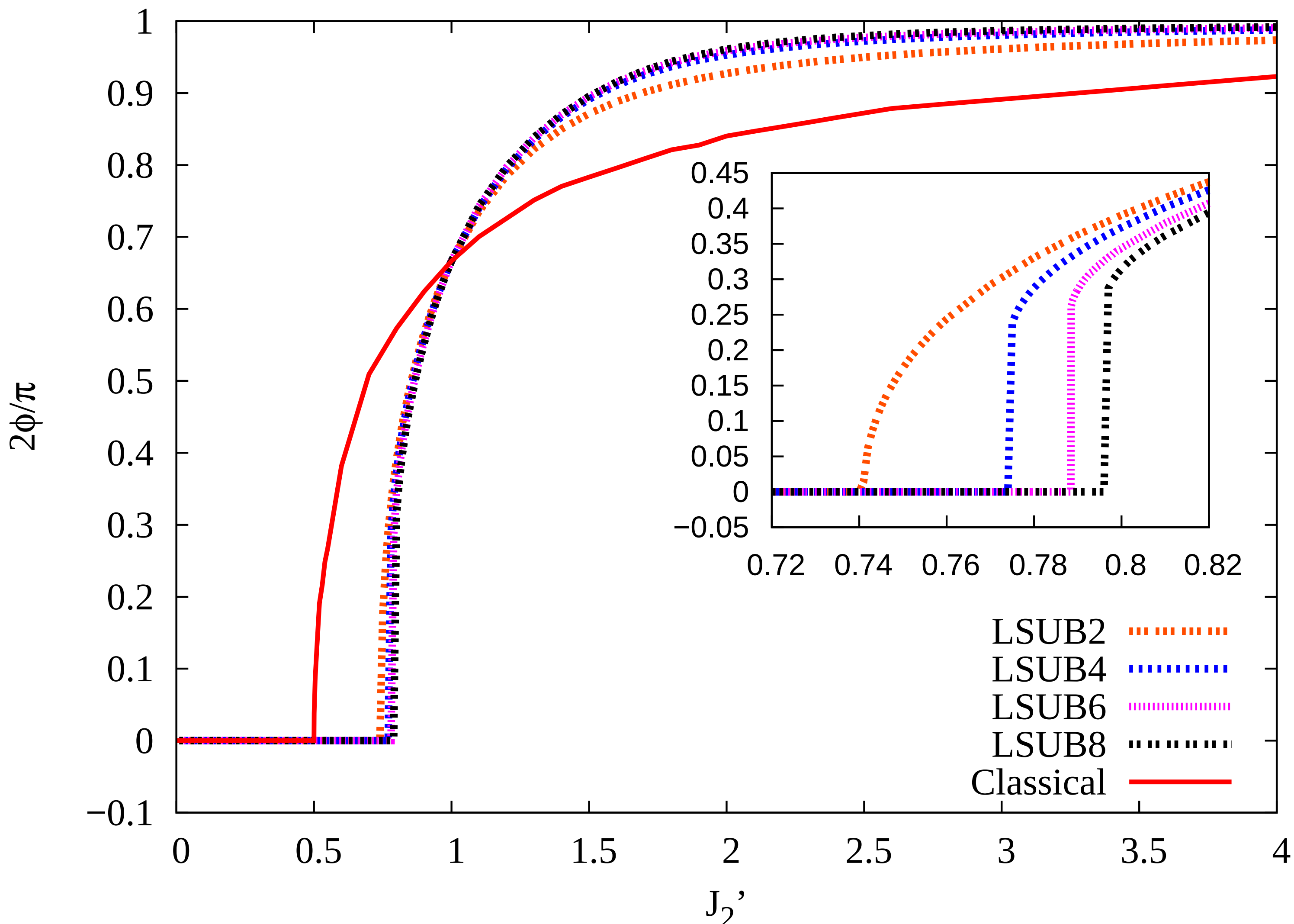
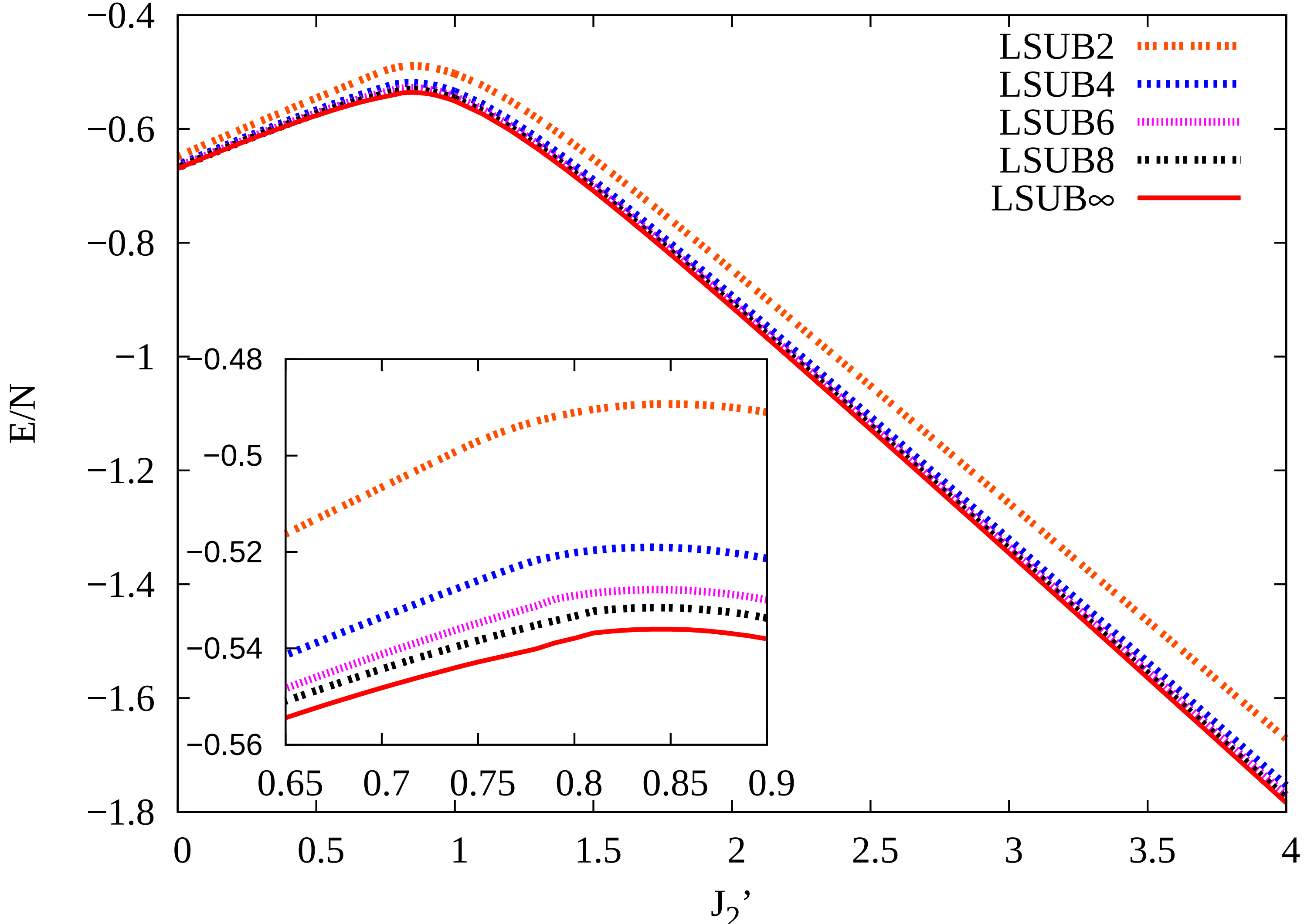
Pitch Angle $\phi = \phi_{\mathrm{LSUBm}}$ of Spiral Phase versus J_2' ($\phi = 0 \Rightarrow$ Néel Phase)

($s = 1/2$ case)



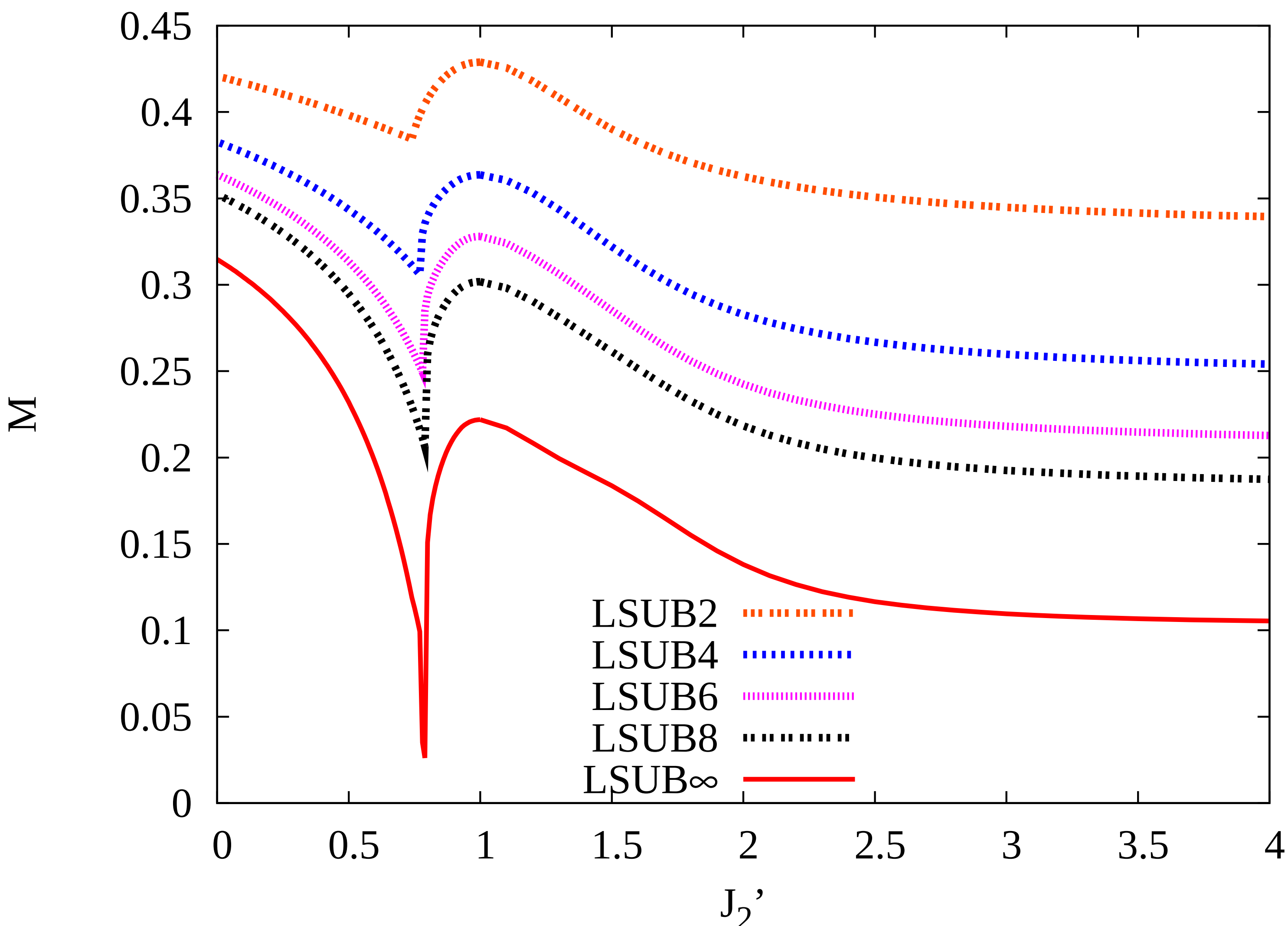
GS Energy versus J_2' in Néel and Spiral Phases

$(s = 1/2$ case$)$



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

($s = 1/2$ case)



Results for Isotropic HAF on Square and Triangular Lattices

($s = 1/2$ case)

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] Using LSUBm; $m = \{4, 6, 8\}$ [b] Using LSUBm; $m = \{3, 5, 7\}$

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- 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 $|\Phi\rangle \rightarrow |\Phi_{\text{stripe}}\rangle$ 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

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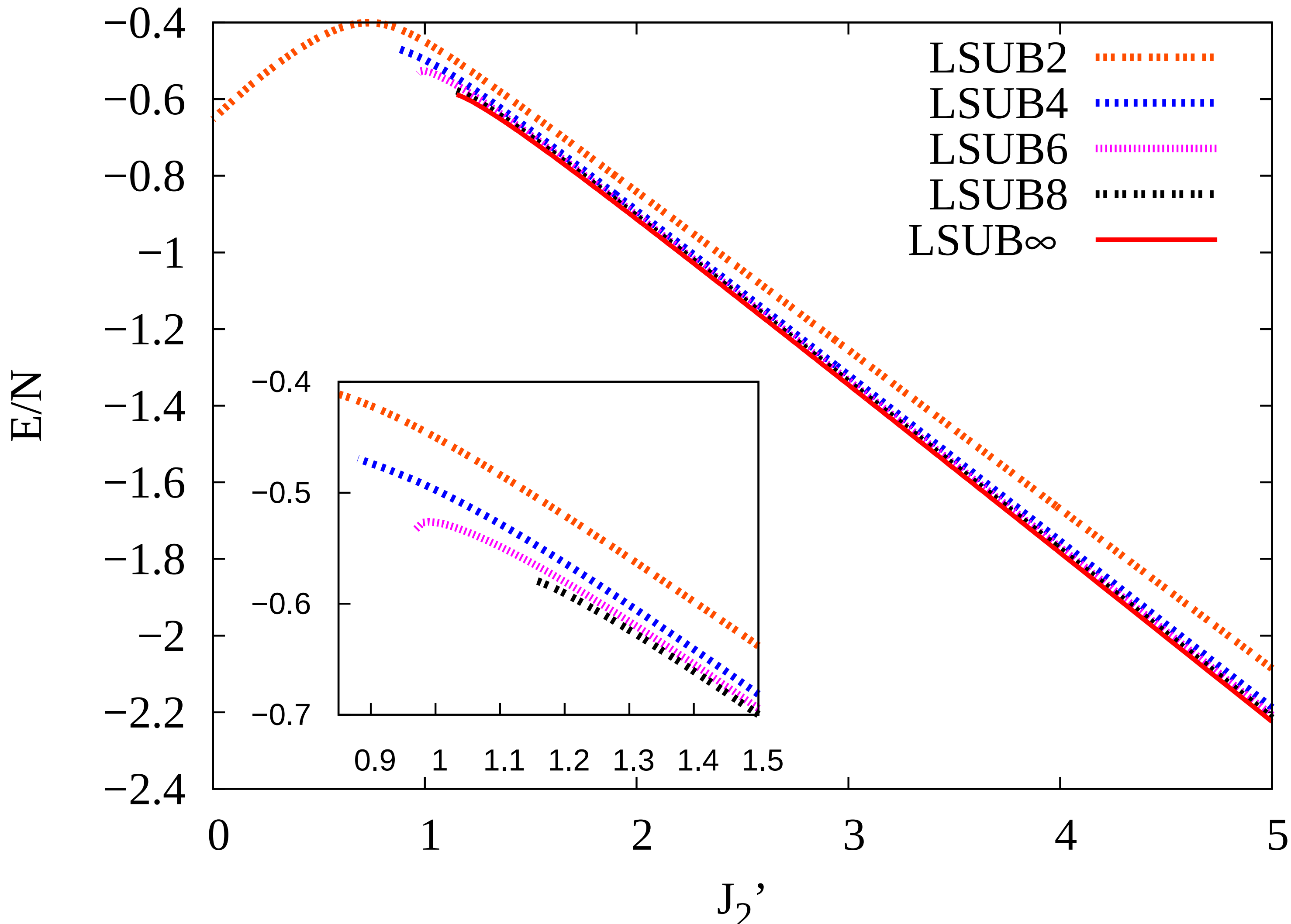
GS Energy versus J_2' in Striped Phase

($s = 1/2$ case)



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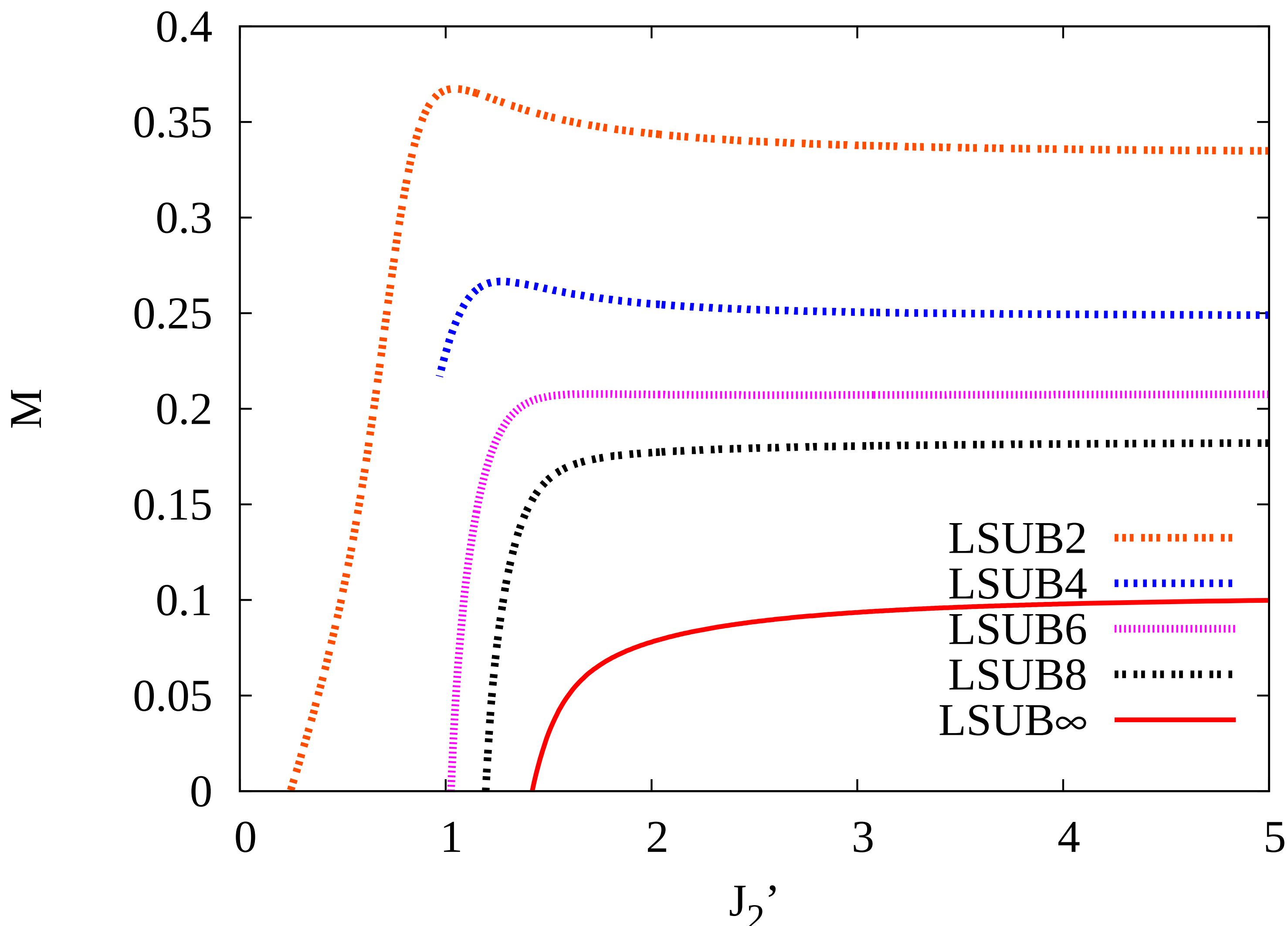
Onsite Magnetization (Order Parameter) versus J_2' in Striped Phases

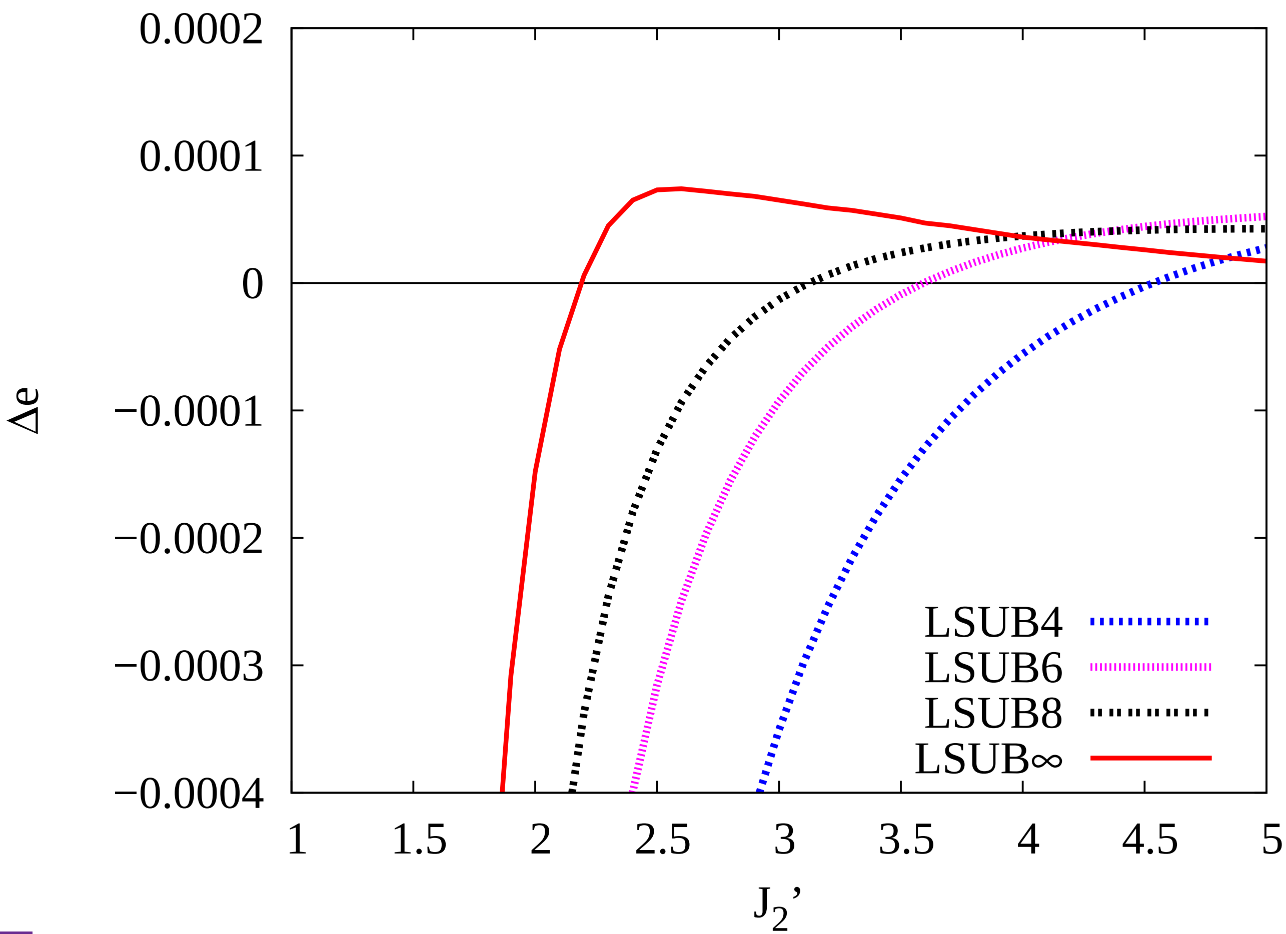
($s = 1/2$ case)



Energy Difference Between Spiral and Striped Phases versus J_2'

($s = 1/2$ case)

- 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

SPIN-1 CASE

1. Néel and Spiral Phases

- again, for $|\Phi\rangle = |\Phi_{\text{spiral}}\rangle$ we treat pitch angle ϕ as a variable to be chosen so that $E_{\text{SUB}m-m}(\phi) =$ min at $\phi = \phi_{\text{SUB}m-m}$
- again, we observe how $\phi \rightarrow \frac{1}{2}\pi$ as $J_2' \rightarrow \infty$ faster than for the corresponding classical case, but by no means as fast as for the $s = 1/2$ case considered previously
- again, we often obtain (real) solutions only for certain ranges of ϕ depending on the value of $\kappa \equiv J_2'/J_1$, with termination points clearly seen, exactly as in the $s = 1/2$ case considered previously

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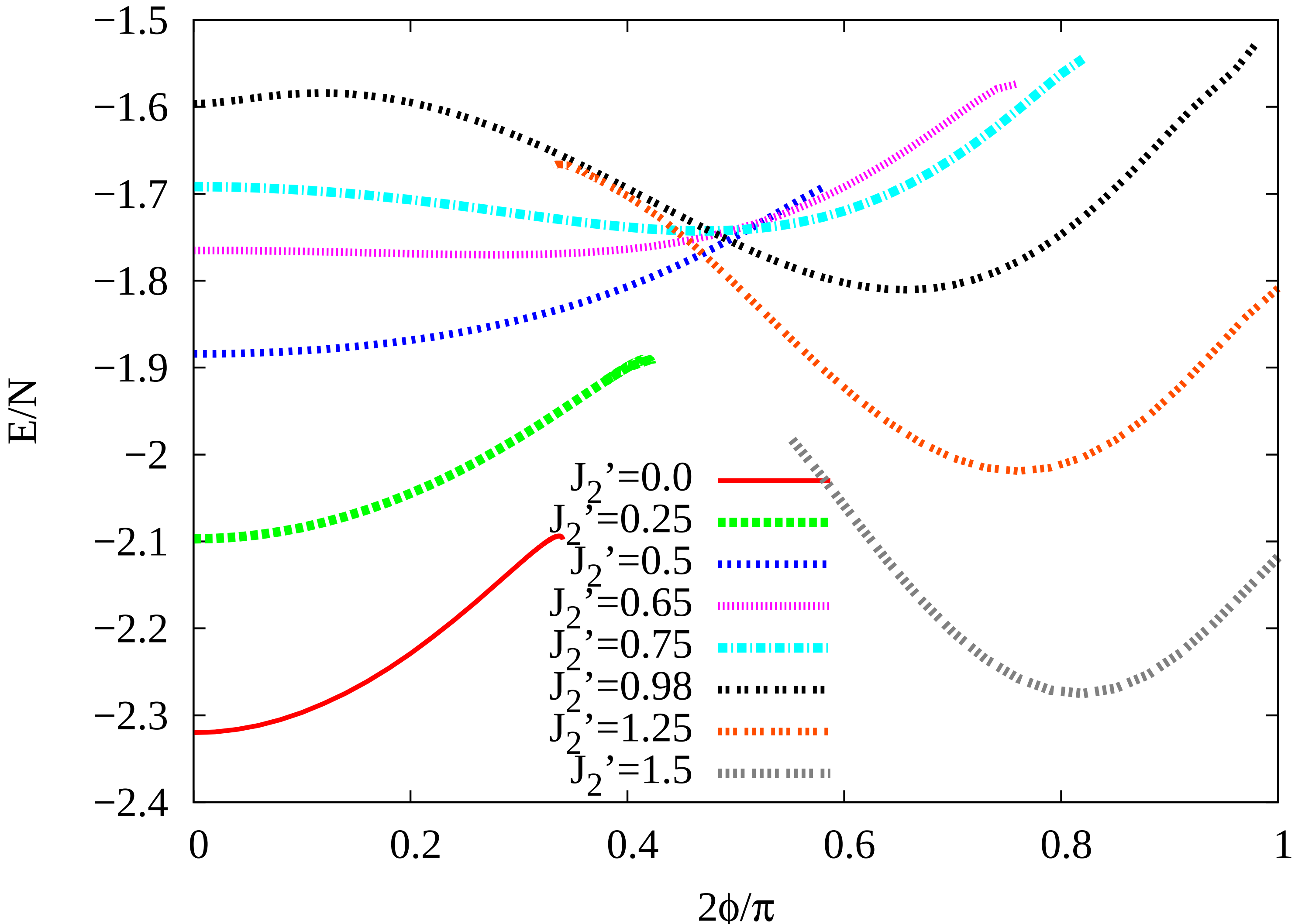
GS Energy versus Pitch Angle for Spiral Phase

($s = 1$ case; SUB4–4 results shown)



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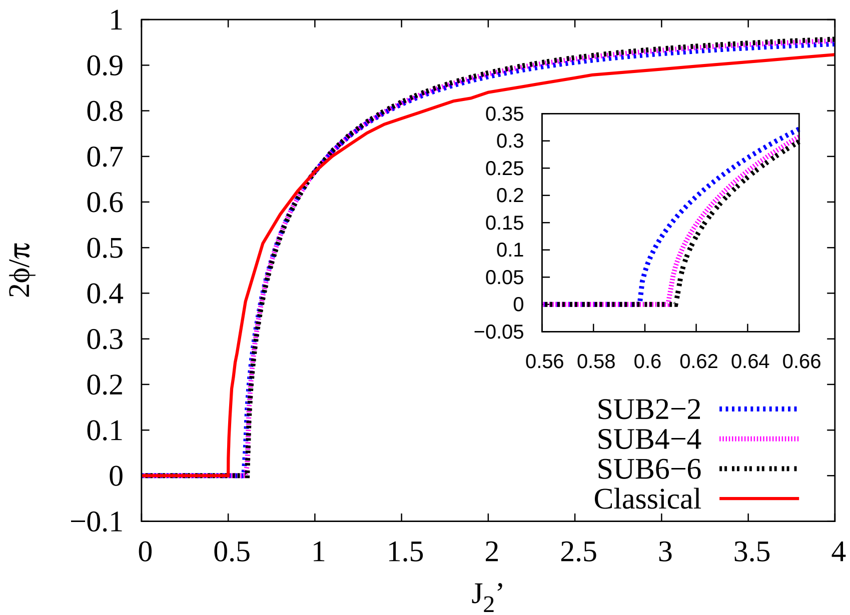
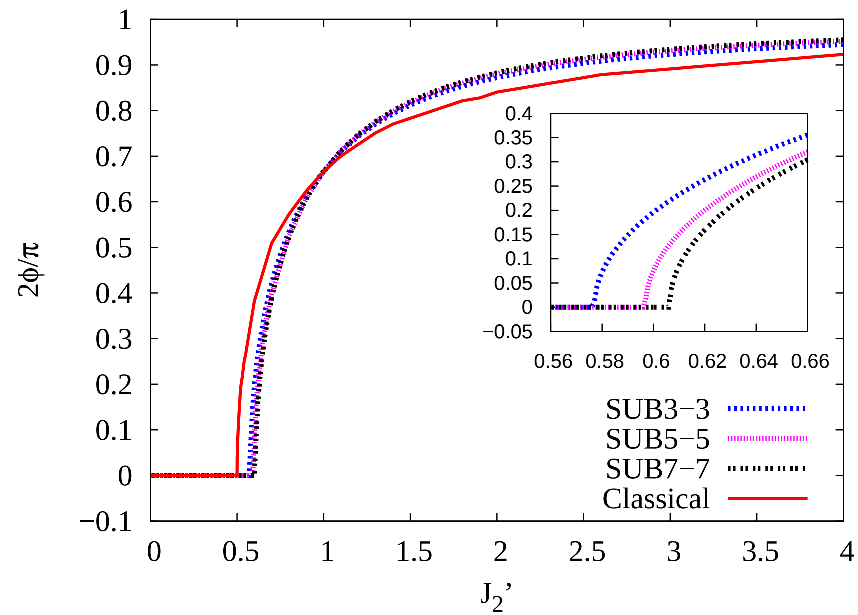
Pitch Angle $\phi = \phi_{\mathrm{SUBm-m}}$ of Spiral Phase versus J_2' ($\phi = 0 \Rightarrow$ Néel Phase)

($s = 1$ case)



(a) SUBm–m; $m = \{2, 4, 6\}$



(b) SUBm–m; $m = \{3, 5, 7\}$

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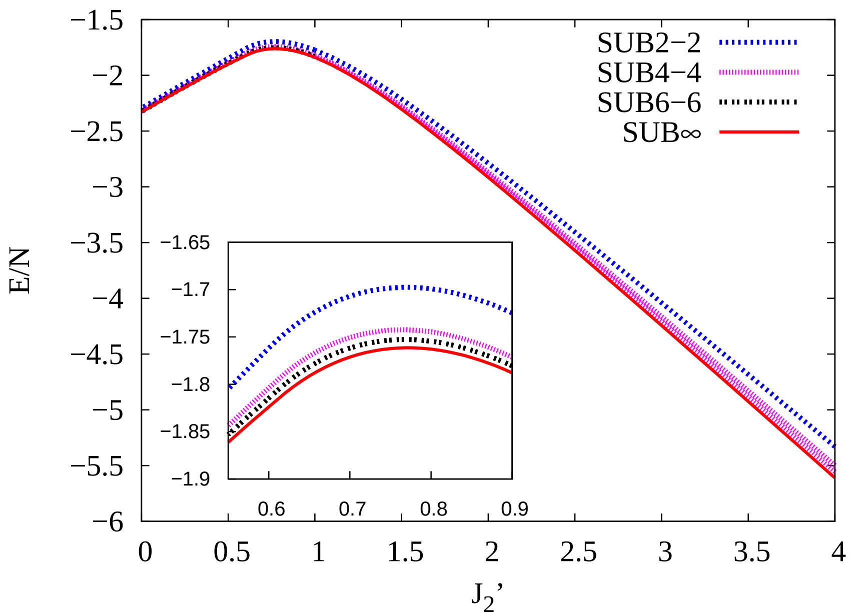
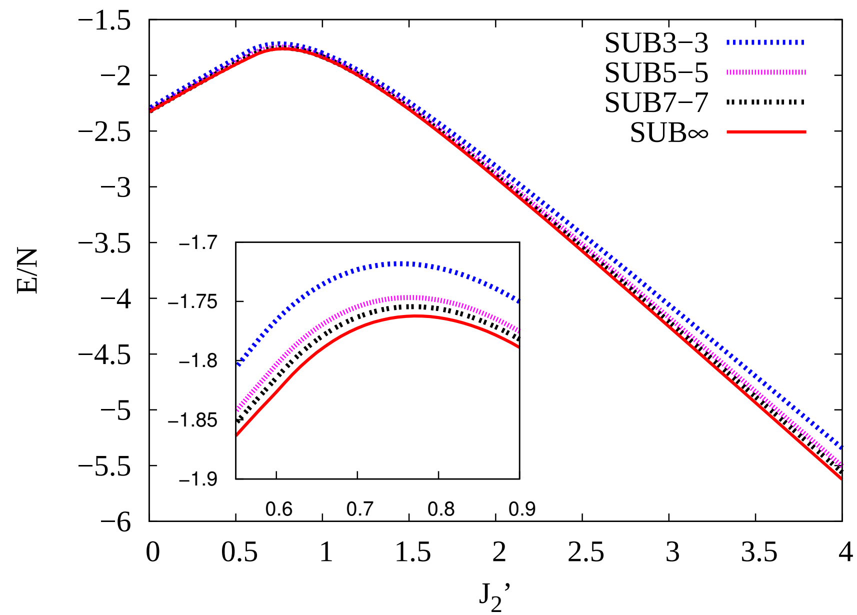
GS Energy versus J_2' in Néel and Spiral Phases

($s = 1$ case)



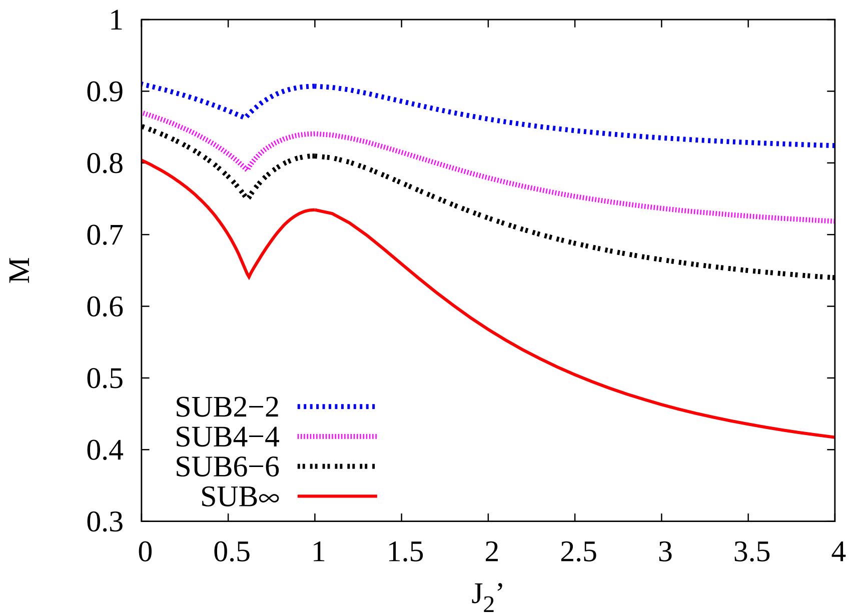
(a) SUBm–m; $m = \{2, 4, 6\}$



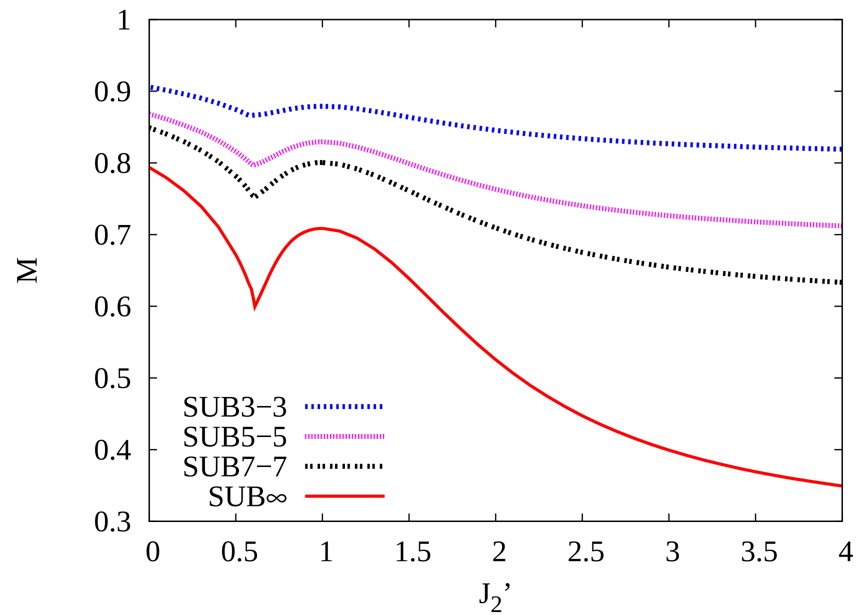
(b) SUBm–m; $m = \{3, 5, 7\}$

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

($s = 1$ case)



(a) SUBm–m; $m = \{2, 4, 6\}$



(b) SUBm–m; $m = \{3, 5, 7\}$

Results for Isotropic HAF on Square and Triangular Lattices

($s = 1$ case)

Method	E/N	M	E/N	M
	square ($\kappa = 0$)		triangular ($\kappa = 1$)	
SUB2–2	-2.29504	0.9100	-1.77400	0.9069
SUB3–3	-2.29763	0.9059	-1.80101	0.8791
SUB4–4	-2.31998	0.8702	-1.82231	0.8405
SUB5–5	-2.32049	0.8682	-1.82623	0.8294
SUB6–6	-2.32507	0.8510	-1.83135	0.8096
SUB7–7	-2.32535	0.8492	-1.83288	0.8006
Extrapolations				
SUB∞ [a]	-2.32924	0.8038	-1.83860	0.7345
SUB∞ [b]	-2.32975	0.7938	-1.83968	0.7086
SWT–3	-2.3282	0.8043		
SE	-2.3279(2)	0.8039(4)		

[a] Using SUBm–m; $m = \{2, 4, 6\}$

[b] Using SUBm–m; $m = \{3, 5, 7\}$

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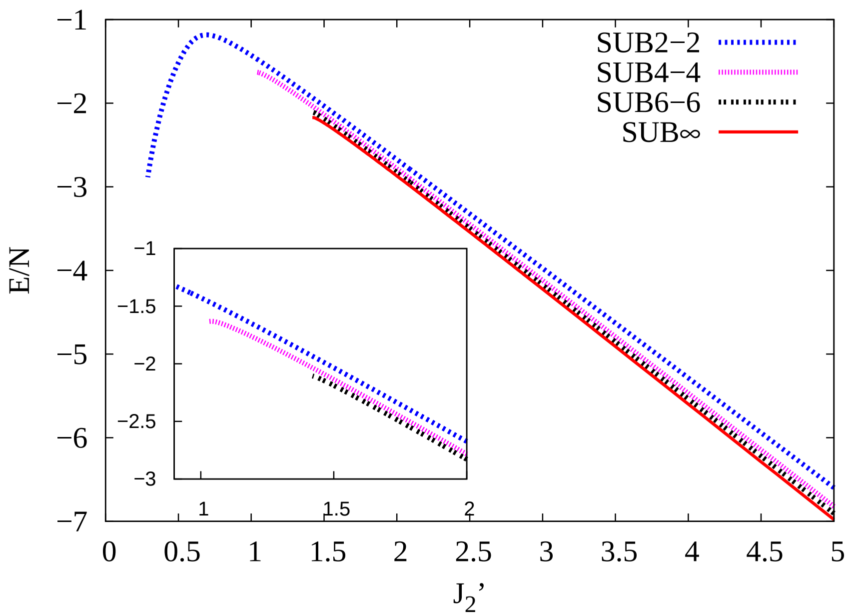
- we observe now a second-order quantum phase transition at a *critical point* $\kappa_c = 0.62 \pm 0.01$ ($\kappa \equiv J_2'/J_1$) [c.f. second-order classical transition at $\kappa_{\rm cl} = 0.5$ for $s \to \infty$ case, and weakly first-order transition at $\kappa_c \equiv 0.80 \pm 0.01$ for $s = 1/2$ case]
- where the collinear Néel order continues to exist to larger frustration than in the classical counterpart, but not to such high value of frustration as for the intrincally more quantum-mechanical $s = 1/2$ counterpart

2. Spiral and Striped Phases

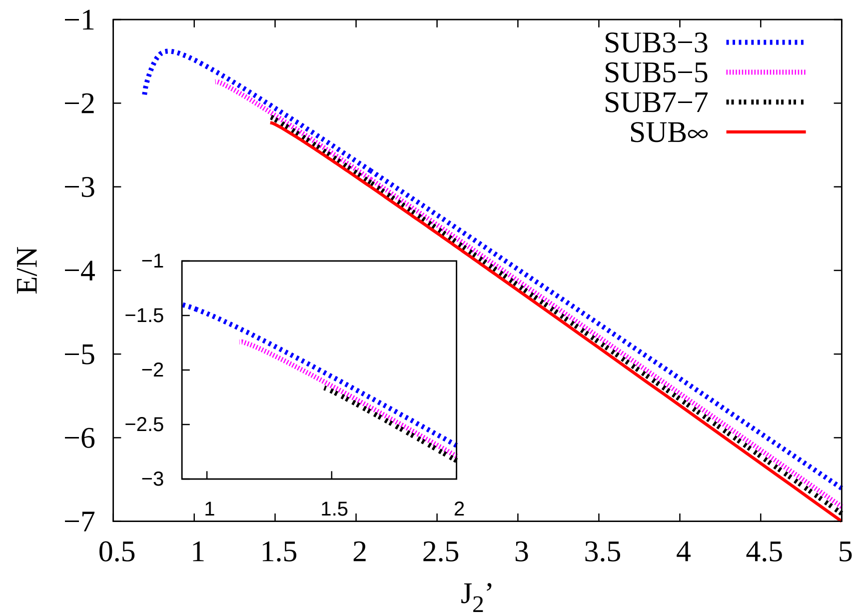
- once again we also use $|\Phi\rangle \rightarrow |\Phi_{\text{stripe}}\rangle$ as an alternative CCM model state
- and now we recall again that although the spiral phase approaches collinearity ($\phi = \frac{1}{2}\pi$) for the uncoupled 1D chain limit (as $J_2' \rightarrow \infty$) faster than in the corresponding classical model, the approach is not as rapid as for the $s = 1/2$ counterpart
  $\rightarrow$ the striped phase, if it exists at all, is likely to be even more fragile than in the $s = 1/2$ case

GS Energy versus J_2' in Striped Phase

($s = 1$ case)



(a) SUBm–m; $m = \{2, 4, 6\}$



(b) SUBm–m; $m = \{3, 5, 7\}$

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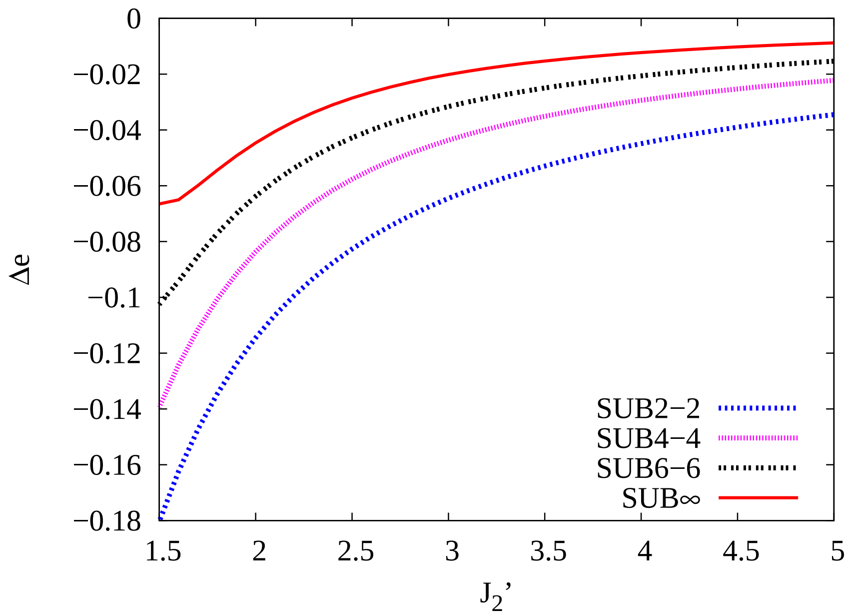
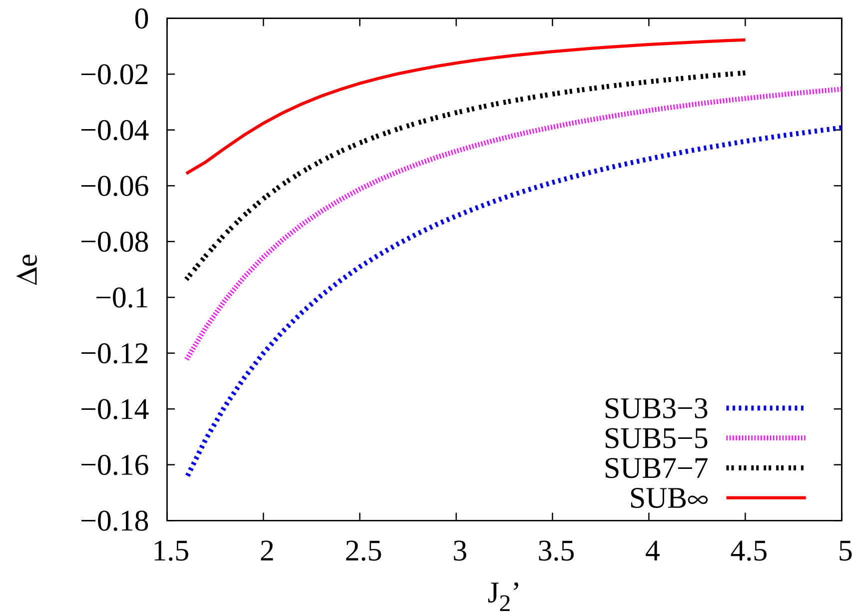
Energy Difference Between Spiral and Striped Phases versus J_2'

($s = 1$ case)

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



(a) SUBm–m; $m = \{2, 4, 6\}$



(b) SUBm–m; $m = \{3, 5, 7\}$

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- we observe now the spiral phase always lies considerably lower in energy than the striped phase for the $s = 1$ case, at all values of J_2', compared with the much smaller energy advantage of the striped phase over the spiral phase for values of $\kappa > \kappa_{c_2} = 1.8 \pm 0.4$ in the $s = 1/2$ case
- and hence, that for the $s = 1$ case, there is no second phase transition from a spiral to a striped phase, unlike in the $s = 1/2$ case

- 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 one example used here for an illustration
- We, and our collaborators, have studied many other spin-lattice models using the CCM – by now there are probably more than 100 papers on such applications

THANK YOU FOR YOUR ATTENTION!