A FRUSTRATED SPIN-1/2 HEISENBERG MAGNET ON A HONEYCOMB BILAYER:

A High-Order Coupled Cluster Study of its Phase Diagram

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Outline of Talk

1. INTRODUCTION
   - J_1–J_2–$J_1^\perp$ Model on a Honeycomb-Lattice Bilayer
   - The Coupled Cluster Method
2. RESULTS
   - Results on the Honeycomb-Lattice Bilayer
     - The spin-1/2 J_1–J_2–$J_1^\perp$ Heisenberg model
3. SUMMARY
   - Conclusions

References

R.F. Bishop and P.H.Y. Li, PRB **95**, 134414 (2017)

P.H.Y. Li and R.F. Bishop, AIP Conf. Proc. **1912**, 020011 (2017)

P.H.Y. Li and R.F. Bishop, JMMM **482**, 262 (2019)

P.H.Y. Li and R.F. Bishop, JMMM **555**, 169307 (2022)

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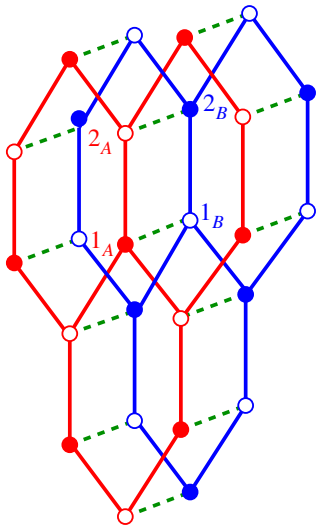
J_1–J_2–$J_1^\perp$ Model on the Honeycomb-Lattice Bilayer

- J_1–J_2–$J_1^\perp$ model on a honeycomb-lattice *AA*-stacked bilayer (i.e., all bonds of Heisenberg type); 4 sites per unit cell
- We'll look at the case with $s = \frac{1}{2}$ spins (viz., the most quantum case)
- $$H = J_1 \sum_{\langle i,j\rangle,\alpha} \mathbf{s}_{i,\alpha} \cdot \mathbf{s}_{j,\alpha} + J_2 \sum_{\langle\langle i,k\rangle\rangle,\alpha} \mathbf{s}_{i,\alpha} \cdot \mathbf{s}_{k,\alpha} + J_1^\perp \sum_i \mathbf{s}_{i,A} \cdot \mathbf{s}_{i,B}$$

  (where $\langle i,j\rangle$ and $\langle\langle i,k\rangle\rangle$ run, respectively, over all NN and NNN intralayer pairs; $\alpha = A, B$ labels the two layers; and we set $J_1 > 0$)



$= = = J_1$: NN intralayer bond

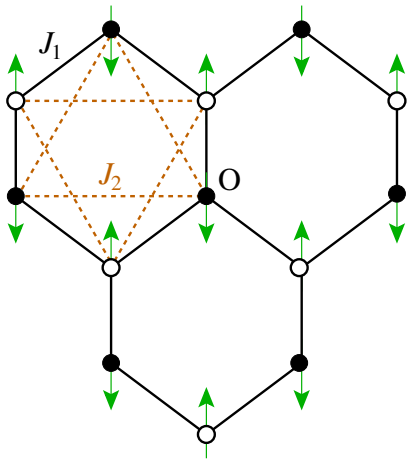
$= = = J_1^\perp$: NN interlayer bond

J_2: NNN intralayer bonds (not shown)

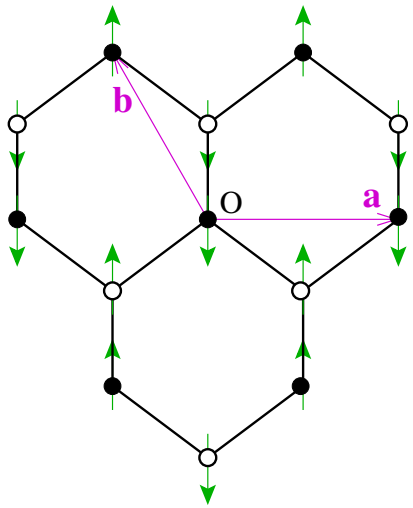
Limiting Cases

- limiting bond cases:
  - $J_2 = 0$: isotropic HAF on 2D honeycomb lattice
  - $J_1 = 0$: two uncoupled isotropic HAFs on two non-overlapping 2D triangular lattices
- classical limit ($s \to \infty$):
  - for $J_1 > 0$; $J_2 \equiv \kappa J_1 > 0$: ground-state (GS) phase diagram contains 2 different ordered phases;
    - Néel: $\kappa \leq \frac{1}{6}$
    - Spiral-I: $\kappa > \frac{1}{6}$
- spin-$\frac{1}{2}$ monolayer case:
  - when $J_1^\perp = 0$ the classical critical point at $\kappa = \frac{1}{6}$ is broken into (at least) 2 quantum critical points, such that:
    - quasiclassical Néel state is the stable GS for $\kappa \leq \kappa_{c_1}^{>} \approx 0.18$
    - another quasiclassical AFM state (viz. the Néel-II state) is the stable GS for $\kappa_{c_2}^{<} \leq \kappa \leq \kappa_{c_2}^{>}$, where $\kappa_{c_1}^{>} < \kappa_{c_2}^{<} \approx 0.44$ and $\kappa_{c_2}^{>} \approx 1.5$

Quasiclassical AFM Phases ($J_1 > 0$)



(a) Néel



(b) Néel-II (one of 3 equivalent states)

- Shown in (a) are the J_1 and J_2 bonds, and in (b) the triangular Bravais lattice vectors
- Even after many studies there is still no consensus on the GS phase diagram for the $s = \frac{1}{2}$ case
- To try to shed more light we now investigate the corresponding J_1–J_2–$J_1^\perp$ bilayer case where the two layers in AA-stacking are now coupled by interlayer NN $J_1^\perp$ bonds of either sign

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The Coupled Cluster Method (CCM)

- The CCM is one of the most pervasive, most powerful and most accurate of all *ab initio* formulations of microscopic quantum many-body theory.
- It has probably been applied to more systems in quantum chemistry, quantum field theory, atomic, nuclear, subnuclear, condensed matter and other areas of physics than *any* other competing method.
- It has yielded numerical results that are among the most accurate available for an incredibly wide range of both finite and extended physical systems defined on a spatial continuum, including, e.g.: $\longrightarrow$

The Coupled Cluster Method

- atoms and molecules of interest in atomic physics and quantum chemistry, where the CCM is the gold standard
- electron gas (or jellium – the one-component Coulomb plasma)
- atomic nuclei
- dense nuclear and baryonic matter
- models in quantum optics and solid-state optoelectronics
- continuum quantum field theories
  - ϕ^4 field theory
  - pions and nucleons with isovector, pseudoscalar coupling
- quantum fluid mechanics of a condensed Bose fluid

$\Rightarrow$ This widespread success motivated us to extend the CCM to deal with systems on a regular spatial lattice, e.g.:

- lattice quantum field theories
  - $\mathrm{O}(4)_{D+1}$ nonlinear sigma model [chiral meson field theory]
  - SU(N) lattice gauge field theories [e.g., lattice QED, QCD]
- spins [spin-lattice problems in **quantum magnetism**] $\rightarrow$
- electrons [e.g., lattice Hubbard model, etc.]

Elements of the CCM: GS Formalism

We use the (normal) coupled cluster method (CCM):

- ground-state (GS) wavefunction:

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

$$S = \sum_{I\neq 0} \mathcal{S}_I C_I^+;\quad \tilde{S} = \mathbb{1} + \sum_{I\neq 0} \tilde{\mathcal{S}}_I C_I^- \quad \left(\Rightarrow\ \langle\Phi|\tilde{\mathcal{S}} = \frac{\langle\Phi|e^{S^\dagger}e^S}{\langle\Phi|e^{S^\dagger}e^S|\Phi\rangle}\right),$$

$$C_0^+ \equiv \mathbb{1};\quad C_I^- \equiv (C_I^+)^\dagger;\quad C_I^-|\Phi\rangle = 0,\ \forall I \neq 0$$

- I is a multi-configurational (i.e., many-body) set index
- choose reference (or model) state $|\Phi\rangle$ to be a generalized vacuum state (or cyclic vector) $\Rightarrow$ $\{C_I^+|\Phi\rangle\}$ is a complete set of wf's; and $[C_I^+, C_J^+] = 0$
- we can always choose the $C_I^+|\Phi\rangle$ to be orthonormalized:

$$\Rightarrow\quad \langle\Phi|C_I^- C_J^+|\Phi\rangle = \delta_{I,J}\,;\quad \sum_I C_I^+|\Phi\rangle\langle\Phi|C_I^- = \mathbb{1}$$

- $\Rightarrow$ explicit expressions: $\mathcal{S}_I = \langle\Phi|C_I^-\mathcal{S}|\Phi\rangle\,;\quad \tilde{\mathcal{S}}_I = \langle\Phi|\tilde{S}C_I^+|\Phi\rangle$
- **example**: for spin-lattice systems choose model (or reference) state $|\Phi\rangle$ to be, e.g., a classical GS [i.e., here Néel and Néel-II on each layer and NN interlayer pairs either aligned (for $\delta < 0$) or anti-aligned (for $\delta > 0$)]
- choose spin axes on each site so $|\Phi\rangle = |\downarrow\downarrow\cdots\downarrow\rangle$ in these local axes $\Longleftrightarrow$ a set of local passive rotations
- $\Rightarrow$ $C_I^+ \to s_{\ell_1}^+ s_{\ell_2}^+ \cdots s_{\ell_m}^+;\quad s_\ell^+ \equiv s_\ell^x + \mathrm{i}s_\ell^y,$ in local axes

Elements of the CCM: GS Formalism

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

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

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

$$\Longrightarrow \quad E = \langle\Phi|\mathrm{e}^{-S}H\,\mathrm{e}^{S}|\Phi\rangle = \langle\Phi|H\,\mathrm{e}^{S}|\Phi\rangle$$

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

$$\Longrightarrow \quad \langle\Phi|\widetilde{S}\,(\mathrm{e}^{-S}H\,\mathrm{e}^{S} - E\mathbb{1})C_I^+|\Phi\rangle = 0\,, \quad \forall I \neq 0$$

$\hookrightarrow$ a coupled set of linear generalized eigenvalue equations for $\{\widetilde{\mathcal{S}}_I\}$ with $\{\mathcal{S}_I\}$ as input

Elements of the CCM: GS Formalism

- 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

  $$\mathrm{e}^{-S} H \mathrm{e}^{S} = H + [H,S] + \tfrac{1}{2!}[[H,S],S] + \tfrac{1}{3!}[[[H,S],S],S] + \cdots$$

  NOTE: This series will terminate exactly after the term bilinear in S for our Heisenberg Hamiltonians $\Longrightarrow$
- CCM satisfies:
  - the Goldstone linked cluster theorem – very important, and
  - the Hellmann-Feynman theorem – equally (or more) important

  for *all* truncations on the complete set $\{I\}$ (same for S and $\widetilde{S}$)
- We use the natural lattice geometry to define the approximation schemes and we retain all distinct fundamental configurations in the set $\{I\}$ with respect to all space- and point-group symmetries of both the Hamiltonian and the model state $|\Phi\rangle$: number N_f
- A similar CCM parametrization also exists for excited states

CCM Truncation Schemes

- The only approximation is to truncate set $\{I\}$
  - for $s = \frac{1}{2}$ case we use the LSUBm scheme where 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$m \equiv$ SUB$2sm$–m for general spin-s case, (i.e., LSUB$m \equiv$ SUBm–m only for $s = \frac{1}{2}$ case)
- For a given LSUBm approximation we have $N_f = N_f(m)$
  - Here, e.g., $N_f(10) \approx 2 \times 10^5$ for the Néel-II model state on each monolayer for both $\delta > 0$ and $\delta < 0$

Universal CCCM code

We have developed a universal code (CCCM) (freely available at https://www-e.uni-magdeburg.de/jschulen/ccm/) for solving *all* such spin-lattice models based on *any* single-spin product state $|\Phi\rangle$, with elements:

- Derive the equations for $\{\mathcal{S}_I, \widetilde{\mathcal{S}}_I;\ \forall I \neq 0\}$ by the following steps:
  - evaluate H in the local rotated axes for chosen model state $|\Phi\rangle$
  - enumerate all $N_f(m)$ independent multispin-flip configurations $I \in$ LSUBm [i.e., find all lattice animals (or polyominos) up to size m and populate them]
  - evaluate $e^{-S} H e^{S} |\Phi\rangle$ by computer algebra at LSUBm level
  - pattern match to find terms in above with a nonzero overlap with $\langle\Phi| C_I^-$, $\forall I \in$ LSUBm, taking into account all available symmetries, and using computer algebra to evaluate
- Solve the corresponding coupled set of nonlinear multinomial equations for the set $\{\mathcal{S}_I\}$, $\langle\Phi| C_I^- e^{-S} H e^{S} |\Phi\rangle = 0$, one for each $I \in$ LSUBm
- Solve the coupled set of linear equations for the set $\{\widetilde{\mathcal{S}}_I\}$, $\langle\Phi| \widetilde{S} e^{-S} H e^{S} - E\mathbb{1}) C_I^+ |\Phi\rangle = 0$, one for each $I \in$ LSUBm, using the set $\{\mathcal{S}_I\,, \forall I \in$ LSUB$m\}$ so obtained above as input

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 $\Longrightarrow$ no finite-size scaling
- for the GS (in the $s_T^z \equiv \sum_{i=1}^{N} s_{l_i}^z = 0$ sector in the original unrotated axes) calculate E/N and magnetic order parameter (i.e., local average onsite magnetization) $M \equiv -\frac{1}{N} \sum_{i=1}^{N} \langle \tilde{\Psi} | s_{\ell_i}^z | \Psi \rangle$ in the local rotated axes, where $\ell_i \equiv (k_i, \alpha)$ labels sites on both layers $\alpha = A, B$
- for excited states (in the $|s_T^z| = 1$ sector) calculate the spin gap Δ to the lowest-lying (triplet) excitation
- 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
  - $M = b_0 + b_1 m^{-1/2} + b_2 m^{-3/2}$ for highly frustrated models or near a QCP
  - $\Delta = d_0 + d_1 m^{-1} + d_2 m^{-2}$

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Preliminaries

- The relevant parameters are now:
  - $\kappa \equiv J_2/J_1 > 0$: the intralayer frustration parameter (when $J_1 > 0$)
  - $\delta \equiv J_1^{\perp}/J_1$: the interlayer coupling parameter
- The effect of δ is to cause competition without frustration:
  - classically ($s \to \infty$) δ has no effect at all
  - for $\delta > 0$ (AFM interlayer coupling) the effect (for $s = \frac{1}{2}$) is to promote spin-singlet NN interlayer dimers $\Rightarrow$ an interlayer dimerized VBC (IDVBC) state as $\delta \to \infty$
  - for $\delta < 0$ (FM interlayer coupling) the effect (for $s = \frac{1}{2}$) is to align the spins of NN interlayer pairs $\Rightarrow$ we expect the system to approach a spin-1 J_1–J_2 honeycomb-lattice monolayer as $\delta \to -\infty$
- So, we examine the GS Néel and Néel-II phases on each layer in the κ-δ half-plane with $\kappa > 0$ [especially their respective boundaries $\kappa_{c_1}(\delta)$ and $\kappa_{c_2}(\delta)$]

RESULTS: Bilayer with $J_1 > 0$

- We study the case $J_1 > 0$; $J_2 \equiv \kappa J_1 > 0$; $J_1^{\perp} \equiv \delta J_1$ of either sign
- We obtain real solutions for a given model state (i.e., Néel or Néel-II) only for certain regions in the κ-δ phase space
- We have calculated E/N, M, Δ and also (the zero-field transverse magnetic susceptibility) χ

References

R.F. Bishop and P.H.Y. Li, PRB **95**, 134414 (2017)
P.H.Y. Li and R.F. Bishop, AIP Conf. Proc. **1912**, 020011 (2017)
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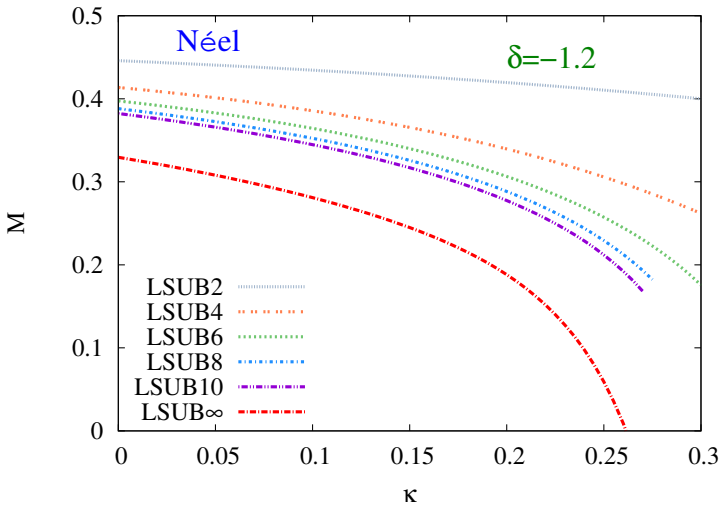
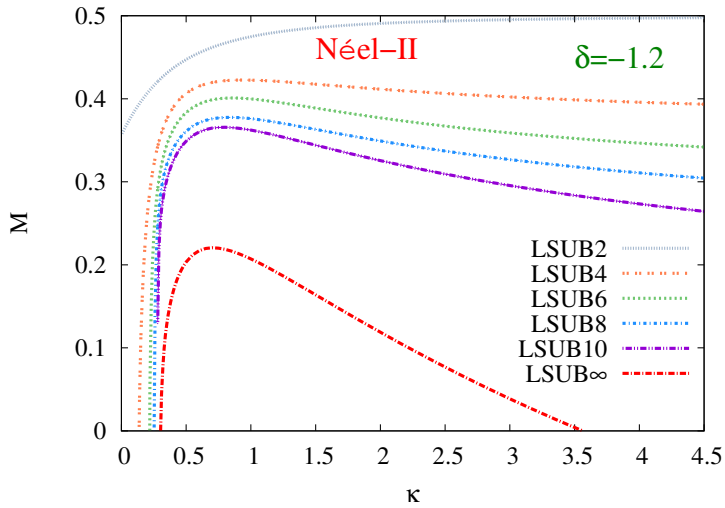
$s = \frac{1}{2}$ J_1–J_2–$J_1^\perp$ Honeycomb-Lattice Bilayer Model:

Order Parameter for the Néel and Néel-II States (for a fixed value of δ)

P.H.Y. Li and R.F. Bishop, JMMM **555**, 169307 (2022)

- $\kappa \equiv J_2/J_1$; $\delta \equiv J_1^\perp/J_1$





NOTES:

- LSUBm curves show both a $2m/(2m-1)$ staggering (as expected, which is why we show only even values of m) and a $4m/(4m-2)$ staggering for the even m values (due to the non-Bravais nature of the honeycomb lattice) $\Longrightarrow$
- LSUB∞ extrapolations are based on LSUBm data sets with $m = \{2, 6, 10\}$

$s = \frac{1}{2}$ J_1–J_2–$J_1^\perp$ Honeycomb-Lattice Bilayer Model:

Extrapolated Order Parameter for the Néel and Néel-II States (for several values of δ)

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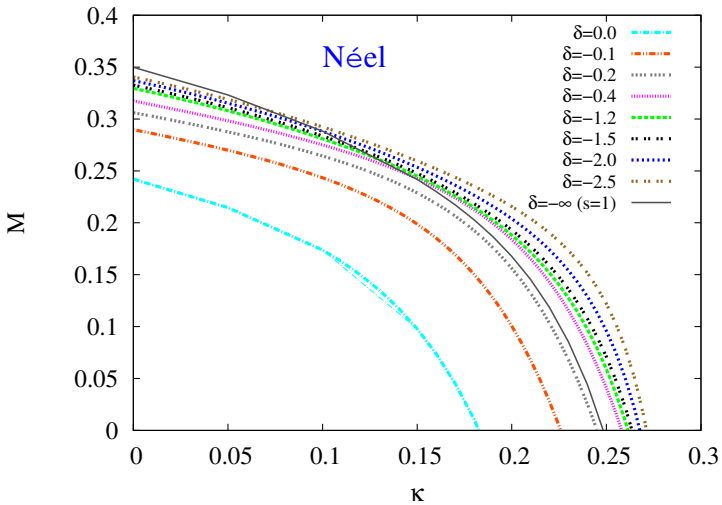
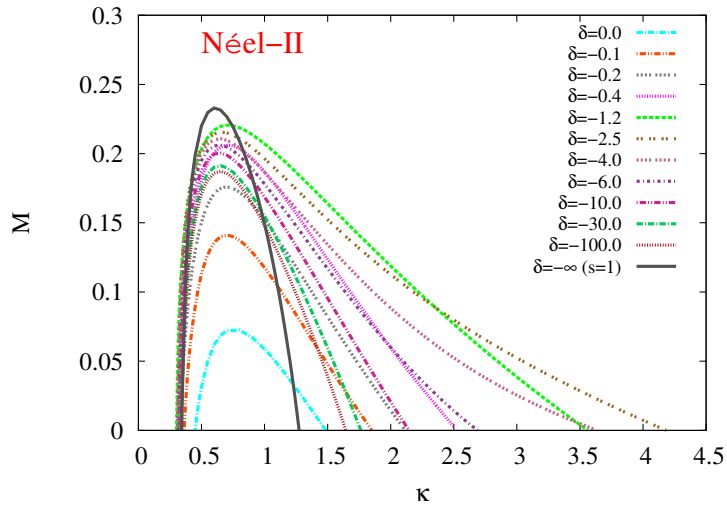
- $\kappa \equiv J_2/J_1$; $\delta \equiv J_1^\perp/J_1$





NOTES:

- LSUB∞ extrapolations are based on LSUBm data sets with $m = \{2, 6, 10\}$
- The curve labelled $\delta = -\infty (s = 1)$ uses SUBm–m data sets with $m = \{2, 6, 10\}$ for the spin-1 version of the model

$s = \frac{1}{2}$ J_1–J_2–$J_1^{\perp}$ Honeycomb-Lattice Bilayer Model:

GS Phase Boundaries of the Quasiclassical AFM States

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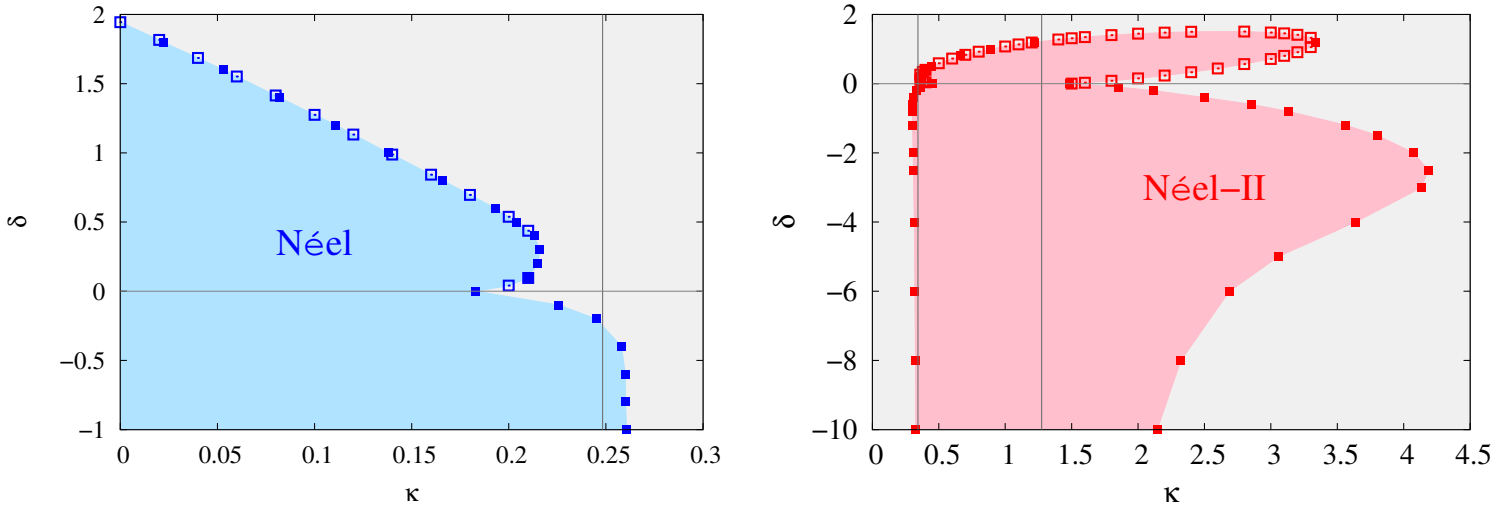
- $\kappa \equiv J_2/J_1$; $\delta \equiv J_1^{\perp}/J_1$



NOTES:

- LSUB∞ extrapolations are based on LSUBm data sets with $m = \{2, 6, 10\}$
- The filled and empty square symbols are points at which the extrapolated GS magnetic order parameter M for the Néel and Néel-II phases vanishes, for specified values of δ and κ, respectively
- The vertical lines at $\kappa = \kappa_{c_1}^{>} \approx 0.248$, $\kappa = \kappa_{c_2}^{<} \approx 0.343$ and $\kappa = \kappa_{c_2}^{>} \approx 1.274$ are taken from the extrapolated spin-1 model results using SUBm–m data sets with $m = \{2, 6, 10\}$

$s = \frac{1}{2}$ J_1–J_2–$J_1^{\perp}$ Honeycomb-Lattice Bilayer Model:

$T = 0$ Quantum Phase Diagram of the Two Collinear Quasiclassical AFM Phases

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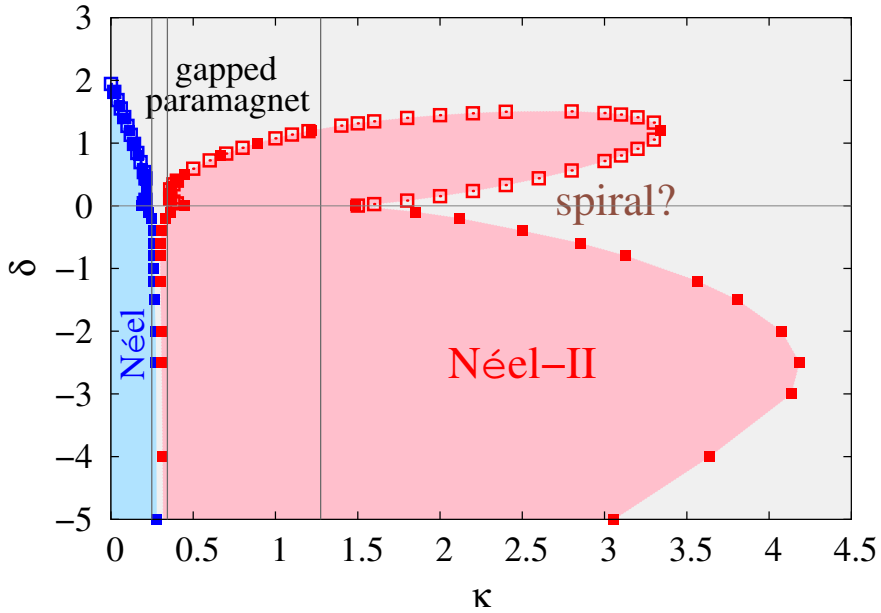
- $\kappa \equiv J_2/J_1$; $\delta \equiv J_1^{\perp}/J_1$



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Discussion

- Both the Néel and Néel-II AFM phases exhibit reentrant regimes around $\delta = 0$
- The phase boundaries of the two quasiclassical AFM phases exhibit a typical avoided crossing behaviour around $\delta = 0 \implies$ the paramagnetic region is singly connected
- The paramagnetic regime is likely to contain a mixture of at least three valence-bond crystal (VBC) phases:
  - IDVBC (interlayer dimers)
  - PVBC (plaquettes in both layers separately)
  - SDVBC (staggered dimers in both layers separately)
- The phase diagram clearly explains the observed extreme sensitivity in calculations of $\kappa^{>}_{c_1}(0)$, $\kappa^{<}_{c_2}(0)$, and $\kappa^{>}_{c_2}(0)$
- We have also calculated the spin gap Δ and the zero-field transverse magnetic susceptibility χ, which corroborate the $T = 0$ quantum phase diagram above obtained from M
- Calculations of Δ also show if a state is gapped or gapless

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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-lattice 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 Heisenberg (J_1) model on all 11 Archimedean lattices
  - the J_1–J_2 model on the square lattice
  - the J_1–J_2 model on the checkerboard lattice
  - the J_1–J_2 model on the Union Jack 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
  - the J_1–J_2–$J_1^{\perp}$ model on the square-lattice bilayer
- By now $\gtrsim$ 150 papers have used the CCM for spin lattices

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THANK YOU FOR YOUR ATTENTION!

For Further Reading

Some references for the CCM methodology and applications

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Landau's pearl of wisdom #1

It is so shameful when you derive an outstanding result and fail to understand its meaning!

Lev Landau

- Given the enormous power and manifold successes of the CCM in dealing with a huge variety of quantum many-body/field-theoretic systems, I would like to end by asking if we can try to understand the reasons for this success at a fundamental level
- In order to do so let us try to rationalize the particular choice of CCM parametrizations of the GS many-body ket and bra states, particularly the seemingly very asymmetric way in which the two fundamental CCM correlation operators S and $\widetilde{S}$ have been introduced $\longrightarrow$
- To do this it is very instructive to consider the generalization of the CCM to its time-dependent version $\longrightarrow$

Elements of the CCM: Time-Dependent Formalism

- Let the CCM correlation coefficients be time-dependent: $\{\mathcal{S}_I(t), \widetilde{\mathcal{S}}_I(t)\}$
- Define the action: $\mathcal{A} \equiv \int_{t_0}^{t_1} \mathrm{d}t \, \langle \widetilde{\Psi}(t) | (\mathrm{i}\overrightarrow{\partial}_t - H) | \Psi(t) \rangle$. Extremization of $\mathcal{A}$ is now equivalent to the time-dependent Schrödinger equations:

$$\delta\mathcal{A}/\delta\langle\widetilde{\Psi}(t)| = 0 \quad \Longrightarrow \quad \mathrm{i}\partial_t|\Psi(t)\rangle = H\,|\Psi(t)\rangle$$
$$\delta\mathcal{A}/|\Psi(t)\rangle = 0 \quad \Longrightarrow \quad -\mathrm{i}\partial_t\langle\widetilde{\Psi}(t)| = \langle\widetilde{\Psi}(t)|H$$

- Now insert the CCM parametrizations of the ket and bra states:

$$\begin{aligned}
\mathcal{A} &= \int_{t_0}^{t_1} \mathrm{d}t \, \langle\phi|\widetilde{S}(t)\,\mathrm{e}^{-S(t)}(\mathrm{i}\overrightarrow{\partial}_t - H)\,\mathrm{e}^{S(t)}|\Phi\rangle \\
&= \int_{t_0}^{t_1} \mathrm{d}t \, \left\{\langle\Phi|\widetilde{S}(t)\,\mathrm{i}\dot{S}|\Phi\rangle - \overline{H}(\mathcal{S}_I, \widetilde{\mathcal{S}}_I)\right\} \\
&= \int_{t_0}^{t_1} \mathrm{d}t \, \left\{\mathrm{i}\sum_{I\neq 0} \widetilde{\mathcal{S}}_I(t)\dot{\mathcal{S}}_I(t) - \overline{H}(\mathcal{S}_I, \widetilde{\mathcal{S}}_I)\right\}
\end{aligned}$$

Elements of the CCM: Time-Dependent Formalism

- Now extremize $\mathcal{A}$ with respect to all parameters $\{\mathcal{S}_I(t), \widetilde{\mathcal{S}}_I(t);\ \forall I \neq 0\}$:

$$\frac{\partial \mathcal{A}}{\partial \widetilde{\mathcal{S}}_I} = 0 \quad \Longrightarrow \quad \mathrm{i}\dot{\mathcal{S}}_I = \frac{\partial \overline{H}}{\partial \widetilde{\mathcal{S}}_I}$$

$$\frac{\partial \mathcal{A}}{\partial \mathcal{S}_I} = 0 \quad \Longrightarrow \quad -\mathrm{i}\dot{\widetilde{\mathcal{S}}}_I = \frac{\partial \overline{H}}{\partial \mathcal{S}_I}$$

- Consider an expectation value of an arbitrary operator $V(t)$:

$$\overline{V}(t) \equiv \langle \phi | \widetilde{\mathcal{S}}(t)\, \mathrm{e}^{-S(t)}\, V(t)\, \mathrm{e}^{S(t)} | \Phi \rangle \equiv \overline{V}(\mathcal{S}_I, \widetilde{\mathcal{S}}_I; t)$$

By the usual chain rule of partial differentiation $\longrightarrow$

$$\frac{\mathrm{d}\overline{V}}{\mathrm{d}t} = \frac{\partial \overline{V}}{\partial t} + \sum_{I \neq 0} \left\{ \frac{\partial \overline{V}}{\partial \mathcal{S}_I} \frac{\mathrm{d}\mathcal{S}_I}{\mathrm{d}t} + \frac{\partial \overline{V}}{\partial \widetilde{\mathcal{S}}_I} \frac{\mathrm{d}\widetilde{\mathcal{S}}_I}{\mathrm{d}t} \right\}$$

Hence, from the above equations of motion for $\{\mathcal{S}_I(t), \widetilde{\mathcal{S}}_I(t)\}$ $\longrightarrow$

Elements of the CCM: Time-Dependent Formalism

- The CCM equation of motion for the expectation value $\overline{V}(t)$:

$$\frac{\mathrm{d}\overline{V}}{\mathrm{d}t} = \frac{\partial \overline{V}}{\partial t} + \{\overline{V}, \overline{H}\}$$

which is just the usual classical Hamilton's equation of motion in terms of the generalized classical Poisson (or Moyal) bracket defined as $\longrightarrow$

$$\{\overline{A}, \overline{B}\} \equiv \frac{1}{\mathrm{i}} \sum_{I \neq 0} \left\{ \frac{\partial \overline{A}}{\partial \mathcal{S}_I} \frac{\partial \overline{B}}{\partial \widetilde{\mathcal{S}}_I} - \frac{\partial \overline{A}}{\partial \widetilde{\mathcal{S}}_I} \frac{\partial \overline{B}}{\partial \mathcal{S}_I} \right\}$$

- The above CCM equation of motion for $\overline{V}(t)$ is just the exactly mapped counterpart in the CCM phase space $\mathscr{P}$ of the usual Heisenberg equation of motion for operator $V(t)$ in the original Hilbert space $\mathscr{H}$:

$$\frac{\mathrm{d}V}{\mathrm{d}t} = \frac{\partial V}{\partial t} + \frac{1}{\mathrm{i}}[V, H]$$

We can now make this exact classicization map $\mathscr{H} \mapsto \mathscr{P}$ even clearer by defining sets of c-number CCM fields $\{\phi_I\}$ and their c-number canonically conjugate CCM momentum densities $\{\pi_I\}$ $\longrightarrow$

$$\phi_I \equiv \frac{1}{\sqrt{2}}(\mathcal{S}_I + \widetilde{\mathcal{S}}_I)\,; \quad \pi_I \equiv -\frac{\mathrm{i}}{\sqrt{2}}(\mathcal{S}_I - \widetilde{\mathcal{S}}_I)$$

Elements of the CCM: Time-Dependent Formalism

- In terms of $\{\phi_I, \pi_I\}$ the generalized Poisson bracket takes the form:

$$\{\overline{A}, \overline{B}\} = \sum_{I \neq 0} \left\{ \frac{\partial \overline{A}}{\partial \phi_I} \frac{\partial \overline{B}}{\partial \pi_I} - \frac{\partial \overline{A}}{\partial \pi_I} \frac{\partial \overline{B}}{\partial \phi_I} \right\}$$

  which is exactly the usual classical Poisson bracket

- Hamilton's equations of motion for the new variables $\{\phi_I, \pi_I\}$ are:

$$\dot{\phi}_I = \frac{\partial \overline{H}}{\partial \pi_I} = \{\phi_I, \overline{H}\}\,; \quad \forall I \neq 0\,,$$

$$\dot{\pi}_I = -\frac{\partial \overline{H}}{\partial \phi_I} = \{\pi_I, \overline{H}\}\,; \quad \forall I \neq 0$$

- The phase space $\mathscr{P} \ni \{\phi_I, \pi_I; \forall I \neq 0\}$ has the symplectic structure,

$$\{\phi_I, \pi_J\} = \delta_{I,J}\,; \quad \forall I \neq 0\,, J \neq 0\,,$$

$$\{\phi_I, \phi_J\} = 0 = \{\pi_I, \pi_J\}\,.$$

- To complete this description of a complete and exact classicization of an arbitrary quantum many-body theory, we need also to show that the expectation value of the commutator between an arbitrary pair of operators A and B in the original Hilbert space $\mathscr{H}$ is also exactly mapped into its corresponding Poisson bracket in $\mathscr{P}$ $\longrightarrow$

Elements of the CCM: Time-Dependent Formalism

- The CCM expectation value of the product of any two operators is:

$$\overline{AB} = \langle\Phi|\widetilde{S}\,\mathrm{e}^{-S}AB\,\mathrm{e}^{S}|\Phi\rangle$$

$$= \sum_I \langle\Phi|\widetilde{S}\underbrace{\mathrm{e}^{-S}A\,\mathrm{e}^{S}C_I^+}|\Phi\rangle\langle\Phi|C_I^-\,\mathrm{e}^{-S}B\,\mathrm{e}^{S}|\Phi\rangle$$

$$= \sum_I \langle\Phi|\widetilde{S}\left[\mathrm{e}^{-S}A\,\mathrm{e}^{S},C_I^+\right]|\Phi\rangle\langle\Phi|C_I^-\,\mathrm{e}^{-S}B\,\mathrm{e}^{S}|\Phi\rangle + \sum_I \langle\Phi|\widetilde{S}C_I^+\,\mathrm{e}^{-S}A\,\mathrm{e}^{S}|\Phi\rangle\langle\Phi|C_I^-\,\mathrm{e}^{-S}B\,\mathrm{e}^{S}|\Phi\rangle$$

$$= \sum_{I\neq 0}\frac{\partial\overline{A}}{\partial\mathcal{S}_I}\frac{\partial\overline{B}}{\partial\widetilde{\mathcal{S}}_I} + \sum_I\sum_J \langle\Phi|\widetilde{S}C_I^+C_J^+|\Phi\rangle\langle\Phi|C_J^-\,\mathrm{e}^{-S}A\,\mathrm{e}^{S}|\Phi\rangle\langle\Phi|C_I^-\,\mathrm{e}^{-S}B\,\mathrm{e}^{S}|\Phi\rangle$$

$\hookrightarrow$ a formula for the CCM phase space star product: $\overline{AB} \equiv \overline{A}\star\overline{B}$

The last term is invariant under interchanges $I \rightleftharpoons J$ and $A \rightleftharpoons B$ $\longrightarrow$

- The CCM expectation value of the commutator of any two operators is:

$$\langle\Phi|\widetilde{S}\mathrm{e}^{-S}[A,B]\mathrm{e}^{S}|\Phi\rangle \equiv \overline{AB} - \overline{BA} = \overline{A}\star\overline{B} - \overline{B}\star\overline{A}$$

$$= \sum_{I\neq 0}\left\{\frac{\partial\overline{A}}{\partial\mathcal{S}_I}\frac{\partial\overline{B}}{\partial\widetilde{\mathcal{S}}_I} - \frac{\partial\overline{A}}{\partial\widetilde{\mathcal{S}}_I}\frac{\partial\overline{B}}{\partial\mathcal{S}_I}\right\} = \mathrm{i}\{\overline{A},\overline{B}\}$$

Elements of the CCM: Time-Dependent Formalism

- In summary, the CCM exactly maps $\mathscr{H} \mapsto \mathscr{P}$, from a quantum many-body theory in the Hilbert space $\mathscr{H}$ into a classical many-body theory in the CCM phase space $\mathscr{P}$, a symplectic differentiable manifold in the modern terminology of classical mechanics, as shown
  - The symplectic nature of the phase space is a direct consequence of the existence of the generalized Poisson (or Moyal) bracket, which is just a skew-symmetric bilinear form that can be used to define a Hamiltonian vector field in the tangent space of the manifold $\Longrightarrow$
  - In other words, the set of trajectories defined by the equations of motion fill the whole of the dynamically allowed region of the phase space
- The exact classicization mapping opens up the possibility of exploiting or extending techniques in classical mechanics for use in the quantum many-body problem, e.g., to make easy contact with conservation laws and the associated sum rules by using the Noether currents
- In principle, the CCM phase space $\mathscr{P}$ can now also be used to generalize to an arbitrary quantum many-body system the well-known Wigner-Weyl-Moyal-Groenewold programme of work to describe the quantum mechanics of a set of particles described by coordinates $\{x_i\}$ and momenta $\{p_i\}$ as a form of non-deterministic statistical mechanics

Elements of the CCM: Time-Dependent Formalism

- It is also intuitively apparent from the existence of this mapping $\mathscr{H} \mapsto \mathscr{P}$ onto classical mechanics that the *c*-number CCM amplitudes $\{\phi_I, \pi_I\}$ or $\{\mathcal{S}_I, \widetilde{\mathcal{S}}_I\}$, which completely characterize and decompose our many-body problem, may be viewed as a set of generalized (quasi-local) mean fields that describe each subsystem of particles (labelled by the configuration-space indices $\{I\}$) in the interacting many-body system, which mutually interact via non-local classical interactions
- Indeed, this interpretation can formally be extended to show how the CCM may very profitably also be viewed as an exact bosonization procedure in which the CCM states may be exactly associated, in a one-to-one fashion, with a set of generalized coherent states in some suitably defined boson space $\longrightarrow$ the usual Glauber coherent states are then just the associates of the lowest-order one-body mean fields
- This CCM bosonization procedure differs from other more well-known such procedures by taking the usual motivation for any bosonization scheme to its ultimate conclusion, viz., that the resultant generalized coherent boson fields are simply classical *c*-number fields with only classical (nonlinear and nonlocal) interactions between them

Landau's pearl of wisdom #2

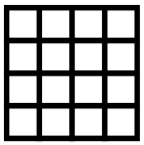
- Let Dau have the last word:

A method is more important than a discovery, since the right method will lead to new and even more important discoveries.

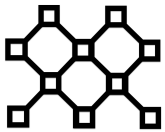
Lev Landau

The 11 Archimedean Lattices in 2D

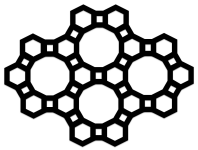
Archimedes was one of the first people to describe regular tilings in two spatial dimensions. Archimedean lattices are infinite and they are composed of arrangements of regular polygons with every site equivalent (but NN bonds may be inequivalent) $\Longrightarrow$ there are 11 uniform 2D Archimedean lattices.

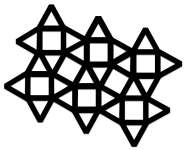

Square

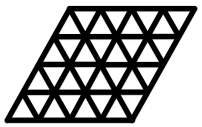

Honeycomb


CaVO

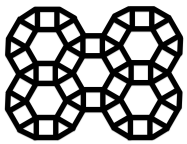
square = 4^4; honeycomb = 6^3; CaVO = $4 \cdot 8^2$

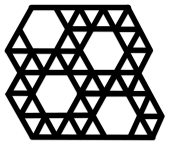

SHD

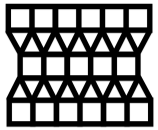

SrCuBO


Triangle

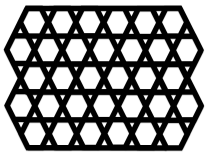
SHD = $4 \cdot 6 \cdot 12$; SrCuBO = $3^2 \cdot 4 \cdot 3 \cdot 4$; triangle = 6^3

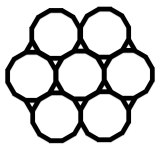

Bounce


Maple-Leaf


Trellis

bounce = $3 \cdot 4 \cdot 6 \cdot 4$; maple-leaf = $3^4 \cdot 6$; trellis = $3^3 \cdot 4^2$


Kagome


Star

kagome = $3 \cdot 6 \cdot 3 \cdot 6$; star = $3 \cdot 12^2$

– The only unfrustrated cases: square, honeycomb, CaVO, SHD
– All bonds are equivalent only on: square, honeycomb, triangle, kagome