Montauk 9/04

Ordering by Spin-wave Fluctuations in the $S \gg 1$ Heisenberg Antiferromagnet on the Pyrochlore Lattice

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Summary: an approach to find (ordered) gr. state

- start: discrete selected states [collinear]

discrete spins $\{\eta_i\}$ are <u>coefficients</u> in an expansion

$\boxed{\Rightarrow \mathcal{H}_{eff}(\{\eta_i\})}$

defined on any (discrete) state, but uncontrolled

Effective Hamiltonian approach

High frustration

$\Leftrightarrow$ macroscopic degeneracy of config.'s
$\Rightarrow$ many ways to select/mix them by small pert. ($\therefore$ rich phase diagrams à la Fermi liquid or Quantum Hall based)

? how to navigate amongst them

E.g. what is ground state in large-S limit?

[at $T < \mathcal{O}(JS)$; classical regime is $\mathcal{O}(JS) < T < \mathcal{O}(JS^2)$

Usual approach:

construct two (or more) high-symm. candidates
evaluate $\mathcal{E}$ as accurately as poss. for each

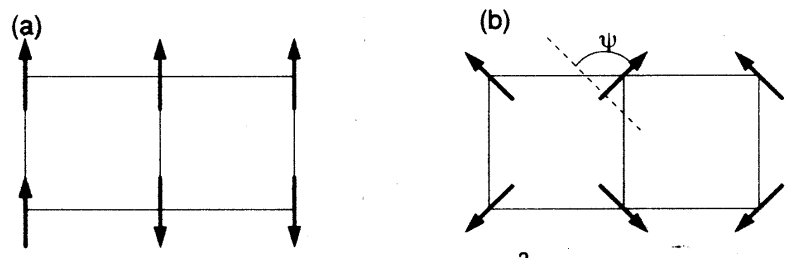
"Eff. Hamiltonian" philosophy

find $\mathcal{H}_{eff}$ defined for every state

[in a subspace defined by a previous level of selection]

Review "order by disorder"

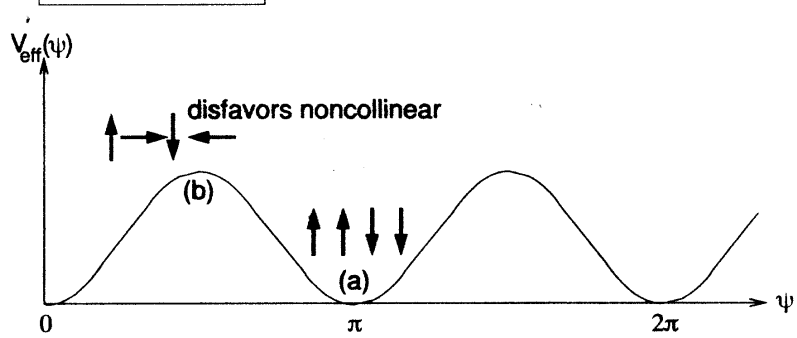
NON highly frustrated (just one global degeneracy parameter ψ)
resolve degeneracy by (harmonic) zero-point E.



same classical energy (O $J(S^2)$)
different harmonic spinwave spectra

Define effective Hamiltonian

$$\boxed{V_{eff}(\psi) = \frac{1}{2}\sum \hbar\, \omega^{\psi}(k)}$$



favors collinear

Side remark: competing selection effects

	small parameter	favors
quantum [as above]	1/S	↑↑↓↓
thermal [classical spins]	T	↑↑↓↓
dilution [quenched]	δx	↑→↓←

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Disadvantages of $\mathcal{H}_{eff}$ approach

- crude form of $\mathcal{H}_{eff}$
  [keep simplest terms — e.g. 2-spin or nearest-neighbors]

- uncontrolled derivation
  ["small parameter" may be numerically small, but can't tune to 0]

Advantages

- perhaps the right answer is not one of the ~2 states you thought of!

- not just an answer — building block for further modeling

  a) $T > 0$: use $e^{-\beta \mathcal{H}_{eff}}$ ensemble

  b) intermediate S regime

  $\mathcal{H}_{eff}$ + "flip" terms
  [e.g. ring exchange due to tunneling among discrete states]
  see von Delft + Henley ('92), Hermele et al ('03)

  $\Rightarrow$ investigate poss. of [part] disordered state

Remarks

One can also apply $\mathcal{H}_{eff}$ approach in a purely empirical fashion:

Database {many config's, their $\mathcal{E}_{eff}$}
$\Rightarrow$ fit to $\mathcal{H}_{eff}$ w/ simplest symm.-allowed terms

Not only for large-S harmonic & anharmonic!

- Kagomé Heisenberg classical low T [CLH, unpublished]

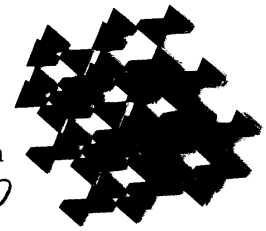
- large-N [+ large "S/N"] for ordered states of pyrochlore Heisenberg [Uzi Hizi, Prashant Sharma, CLH – current]

SEE HIZI POSTER

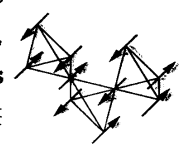
? large-N [disordered limit] for pyrochlore Heisenberg: a degeneracy of spatial config's remains at lowest order [Moessner, Tchernyshyov & Sondhi, recent]

Heisenberg Model on the Pyrochlore lattice

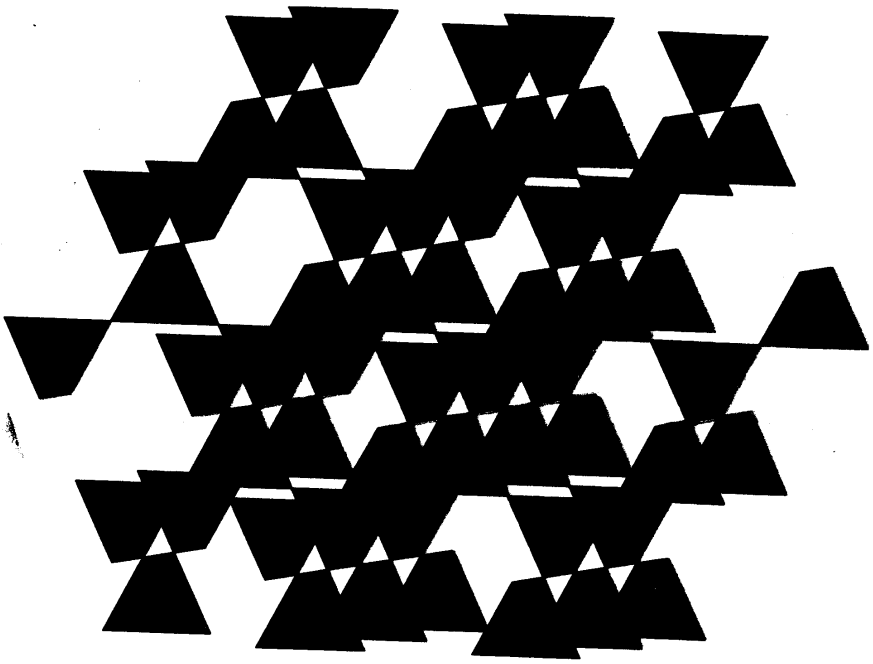
$$\mathcal{H} = J\sum_{\langle ij\rangle}\vec{S}_i\cdot\vec{S}_j = \sum_{\alpha}\left|\overbrace{\sum_{i\in\alpha}\vec{S}_i}^{\vec{L}_\alpha}\right|^2 + \text{const.}$$



- Classically, all states with zero sum in each tetrahedron are degenerate. $\vec{L}_\alpha \equiv 0$
- Thermal fluctuations do not break the degeneracy enough to make LRO (*Reimers 1992, Moessner and Chalker, 1998*).
- In large S limit, quantum fluctuations choose a subset of the collinear ground states (*Henley, APS March Meeting 2001*). Ground state is characterized by Ising variables $\vec{S}_i = \eta_i\hat{z}$, $\eta_i \in \{\pm 1\}$, $\sum_{i\in\alpha}\eta_i = 0$



- Does the large S quantum model possess long range order?



Summary/preview

- Discrete subset = collinear $\boxed{\vec{s}_i = \eta_i \hat{z}}$ $\eta_i = \pm 1$
- $\boxed{\mathcal{H}_{eff} = K \sum_{\hexagon} \prod \eta_i \quad (K>0)}$
- gives correct harmonic sp. wave ground states ($\prod_{\hexagon} \eta_i = -1$) — large unit cell!
- "gauge" symmetry is exact [for $\mathcal{E}_{harmonic}$]
- remaining infinite degeneracy but $< e^{cN}$

[onwards to ANHARMONIC – see $\boxed{\text{Uzi Hizi poster}}$]

Zero-point energy

linearize dynamics: $\boxed{\delta \dot{\vec{s}}_i = (\cdots)\, \delta \vec{s}_j}$

(details later)

$\Rightarrow$ spin wave (normal modes) $\{\omega\}$

[Note: some directions $\{\delta \vec{s}_i\}$ keep you in the ground-state manifold (though not symmetry). They have no "restoring force" $\Rightarrow \omega = 0$]

Quantize as <u>harmonic</u> <u>oscillators</u>

$\Rightarrow$ magnons (analog of phonons)

(In fact $\hbar\omega \sim |J| s \ll |E_0| \sim |J| s^2$: $\frac{1}{s}$ is the small parameter)

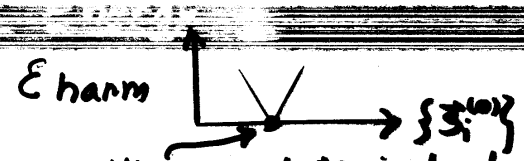
$$\boxed{E_{harm} \equiv \sum \tfrac{1}{2} \hbar \omega}$$

Different classical ground states $\{\vec{s}_i^{\,(0)}\}$ have different E_{harm} $\therefore$

$\therefore$ consider $\boxed{E_{harm}(\{\vec{s}_i^{\,(0)}\})}$ as an effective Hamiltonian (defined only on class. ground states)

True ground state has <u>E_{harm} = minimum</u>

"<u>Order</u> <u>by</u> <u>disorder</u>" (by fluctuations)



every collinear state is local minimum
[coplanar spin state on Kagomé]

collinear: $\vec{S}_i^{(0)} = s\,\eta_i \uparrow$ ± 1

<u>Mapping</u>: consider only collinear subspace (<u>discrete</u>)

(But still many: n° discrete gr. states $\sim e^{\text{const}\,N}$)

Consider $\mathcal{E}_{harm}(\{\eta_i\})$ as <u>effective</u> <u>Hamiltonian</u> on the discrete subspace

a) <u>Kagomé</u> <u>case</u>: <u>all</u> $e^{0.1N}$ coplanar states have <u>same</u> spectrum $\{\omega\} \Rightarrow$ <u>same</u> $\mathcal{E}_{harm}$!

$\Rightarrow$ need anharmonic terms to get a final unique gr. state

(E.P. Chan thesis, 1994 (with CLH))

b) <u>Pyruchlore</u> <u>case</u>: this calculation

preview of answer: collinear states have <u>different</u> $\mathcal{E}_{harm}$, but there are <u>still</u> $e^{(\text{const}\,L)}$ of minimum energy ($L \sim N^{1/3}$) DEGENERATE

at least

Dynamics (to get ω's): (semi) classical

$$\boxed{\hbar\, \dot{\vec{s}}_i = \vec{s}_i \times \vec{h}_i}$$

force

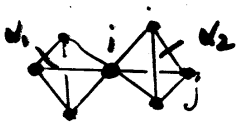
precess around this "local field"

$$\boxed{\vec{h}_i \equiv -\frac{\delta \mathcal{H}}{\delta \vec{s}_i} \equiv -|J| \sum_{\substack{\text{nearest}\\ \text{neighbor}\\ \text{of } i}} \vec{s}_j}$$

Moessner-Chalker eq. of motion (for simplex spins $\vec{L}_\alpha$)

(1998)

$$\vec{h}_i \equiv |J| \left[(L_{\alpha_1} - \vec{s}_i) + (L_{\alpha_2} - \vec{s}_i) \right]$$



$$\Rightarrow \quad \hbar\, \dot{\vec{s}}_i = -\vec{s}_i \times |J| \sum_{\alpha : i \in \alpha} \vec{L}_\alpha$$

$\vec{s}_i \times \vec{s}_i = 0$

neighbor connected by i

$$\boxed{\begin{aligned} \hbar \dot{L}_\alpha &\equiv \hbar \sum_{i \in \alpha} \dot{\vec{s}}_i \equiv |J| \sum_{i \in \alpha} \vec{s}_i \times (\vec{L}_\alpha + \vec{L}_{\beta(i)}) \\ &\equiv |J| \Big(\underbrace{\cancel{\vec{L}_\alpha \times \vec{L}_\alpha}}_{0} + \sum_{\beta \text{ nbr. to } \alpha} \vec{s}_{i(\alpha\beta)} \times \vec{L}_\beta \Big) \end{aligned}}$$

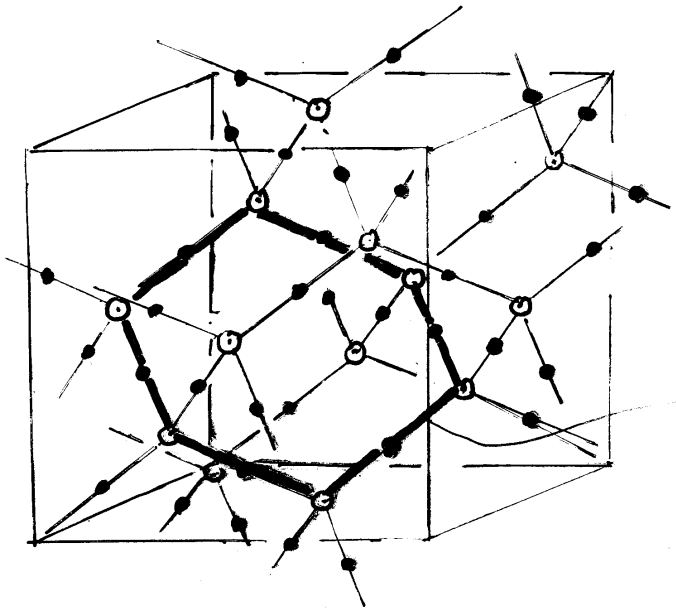
site connecting simplex α to β

linearize

$$\boxed{\hbar\, \delta \dot{\vec{L}}_\alpha = |J| \sum_\beta \vec{s}_i^{(0)}{}_{(\alpha\beta)} \times \delta \vec{L}_\beta}$$

Remark: only involves $\{\vec{L}_\alpha\}$ which live on a diamond lattice (simpler). The degrees of freedom we threw away all have $\omega \equiv 0$ $\therefore$ don't matter for E_{harm}.

EXPANDED MEDIAL LATTICE OF THE DIAMOND LATTICE.



smallest loop is 6

PYR. AS MEMBER
LATTICE OF THE
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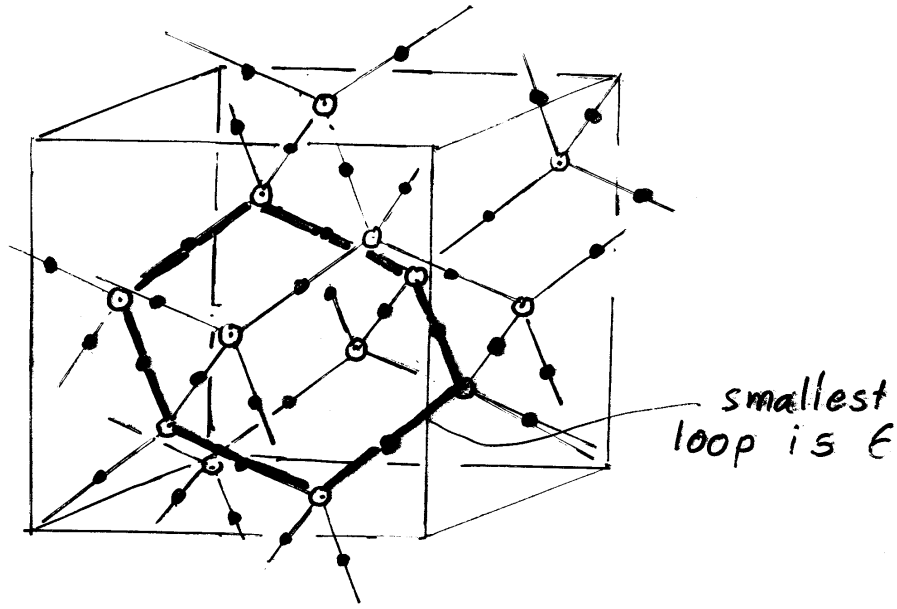


<u>Collinear case</u> $\quad \vec{S}_i^{(0)} \equiv \eta_i \hat{z}$

$$\boxed{\begin{cases} \hbar\, \delta \dot{L}_{\alpha x} = s|J| \sum_\beta \eta_{\alpha\beta}\, \delta L_{\beta y} \\ \hbar\, \delta \dot{L}_{\alpha y} = -s|J| \sum_\beta \eta_{\alpha\beta}\, \delta L_{\alpha x} \end{cases}}$$

matrix elements $\eta_{\alpha\beta} \equiv \eta_{i(\alpha\beta)}$

<u>eigenvalue eq^n</u> for frequencies

matrix square

$$\boxed{(\hbar\omega)^2 \delta L_{\alpha x} = -\hbar^2 \delta \ddot{L}_{\alpha x} = (s|J|)^2 (\underset{\sim}{\eta}^2)_{\alpha\gamma}\, \delta L_{\gamma x}}$$

$$\hbar\omega \equiv s|J| \cdot (\text{eigenvalue of } \eta^2)^{1/2}$$

$$\boxed{E_{harm}(\{\eta_i\}) \equiv \tfrac{1}{2} \sum \hbar\omega \equiv \tfrac{1}{2} \mathrm{Tr}\left((\underset{\sim}{\eta}^2)^{1/2}\right)}$$

(the matrix <u>is</u> the Ising spin configuration)

<u>Remarks</u>

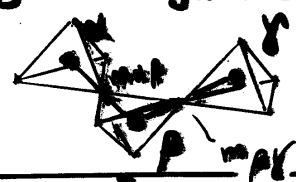
1. $\underset{\sim}{\eta}^2$ only connects even sites α, γ of diamond
   $\Rightarrow$ acts on <u>fcc</u> lattice (Bravais lattice)
   EASIER technically
2. This is <u>gauge-invariant</u>.
   Let $\sigma_\alpha = \pm 1$ on each diamond site
   set $\eta'_{\alpha\beta} \equiv \sigma_\alpha \sigma_\beta\, \eta_{\alpha\beta}$
   ($\underset{\sim}{\eta}' = \underset{\sim}{\mathcal{O}}\, \underset{\sim}{\eta}\, \underset{\sim}{\mathcal{O}}^{-1}$ orthog. matrix $\mathcal{O}$)

$$\left\{ \begin{array}{l} \underline{\text{Same}} \text{ eigenvalues} \\ \underline{\text{Same}}\ E_{harm}(\{\eta_i\}) \end{array} \right\} \Rightarrow \underline{\text{DEGENERACY}}$$

write $\quad \underset{\sim}{\eta}^2 = 4\,\underset{\sim}{I} + \underset{\sim}{W}$

off diagonal terms connecting fcc neighbors

$$W_{\alpha\gamma} \equiv \eta_{\alpha\beta}\,\eta_{\beta\gamma} = \pm 1$$

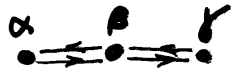


$$E_{harm} = \tfrac{1}{2}|J|s\,\mathrm{Tr}\,(4+\underset{\sim}{W})^{1/2}$$

$$\boxed{E_{harm} = \tfrac{1}{2}|J|s\,\mathrm{Tr}\left\{4^{1/2}\left(1 + \frac{W}{8} - \frac{W^2}{2^7} + \frac{W^3}{2^{10}} - \frac{5}{2^{15}}W^4 + \cdots\right)\right\}}$$

[Note diag. terms in $\underset{\sim}{\eta}^2$ independent of config. since $(\eta^2)_{\alpha\alpha} = \sum_\beta (\eta_{\alpha\beta})^2 = \sum_{\text{neighbors}} 1$]

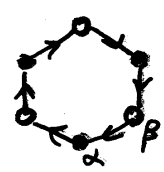
Similarly terms in W^2, e.g.



$$\eta_{\alpha\beta}\,\eta_{\beta\gamma}\cdot\eta_{\beta\gamma}\,\eta_{\alpha\beta}$$

The 1st nontrivial term comes in η^6 or $\underset{\sim}{W}^3$, since the smallest loop in diamond lattice is a hexagon
or pyrochlore

[There are also rings of length 8]



each arrow is a factor $\eta_{\alpha\beta}$

Mapping: let $\boxed{\tau_\mu = \prod_{i \in \text{Hexagon } \mu} \eta_i = \pm 1}$

site of μ at center of hexagon

It turns out $\{\mu\}$ is a new pyrochlore lattice interpenetrating the old one!

plug in ⇒

$$\boxed{E_{harm} \cong |J| s \left\{ 1 - \frac{1}{2^7}\cdot \overset{\mathrm{Tr}\,W^2}{12} + \frac{1}{2^{10}}\cdot 48 \overset{\mathrm{Tr}\,W^3}{\langle \tau_\mu \rangle} - \frac{5}{2^{15}}\cdot 12 \underbrace{\left[25 + 12\langle \tau_\mu \rangle + 4 \langle \tau_\mu \tau_\nu \rangle \right]}_{\mathrm{Tr}\,W^4} \right\}}$$

(here $\langle \cdots \rangle$ means average over space)

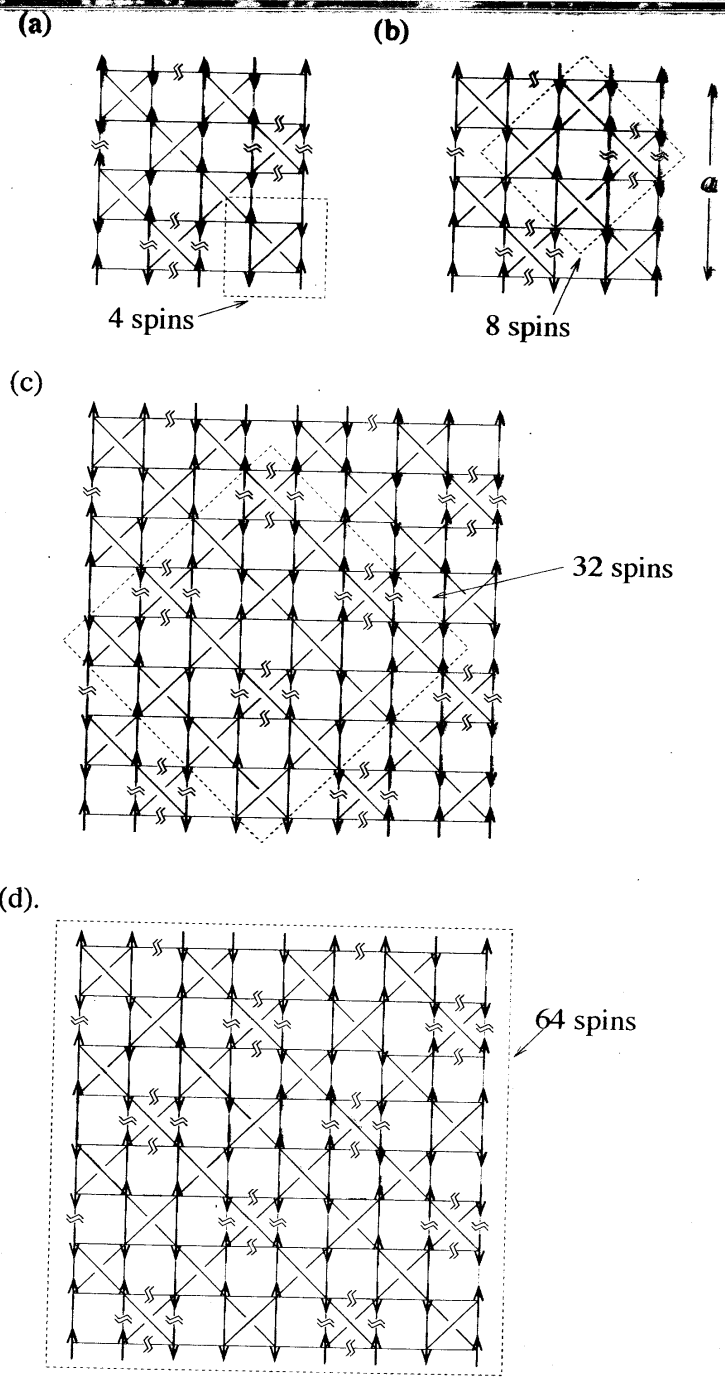
i.e. $\boxed{E_{harm} \simeq \text{const} + \tilde{h} \sum \tau_\mu - \tilde{J} \sum_{\langle \mu\nu \rangle} \tau_\mu \tau_\nu}$

It looks just like ferromagnetic Ising spins $\{\tau_\mu\}$ in an external field $\tilde{h}$.

∴ ground state is $\boxed{\tau_\mu \equiv -1}$

Indeed, we can find a set of $\{m_i\text{'s}\}$ that realize this, while still keeping $\sum_{i \in \alpha} \eta_i = 0$ (condition of classical ground state)

This is a surprisingly complicated ordering pattern. (Some simpler states all have $\tau_\mu \equiv +1$).


(a)
(b)
4 spins
8 spins
a
(c)
32 spins
(d).
64 spins

Random concluding remarks

- Checkerboard [$d=2$ pyrochlore] also works
- Capped Kagomé – does not give right ans [O. Tchernyshov] ↳ from smallest loop
- Hexagon centers (sites of $\prod \eta_i$) form a complementary pyrochlore — can someone concoct an exactly self dual model?