Frustrated about Frustration

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An attempt will be made to sharpen the term **frustration** which appears very often in connection with antiferromagnetically coupled spin systems. Usage of this term is very sloppy, observable properties, which hold in general, obscure.

Typical statement: "It is known that frustrated spin systems exhibit spectacular phenomena: high ground state degeneracy, re-entrance, partial disorder, controversial nature of the phase transition, order by the disorder, etc."

http://obelix.physik.uni-osnabrueck.de/∼schnack/

Hamilton Operator

Hamilton operator; AF $J < 0$, F: $J > 0$

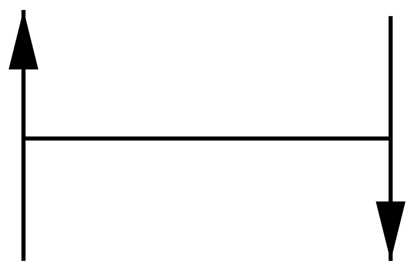
$$\begin{aligned}
\underset{\sim}{H}(\gamma) &= -2\,J \sum_x \left\{ \underset{\sim}{s}^3(x)\underset{\sim}{s}^3(x+1) + \gamma\left[\underset{\sim}{s}^1(x)\underset{\sim}{s}^1(x+1) + \underset{\sim}{s}^2(x)\underset{\sim}{s}^2(x+1)\right]\right\} \\
&= -2\,J \sum_x \left\{ \underset{\sim}{s}^3(x)\underset{\sim}{s}^3(x+1) + \frac{\gamma}{2}\left[\underset{\sim}{s}^+(x)\underset{\sim}{s}^-(x+1) + \underset{\sim}{s}^-(x)\underset{\sim}{s}^+(x+1)\right]\right\} \\
\underset{\sim}{H}(1) &= -2\,J \sum_x \underset{\sim}{\vec{s}}(x)\cdot\underset{\sim}{\vec{s}}(x+1)
\end{aligned}$$

Classical Hamilton function

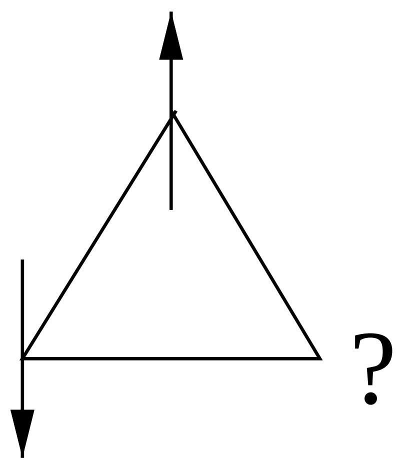
$$\begin{aligned}
H(\gamma) &= -2\,J_c \sum_x \left\{ e^3(x)e^3(x+1) + \gamma\left[e^1(x)e^1(x+1) + e^2(x)e^2(x+1)\right]\right\} \\
H(1) &= -2\,J_c \sum_x \vec{e}(x)\cdot\vec{e}(x+1)
\end{aligned}$$

Classical Heisenberg Spin Systems I

Dimer & trimer



$$E_{GS} = -2J(\vec{e}(1) \cdot \vec{e}(2) + \vec{e}(2) \cdot \vec{e}(1)) = 4J$$

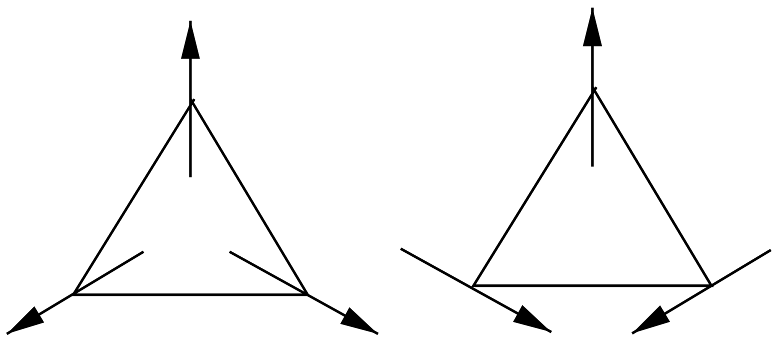


Very simple definition of frustration:

The last spin is frustrated because it does not know how to align.

Classical Heisenberg Spin Systems II

Non-trivial degeneracy

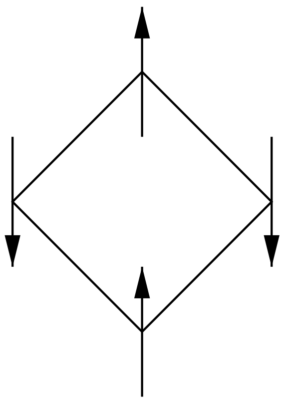


Definition I: The ground state possesses a non-trivial degeneracy.

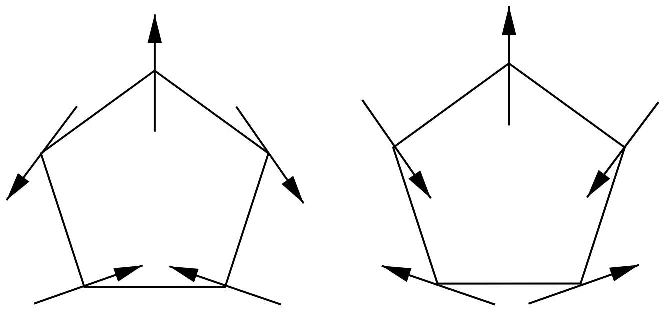
Definition II: $\langle\langle\, \vec{e}(x) \cdot \vec{e}(x+1)\, \rangle\rangle(T=0) > \langle\langle\, \vec{e}(1) \cdot \vec{e}(2)\, \rangle\rangle_D(T=0) = -1$, i.e. anti-correlation weaker than in the dimer.

Classical Heisenberg Spin Systems III

Square & pentagon



only trivial degeneracy and $\langle\langle\, \vec{e}(x) \cdot \vec{e}(x+1)\, \rangle\rangle(T=0) = -1$



non-trivial degeneracy and
$\langle\langle\, \vec{e}(x) \cdot \vec{e}(x+1)\, \rangle\rangle(T=0) = \cos\left(\frac{4\pi}{5}\right) \approx -0.8 > -1$

Definitions work!?

Ising Model

Hamilton operator of the q-states Potts model; $q = 2 \Rightarrow$ Ising

$$\underset{\sim}{H} = \underset{\sim}{H}(\gamma = 0) = -2\,J \sum_x \underset{\sim}{s}^3(x)\underset{\sim}{s}^3(x+1)$$

$N = 2, s = \frac{1}{2}$ ground state energy $E_{GS} = J$ twofold degenerate;
ground states: $|\,\frac{1}{2}, -\frac{1}{2}\,\rangle, |\,-\frac{1}{2}, \frac{1}{2}\,\rangle$
correlation: $\langle\langle\, \underset{\sim}{s}^3(x) \cdot \underset{\sim}{s}^3(x+1)\,\rangle\rangle(T=0)/s^2 = -1$

$N = 3, s = \frac{1}{2}$ ground state energy $E_{GS} = J/2$ $2 \cdot N$-fold degenerate;
ground states: $|\,\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}\,\rangle, |\,\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}\,\rangle$ and cyclic shifts thereof
correlation: $\langle\langle\, \underset{\sim}{s}^3(x) \cdot \underset{\sim}{s}^3(x+1)\,\rangle\rangle(T=0)/s^2 = -1/3$

$N = 4, s = \frac{1}{2}$ ground state energy $E_{GS} = 2\,J$ twofold degenerate;
ground states: $|\,\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}\,\rangle, |\,-\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}, \frac{1}{2}\,\rangle$
correlation: $\langle\langle\, \underset{\sim}{s}^3(x) \cdot \underset{\sim}{s}^3(x+1)\,\rangle\rangle(T=0)/s^2 = -1$

Definition I (non-trivial degeneracy) applicable! Definiton II (correlation) applicable!

Heisenberg Model I

Hamilton operator

$$\underset{\sim}{H} = \underset{\sim}{H}(\gamma = 1) = -2\,J \sum_x \underset{\sim}{\vec{s}}(x) \cdot \underset{\sim}{\vec{s}}(x+1)$$

$N = 2, s = \frac{1}{2}$ ground state energy $E_{GS} = 3J$ non-degenerate;
ground state: $|\,GS\,\rangle = \frac{1}{\sqrt{2}} \left(|\,\frac{1}{2}, -\frac{1}{2}\,\rangle - |\,-\frac{1}{2}, \frac{1}{2}\,\rangle\right)$
correlation: $\langle\langle\, \underset{\sim}{\vec{s}}(x) \cdot \underset{\sim}{\vec{s}}(x+1)\,\rangle\rangle(T=0)/\sqrt{s(s+1)}^2 = -1$

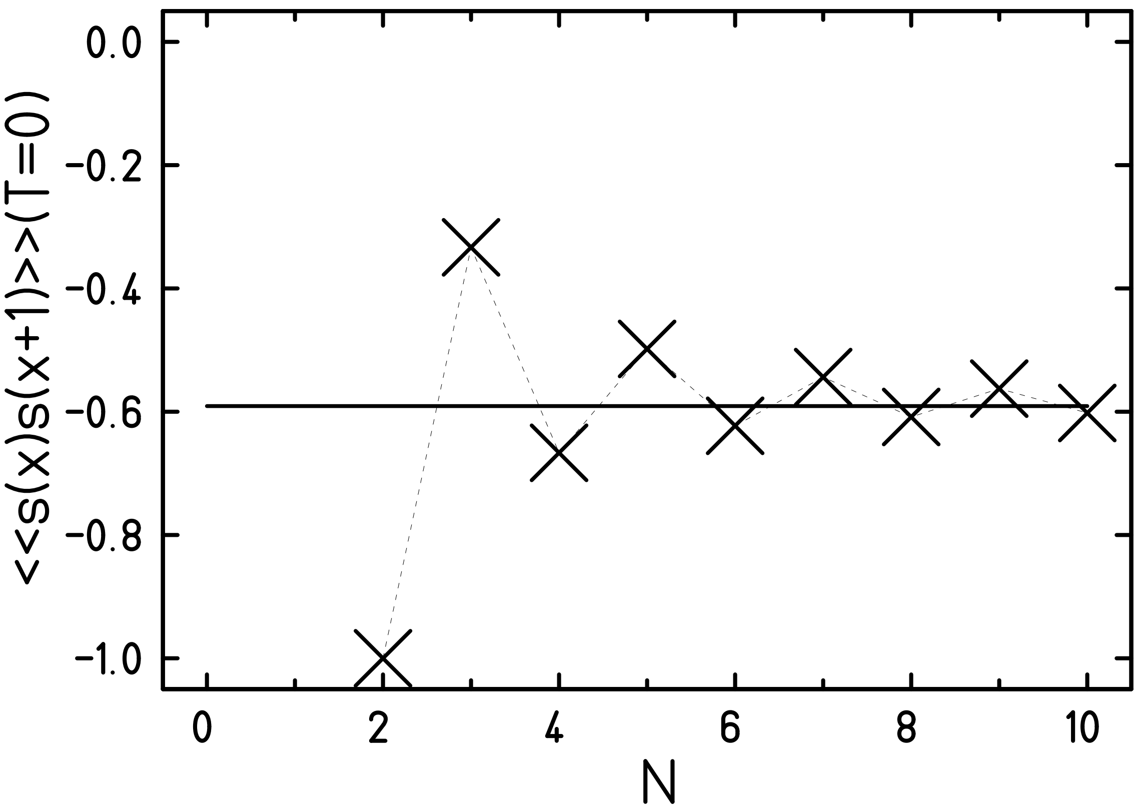
$N = 3, s = \frac{1}{2}$ ground state energy $E_{GS} = 3\,J/2$ fourfold degenerate;
ground states: $|\,GS1\,\rangle = \frac{1}{\sqrt{3}} \left(|\,\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}\,\rangle + e^{i\frac{2\pi}{3}}\,|\,-\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\,\rangle + e^{i\frac{4\pi}{3}}\,|\,\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}\,\rangle\right)$
$|\,GS2\,\rangle = \frac{1}{\sqrt{3}} \left(|\,\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}\,\rangle + e^{-i\frac{2\pi}{3}}\,|\,-\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\,\rangle + e^{-i\frac{4\pi}{3}}\,|\,\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}\,\rangle\right)$
etc.
correlation: $\langle\langle\, \underset{\sim}{\vec{s}}(x) \cdot \underset{\sim}{\vec{s}}(x+1)\,\rangle\rangle(T=0)/\sqrt{s(s+1)}^2 = -\frac{1}{4}$

$N = 4, s = \frac{1}{2}$ ground state energy $E_{GS} = 4\,J$ non-degenerate;
ground states: $|\,GS\,\rangle = \frac{1}{\sqrt{3}} \left(|\,\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}\,\rangle + |\,-\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}, \frac{1}{2}\,\rangle\right) +$
$\frac{1}{\sqrt{12}} \left(|\,\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}\,\rangle + |\,-\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, -\frac{1}{2}\,\rangle + |\,-\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\,\rangle + |\,\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}\,\rangle\right)$
correlation: $\langle\langle\, \underset{\sim}{\vec{s}}(x) \cdot \underset{\sim}{\vec{s}}(x+1)\,\rangle\rangle(T=0)/\sqrt{s(s+1)}^2 = -\frac{2}{3}$

Definition I (non-trivial degeneracy) applicable! Definiton II (correlation) applicable?

Heisenberg Model II

Next-neighbour correlation $s = 1/2$



The next-neighbour spin-spin correlation does not serve as a measure of frustration.

Heisenberg Model III

Hamilton operator

$$\underset{\sim}{H} = \underset{\sim}{H}(\gamma = 1) = -2\,J \sum_x \underset{\sim}{\vec{s}}(x) \cdot \underset{\sim}{\vec{s}}(x+1)$$

$N = 2, s = 1$ ground state energy $E_{GS} = 8\,J$ non-degenerate;
ground state: $|\,GS\,\rangle = \frac{1}{\sqrt{3}}\left(|\,1,-1\,\rangle + |\,-1,1\,\rangle - |\,0,0\,\rangle\right)$
correlation: $\langle\langle\, \underset{\sim}{\vec{s}}(x) \cdot \underset{\sim}{\vec{s}}(x+1)\,\rangle\rangle(T=0)/\sqrt{s(s+1)}^2 = -1$

$N = 3, s = 1$ ground state energy $E_{GS} = 6\,J$ non-degenerate;
ground states: $|\,GS\,\rangle = \frac{1}{\sqrt{6}}\big(|\,1,0,-1\,\rangle + |\,-1,1,0\,\rangle + |\,0,-1,1\,\rangle + |\,-1,0,1\,\rangle + |\,1,-1,0\,\rangle + |\,0,1,-1\,\rangle\big)$
correlation: $\langle\langle\, \underset{\sim}{\vec{s}}(x) \cdot \underset{\sim}{\vec{s}}(x+1)\,\rangle\rangle(T=0)/\sqrt{s(s+1)}^2 = -\frac{1}{2}$

$N = 4, s = 1$ ground state energy $E_{GS} = 12\,J$ non-degenerate;
correlation: $\langle\langle\, \underset{\sim}{\vec{s}}(x) \cdot \underset{\sim}{\vec{s}}(x+1)\,\rangle\rangle(T=0)/\sqrt{s(s+1)}^2 = -\frac{3}{4}$

Definition I (non-trivial degeneracy) applicable? Definiton II (correlation) applicable?

Way Out ?

Definition III

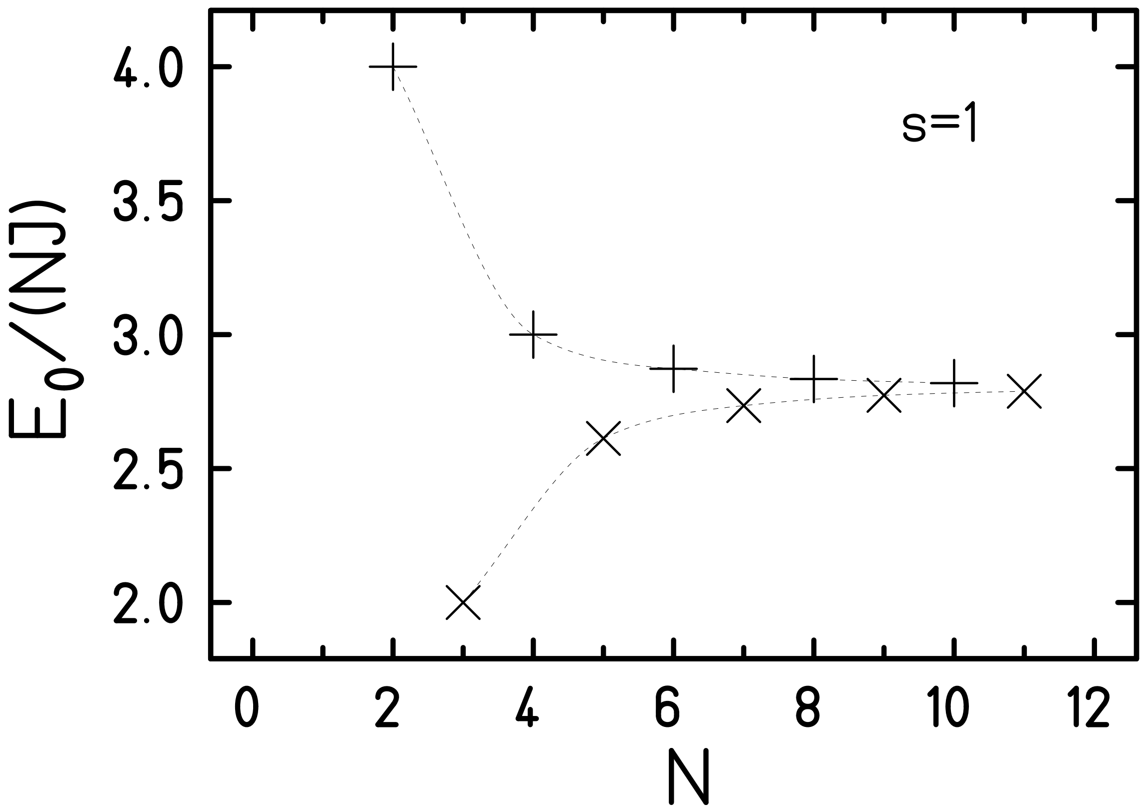
A quantum spin system is frustrated if the corresponding classical system is frustrated.

Problem

- Not very satisfactory. Reminds of the problems one has with “quantum chaos”. There one says that the spectrum should have some special properties like being a GOE.
- Are there any common observable phenomena caused by frustration?
- Or does the pessimistic statement hold, that the classical term frustration is without value in quantum mechanics except for Ising systems?
- One suggestion: weaker binding per bond compared to “neighbouring”, non-frustrated systems

Binding Energy per Bond

Heisenberg ring $s = 1$



Heisenberg ring with e.g. $N = 5$ has a weaker binding per bond than the neighbouring rings with $N = 4$ and $N = 6$. Property holds for arbitrary spin quantum number.

Measure of Frustration

O.k., we still don't know what frustration exactly means, but may be we can quatify it?[a]

Satisfied and unsatisfied bonds

satisfied $$\text{sign}\left(\langle\langle\, \underset{\sim}{\vec{s}}(x)\cdot\underset{\sim}{\vec{s}}(y)\,\rangle\rangle(T=0)\right) = +\text{sign}\left(J(x,y)\right)\ ,\ J(x,y)\neq 0$$

unsatisfied $$\text{sign}\left(\langle\langle\, \underset{\sim}{\vec{s}}(x)\cdot\underset{\sim}{\vec{s}}(y)\,\rangle\rangle(T=0)\right) = -\text{sign}\left(J(x,y)\right)\ ,\ J(x,y)\neq 0$$

Misfit parameter

$$m = 2\,\frac{E_u}{E_u + |E_s|} \qquad E_u = -\sum_{unsatisfied\ bonds} J(x,y)\,\langle\langle\, \underset{\sim}{\vec{s}}(x)\cdot\underset{\sim}{\vec{s}}(y)\,\rangle\rangle(T=0)$$

$$E_s = -\sum_{satisfied\ bonds} J(x,y)\,\langle\langle\, \underset{\sim}{\vec{s}}(x)\cdot\underset{\sim}{\vec{s}}(y)\,\rangle\rangle(T=0)$$

⇒ Heisenberg spin rings always have $m = 0$! Misfit parameter works for Ising model.

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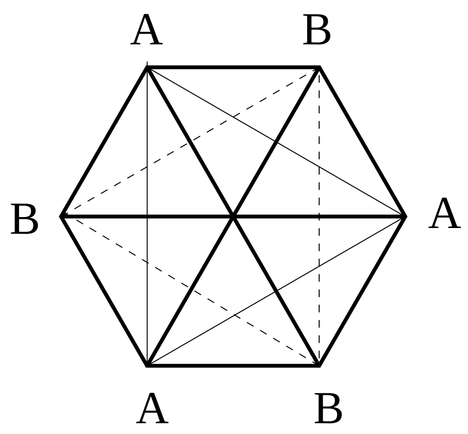
[a] J. Richter, S. Kobe, J. Phys. C: Solid State Phys. **15** (1982) 2193

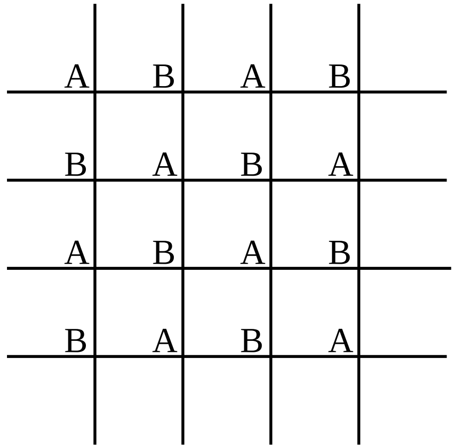
Definition by Geometry of Interaction I

"Bipartiteness"

Definition IV: A non-bipartite system is called frustrated.
(see e.g. Johannes Richtes, Magdeburg)

Bipartite: If the system can be decomposed into subsystems A and B such that the coupling constants fulfil $J(x_A, y_B) \leq g^2$, $J(x_A, y_A) \geq g^2$, $J(x_B, y_B) \geq g^2$, the system is called bipartite.





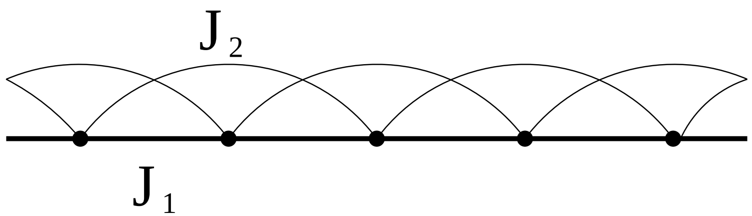
Definition by Geometry of Interaction II

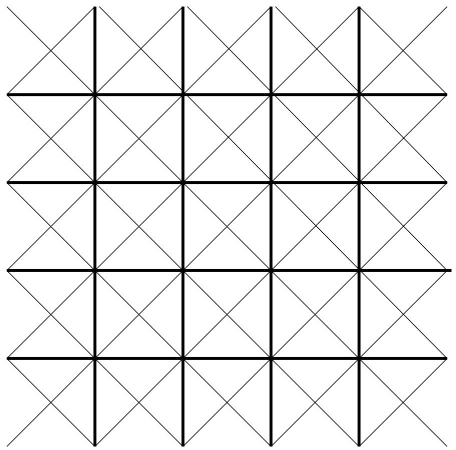
Examples

$$\underset{\sim}{H} \quad = \quad -2\,J_1 \sum_{nn} \underset{\sim}{\vec{s}}(x) \cdot \underset{\sim}{\vec{s}}(y) - 2\,J_2 \sum_{nnn} \underset{\sim}{\vec{s}}(x) \cdot \underset{\sim}{\vec{s}}(y)$$

Consider e.g. rings with an even number of sites or infinite lattices, i.e. $J_1 < 0$ & $J_2 = 0$ should allow a bipartite lattice.

- $J_1 < 0$ & $J_2 > 0$ results in a bipartite lattice, the system is not frustrated.
- $J_1 < 0$ & $J_2 < 0$ results in a non-bipartite lattice, the system is frustrated and the coupling strength J_2 is sometimes itself called frustration.





Summary

Classical Heisenberg and Ising models

- term frustration well defined;
- phenomena like non-trivial ground state degeneracy, weakening of binding energy, spin-spin correlation not -1 etc.;

Quantum Heisenberg models

- term frustration may be defined like in definition IV: non-bipartite $\equiv$ frustrated;
- but resulting general phenomena unclear: ground state energy sometimes degenerate, spin-spin correlation almost always not -1, weakening of binding compared to "neighbouring" non-frustrated systems - but what is "neighbouring"?