Order and disorder in low–dimensional quantum spin systems

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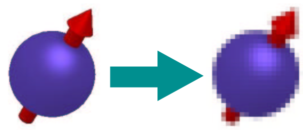
Overview

- introduction + motivation
- numerical methods
- results
  - The Heisenberg–Star
  - The Sierpinski–gasket
- conclusion

Introduction

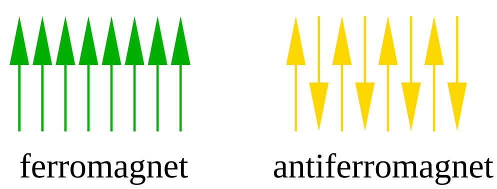
- quantum spin systems = quantum many-body systems
- basic element = magnetic moment of particles = spin
- spin - quantum object with ,,fluctuation"



- interaction = exchange between spins $\hat{\mathbf{s}}_\mathbf{i} \leftrightarrow \hat{\mathbf{s}}_\mathbf{j}$
  - isotropic Heisenberg exchange J

$$J(\hat{\mathbf{s}}_\mathbf{i}\hat{\mathbf{s}}_\mathbf{j}) = J(\hat{\mathbf{s}}_\mathbf{i}^\mathbf{x}\hat{\mathbf{s}}_\mathbf{j}^\mathbf{x} + \hat{\mathbf{s}}_\mathbf{i}^\mathbf{y}\hat{\mathbf{s}}_\mathbf{j}^\mathbf{y} + \hat{\mathbf{s}}_\mathbf{i}^\mathbf{z}\hat{\mathbf{s}}_\mathbf{j}^\mathbf{z})$$

- different kinds of magnetic order

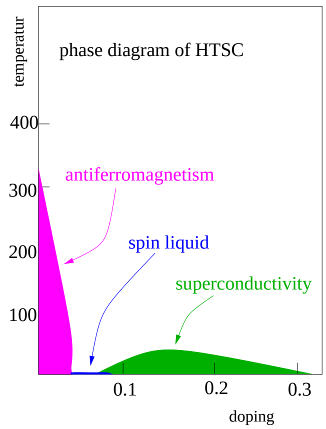


- parameters which influences the magnetic order

f ... frustration, T ... temperatur

d ... dimension,z ... coordination number, S ... spin quantum number

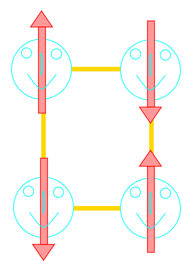
Motivation



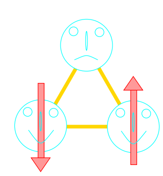
- high temperature superconductivity (HTSC)
- discovery by Bednorz & Müller 1986 on doped La_2CuO_4 with T_c=35K (recent progress: T_c^{max}=125K)
- BCS theory not able to describe this phenomenon
- current research $\longrightarrow$ magnetic correlations are essential for describing HTSC
- magnetic properties of the undoped cuprates are well described by Heisenberg quantum spin systems
- magnetic order – destroyed by doping
- doping $\leftrightarrow$ frustration

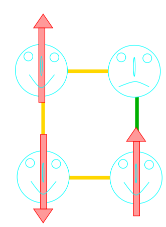
What about frustration?

- dictionary: ,,a deep chronic sense or state of insecurity and dissatisfaction arising from unresolved problems or unfulfilled needs“
- physics: competing interaction



unfrustrated
antiferromagnet





frustration due to:

- geometry
- different interaction

What is known about the magnetic order of Heisenberg quantum spin systems with spin 1/2 ?

- Mermin-Wagner theorem for Heisenberg spin systems with d = 1 or 2

  $T > 0 \rightarrow$ long–range magnetic order (LRO) impossible

  T=0 (ground state) $\rightarrow$ LRO possible

- ground state magnetic order:
  - d=1 spin chain with nearest–neighbour interaction
    - exact solution (Bethe-Ansatz): no LRO
  - d=2 systems (square lattice, triangular lattice, honeycomb lattice)
    - no exact solution known
    - considerations using different methods (exact diagonalization, spin wave theory, renormalization group theory, quantum Monte-Carlo methods, Coupled-Cluster method etc.): LRO present

Aim

analytic solution are rare

1. search for models with analytic solution

Heisenberg–Star

2. How does frustration influence the magnetic order?

d=1: no LRO $\leftrightarrow$ d=2: LRO present

3. What about the transition between d=1 and d=2?

Sierpinski–gasket

Numerical methods

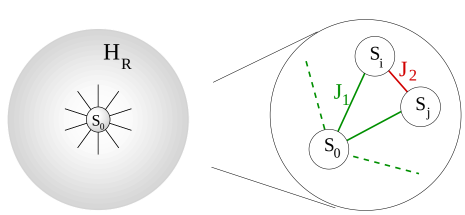
1. full diagonalization of small systems (N≤15)
   - calculation of thermodynamic properties
2. exact diagonalization with Lanczos for systems up to N=36
   - calculation of the ground state and some excitations
3. Decoupled-Cell quantum Monte-Carlo method for systems up to N≈1000
   - "importance sampling" method for calculating thermodynamical properties
   - single spin flip due to a local surrounding (decoupled cell) avoiding „sign“ problem
4. variational wave function calculation for systems up to N≈1000
   - improving variational parameters for an ansatz wave function
   - calculation of the ground state and first excitation

Results

The Heisenberg–Star

- spin model: central spin $\mathbf{s_0}$ + surrounding $H_R\{\mathbf{s}_i\}$

$$H = \frac{J_1}{N}\sum_{i=1}^{N} \mathbf{s}_0\mathbf{s}_i + J_2 H_R\{\mathbf{s}_i\}$$

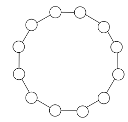


- N+1 spins with s=1/2
- antiferromagnetic interaction: J_1,$J_2 > 0$
- basic element = triangle → frustration

• surrounding $H_R\{\mathbf{s}_i\}$

linear chain
z=2
if J_1=0: no LRO

$$H_R^{LK} = \frac{1}{N}\sum_{i=1}^{N}\mathbf{s}_i\mathbf{s}_{i+1}$$



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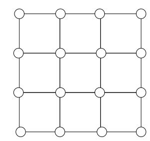
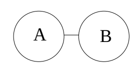
square lattice
z=4
if J_1=0: LRO present

$$H_R^{QG} = \frac{1}{2N}\sum_{i=1}^{N}(\mathbf{s}_i\mathbf{s}_{i+\hat{x}} + \mathbf{s}_i\mathbf{s}_{i+\hat{y}})$$



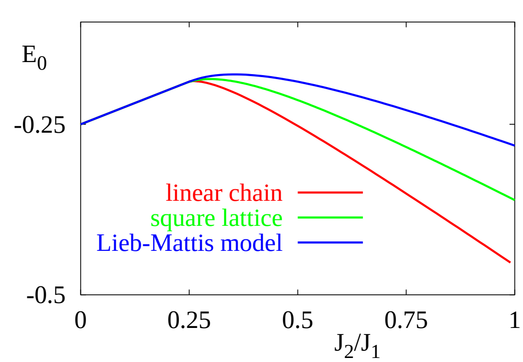
Lieb-Mattis model
z=N/2
if J_1=0: LRO present

$$H_R^{LM} = \frac{4}{N^2}\sum_{\substack{i,j=1 \\ i\in A, j\in B}}^{N}\mathbf{s}_i\mathbf{s}_j$$



• ground state energy vs. J_2/J_1

- linear chain: quasi-analytic solution with Bethe-Ansatz
- square lattice: exact diagonalization with N≤26 and extrapolation N→ ∞
- Lieb-Mattis model: analytic solution

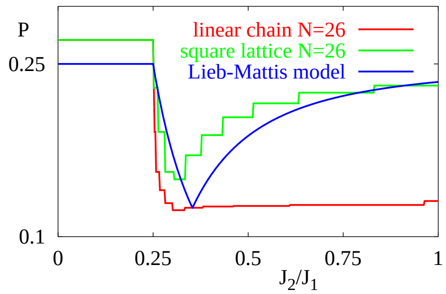


- maximum of energy → maximum of frustration

• total magnetic correlation P vs. J_2/J_1

$$P = \frac{1}{N^2} \sum_{i,j=1}^{N} |\langle \mathbf{s}_i \mathbf{s}_j \rangle|.$$

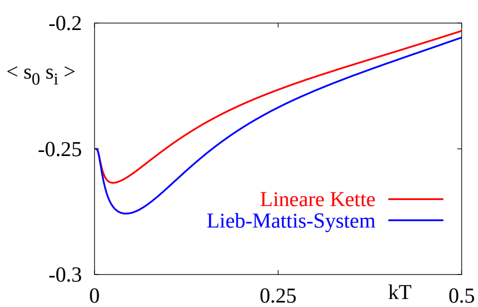
○ measures a global magnetic order of the system



- first transition analytically soluble (independent of surrounding and system size)
- surrounding ferromagnetic until $J_2/J_1 = \frac{1}{4}$
- minimum $P \leftrightarrow$ maximum E_0
- strong frustration $\longrightarrow$ rapid change of P
- $N \longrightarrow \infty$: destruction of LRO for linear chain and square lattice by frustration
- $J_2 >> J_1$: central spin decouples $\longrightarrow$ magnetic order is known:
  linear chain - no LRO
  square lattice and Lieb-Mattis - LRO present

• spin correlation $\langle \mathbf{s}_i \mathbf{s}_j \rangle$ vs. temperature kT

- full diagonalization of small systems (N=8)
- J_2/J_1=0.26 (strong frustration)
- Lieb-Mattis model and square lattice by chance identical



- ”order-from-disorder” effect
  - strong frustration
    $\longrightarrow$ high degeneracy of the ground state
  - thermal fluctuations
    $\longrightarrow$ lifting of degeneracy
    $\longrightarrow$ the state is more symmetric
    $\longrightarrow$ spin correlations are increasing
- $T \longrightarrow \infty$: paramagnet

Heisenberg–Star

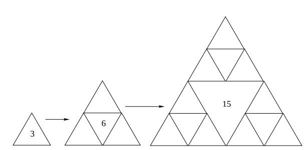
- analytic solution
- frustration reduces or destroys the magnetic order
- frustration + thermal fluctuations → ”order-from-disorder” effect

The Sierpinski–gasket

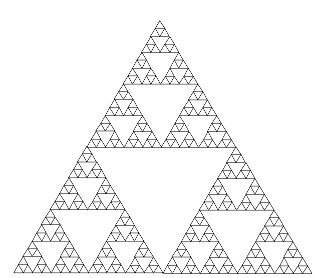
- spin system on a fractal lattice with dimension $1 < d < 2$
  [Tomczak & Ferchmin (1995)]

$$H = J \sum_{i,j=1}^{N} \mathbf{s}_i \mathbf{s}_j$$

- J=1 antiferromagnetic
- basic element = triangle → frustration
- fractal dimension:
  $d_f = \frac{\ln 3}{\ln 2} \approx 1.58$

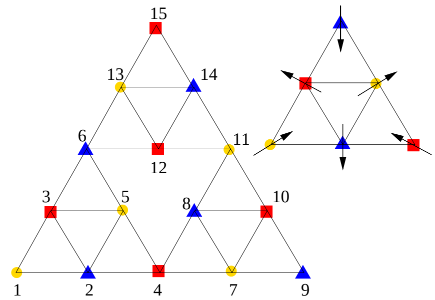


- basic building steps



- system after 6 steps with N=366

• The classical ground state



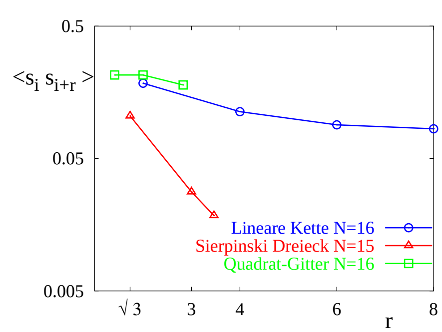
- classical long–range order with 3–sublattice structure
- 120° angle between the classical spins

Are the quantum fluctuations able to destroy the classical long–range order?

- consideration of spin correlation, ground state energy, energy spectra, low–temperature specific heat of signatures for magnetic ordering

• spin correlations $< s_i s_{i+r} >$ vs. distance r

- $\lim_{r\to\infty} < s_i s_{i+r} > = \begin{matrix} 0 \\ const. \end{matrix}$ *disordered* / *ordered*
- exact diagonalization of small systems

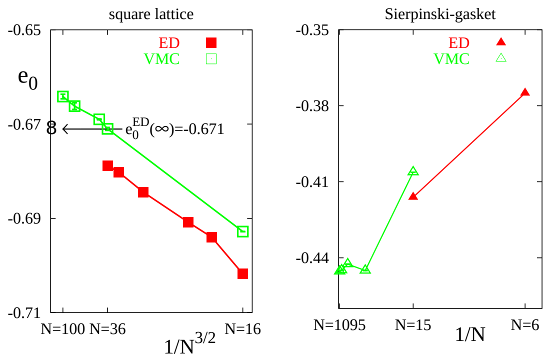


- linear chain: power law decay (analytical solution)
- square lattice: slight decay to a constant (not seen due to small lattice)
- Sierpinski–gasket: strong (exponential) decay

→ first hint for disordered ground state

• ground state energy e_o vs. system size N

- if e_0 is independent of $N \rightarrow$ hint for a disordered ground state
- exact diagonalization and variational calculations



- square lattice: e_o scales as expected with $N^{-3/2}$
- Sierpinski–gasket: no scaling of e_0 with system size

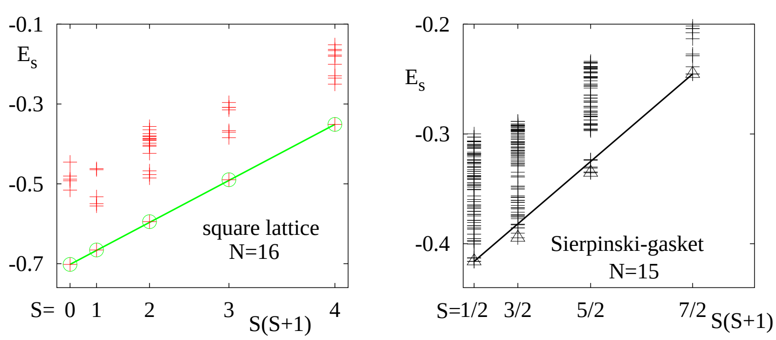
$\rightarrow$ hint for disordered ground state

• energy spectrum

- for lattices with LRO: Pisa–tower structure of the low lying energy levels

$$E_{min}(S) = E_0 + AS(S+1) \quad ; \quad A \propto 1/N$$

- N$\rightarrow \infty$: degeneracy of the low lying states $\rightarrow$ symmetry broken ground state with LRO

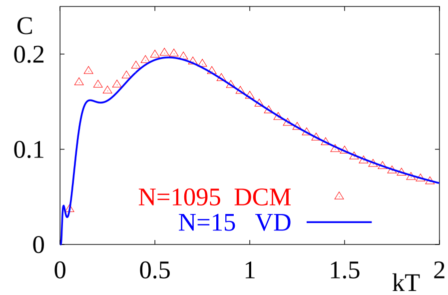


- no Pisa–tower for Sierpinski–gasket
- additional states wit S=1/2 below the first S=3/2 excitation

$\rightarrow$ hint for disordered ground state

• specific heat vs. temperature kT

- full diagonalization for N=15
- Decoupled-Cell quantum Monte-Carlo method for N≤1095



- ordered systems → one broad maximum
- Sierpinski-gasket: additional maxima for $kT < 0.5$
- very similar to the d=2 *kagome* lattice (disordered lattice?)

→ hint for disordered ground state

Conclusion

- investigation of ground state and thermodynamics of antiferromagnetic Heisenberg quantum spin systems with s=1/2

??? How does frustration or dimension influence the magnetic order ???

- – Heisenberg-Star: analytic solution
  – frustration → weakening or destruction of long–range magnetic order
  – frustration + thermal fluctuations → ”order-from-disorder” effect
  – increase of dimension or coordination number
  → stabilization of magnetic order
- – Sierpinski–gasket with dimension $d_f < 2$ + frustration
  → destruction of magnetic order