# Coupled Cluster Method for Quantum Spin Systems

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# Organization of the talk

- Heisenberg model and CCM
- Coupled cluster method
  - application to quantum spin systems
  - spin stiffness
  - excited state
- Results
  - $J$–$J'$ model
  - $J_1$–$J_2$ model
  - square lattice, triangular lattice
- Conclusions

# Heisenberg model, spin $1/2$, two dimensional

$$H = \sum_{i,j} J_{ij} \mathbf{s}_i \mathbf{s}_j$$

*ground state* HAFM on square and triangular lattice:

$\longrightarrow$ Néel ordered

important mechanisms to destroy magnetic long-range order (LRO):

*competition of bonds*:

- higher quantum fluctuations $\longrightarrow$ suppression of long-range order, formation of *local singlets*; e.g., $CaV_4O_9$, $SrCu_2(BO_3)_2$
- *frustration* $\longrightarrow$ my yield to PT to noncollinear (spiral) states in the classical model; quantum fluctuations – favor collinear order
  $\longrightarrow$ my yield (together with quantum fluctuations) to quantum paramagnetic phase

# Heisenberg model and CCM

with CCM it can be calculated in higher orders:

- ground state energy, magnetization
- new: stiffness, gap

CCM is able to describe (for example in the $J$–$J'$ model)

- frustrated incommensurate spiral phase
- quantum phase transition without frustration

here: quantum phase transition *with* frustration
$\rightarrow$ $J_1$–$J_2$ model

# Coupled cluster method – CCM

**I.** choose a *model state* $|\Phi\rangle$ and a set of *creation operators* $(C_I^+)$

$$C_I|\Phi\rangle = 0 \quad \forall I \neq 0, \quad \sum_I C_I^+ |\Phi\rangle\langle\Phi| C_I = 1$$

**II.** ansatz for the ground state $|\Psi\rangle$ with the *correlation operator* $S$

$$|\Psi\rangle = e^S|\Phi\rangle, \;\; S = \sum_{I\neq 0} \mathcal{S}_I C_I^+; \qquad \langle\tilde{\Psi}| = \langle\Phi|\tilde{S}e^{-S}, \;\; \tilde{S} = 1 + \sum_{I\neq 0} \tilde{\mathcal{S}}_I C_I$$

**III.** ket-state equations (non linear), with $\bar{H} = \langle\tilde{\Psi}|H|\Psi\rangle$

$$\frac{\partial \bar{H}}{\partial \tilde{\mathcal{S}}_I} = 0 \Leftrightarrow \langle\Phi|C_I e^{-S} H e^S|\Phi\rangle = 0, \Rightarrow \text{ket coefficients } \mathcal{S}_I, \Rightarrow |\Psi\rangle,$$

$$\Rightarrow E = \langle\Phi|e^{-S} H e^S|\Phi\rangle$$

**IV.** bra-state equations (linear):

$$\frac{\partial \bar{H}}{\partial \mathcal{S}_I} = 0, \Rightarrow \text{bra coefficients } \tilde{\mathcal{S}}_I, \Rightarrow \langle\tilde{\Psi}|, \Rightarrow \bar{A} = \langle\tilde{\Psi}|A|\Psi\rangle$$

# CCM – application on spin systems

**I.** Selection of $|\Phi\rangle$: classical spin state

$$\Rightarrow S = \sum_{i_1} \mathcal{S}_{i_1} s^+_{i_1} + \sum_{i_1 i_2} \mathcal{S}_{i_1 i_2} s^+_{i_1} s^+_{i_2} + \sum_{i_1 i_2 i_3} \mathcal{S}_{i_1 i_2 i_3} s^+_{i_1} s^+_{i_2} s^+_{i_3} + \cdots$$

**II.** approximation of $S$ – LSUB$n$

- approximation of $S$ is the *only* approximation in the CCM
- LSUB$n$: *local* approximation, including correlations with up to $n$ spins
- hierarchical approximation, LSUB$\infty$ becomes exact

# CCM – Fundamental configurations

## example for square lattice:

LSUB8 with 259 types of *connected* fundamental confi gurations

# Spin stiffness

- spin stiffness $\rho_s$ measures the rigidity of the spins with respect to a small twist $\theta$ of the direction of spin between every pair of neighboring rows:

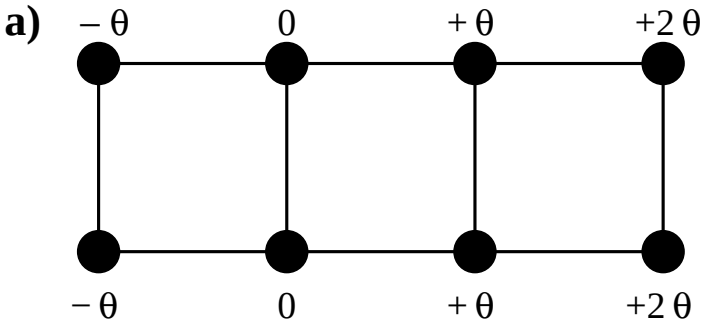
$$\rho_s = \left. \frac{d^2}{d\theta^2} \frac{E_0(\theta)}{N} \right|_{\theta=0}$$

- $\rho_s > 0 \rightarrow$ LRO, systems are stiff
- $\rho_s = 0 \rightarrow$ no LRO, systems are not stiff

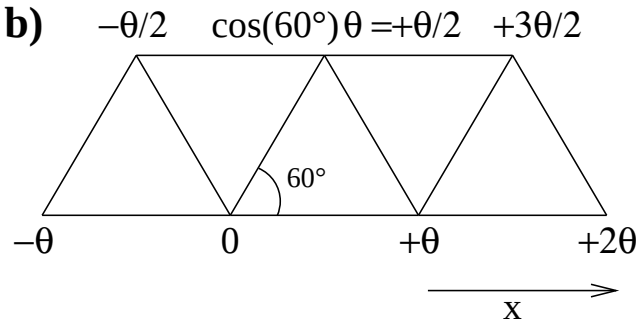
# CCM – calculation of the spin stiffness

- introducing the twist $\theta$: appropriate changing of the classical spin state of $|\Phi\rangle$, $\rightarrow$ doing the CCM, $\rightarrow$ ground-state energy in dependence of $\theta$

- twist $\theta$ for the square lattice:




- twist $\theta$ for the triangular lattice:




- twist is introduced along rows in $x$ direction.

# CCM – Excited-State Formalism

- apply linearly an excitation operator $X^e$ to the ket-state wave function:

$$|\Psi_e\rangle = X^e|\Psi\rangle = X^e e^S|\Phi\rangle, \quad X^e = \sum_{I\neq 0} \mathcal{X}_I^e C_I^+$$

- using Schrödinger equation $E_e|\Psi_e\rangle = H|\Psi_e\rangle$ gives for the excitation energy $\epsilon_e \equiv E_e - E_g$

$$\epsilon_e X^e|\Phi\rangle = e^{-S}[H, X^e]e^S|\Phi\rangle$$

- apply $\langle\Phi|C_I$

  $\Rightarrow$ set of eigenvalue equations

$$\epsilon_e \mathcal{X}_I^e = \langle\Phi|C_I e^{-S}[H, X^e]e^S|\Phi\rangle \quad , \forall I \neq 0$$

# CCM – Excited-State Formalism:
## application on spin systems

**I.** Selection of $X^e$: classical spin state

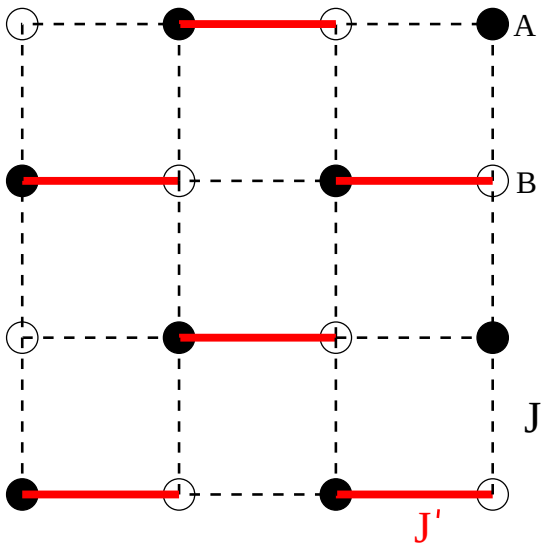
$$\Rightarrow X^e = \sum_{i_1} \mathcal{X}_{i_1} s^+_{i_1} + \sum_{i_1 i_2} \mathcal{X}_{i_1 i_2} s^+_{i_1} s^+_{i_2} + \sum_{i_1 i_2 i_3} \mathcal{X}_{i_1 i_2 i_3} s^+_{i_1} s^+_{i_2} s^+_{i_3} + \cdots$$

**II.** approximation of $X$:

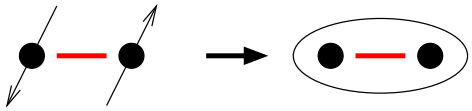
- similar to the ground state
- but: choose confi gurations which change $s^T_z$ by $\pm 1$
- use the same approximation level (e.g., LSUB$n$) as for ground state

# Applications and Results

# $J - J'$ model




- $J = 1$, $J' > J$: *quantum* competition;
  at $J' = J'_s$ phase transition
  LRO $\leftrightarrow$ dimerized paramagnetic phase
  with local singlets:



- $J$, $J'$ different signs: frustration $\rightarrow$ spiral state

known results with CCM:

- phase transition to the dimerized phase can be described by magnetization, gap, and spin stiffness
- frustrated region: quantum fluctuations favor *collinear* order

PRB **61**, 14607 (2000); PRB **64**, 0244331 (2001)

# $J - J'$ model: new results with CMM

## $J = 1$, $J' > J$, transition to the dimerized paramagnetic phase

- influence of the Ising anisotropy $\Delta$

  $\mathbf{s}_i \mathbf{s}_j \rightarrow s_i^x s_j^x + s_i^y s_j^y + \Delta s_i^z s_j^z$

  on the position of the quantum critical point $J'_s$:

  $\rightarrow$ *linear* relation $J'_s(\Delta) \propto \alpha\Delta$ with $\alpha \approx 2.3 \ldots 3.0$

  R. Darradi, J. Richter and S.E. Krüger, J. Phys. Condens. Matter **16**, 2681-2687 (2004))

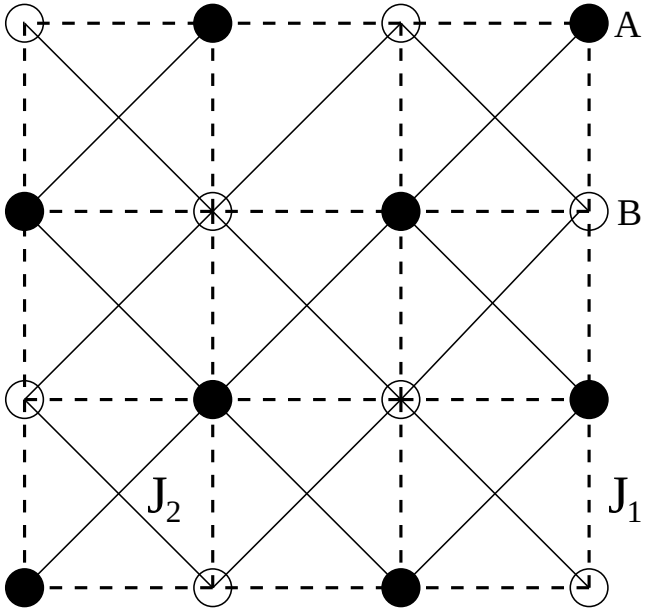
- influence of the spin quantum number $s$ on the position of the quantum critical point $J'_s$:

  $J'_s \propto s(s+1)$

  increase of $J'_s$ with $s \rightarrow$ diminishing of quantum effects

  R. Darradi, J. Richter and D.J.J. Farnell, J. Phys. Condens. Matter **17**, 341-350 (2005)

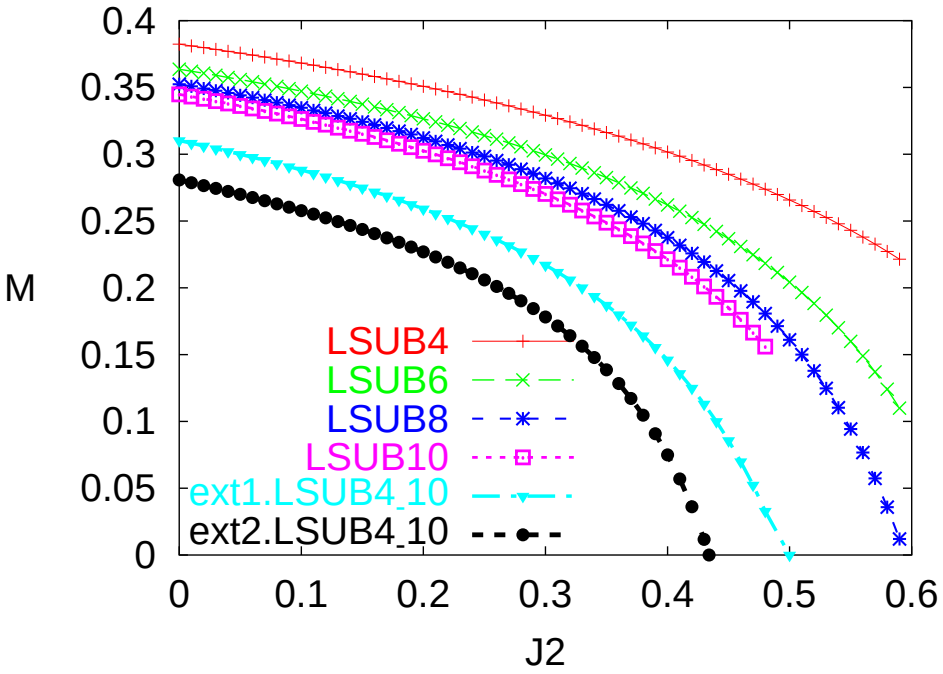
# $J_1$–$J_2$ model




- $J = 1$ – antiferromagnetic
- $J_2 > 0$ parameter, frustration
- at $J_2 = J_2^c$ frustration (together with quantum fluctuations) destroys LRO
  $\rightarrow$ quantum paramagnet (magnetically disordered phase)

# $J_1$–$J_2$ model: magnetization

- sublattice magnetization $M$ versus $J_2$ obtained by CCM-LSUB$n$
- Néel LRO disappears at $J_2^c \approx 0.50$ with extr1, and at $J_2^c \approx 0.434$ with extr2
- new: up to LSUB10 with 29605 confi guration (using the code of Damian Farnell)




$$\text{extr1} \equiv a_0 + a_1(1/n) + a_2(1/n)^2$$

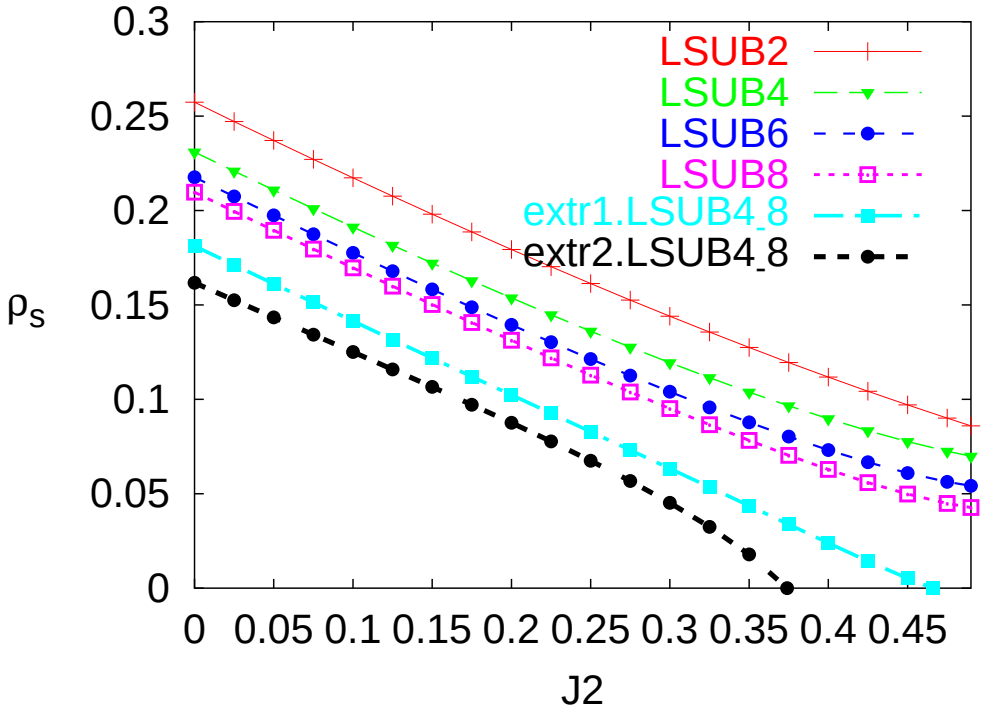
$$\text{extr2} \equiv a_0 + b_1(1/n)^{b_2}$$

- at $J_2 = 1$ extr1 is better approximation
- at the critical point $J_2^c$ extr2 seems to yield better results
- reason: scaling rules often change at a phase transition

  $\rightarrow$ use an approximation (extr2) with variable exponents

# $J_1$–$J_2$ model: spin stiffness

- spin stiffness $\rho_s$ versus $J_2$ obtained by CCM-LSUB$n$
- Néel LRO disappears at $J_2^c \approx 0.466$ with extr1. and $J_2^c \approx 0.374$ with extr2.



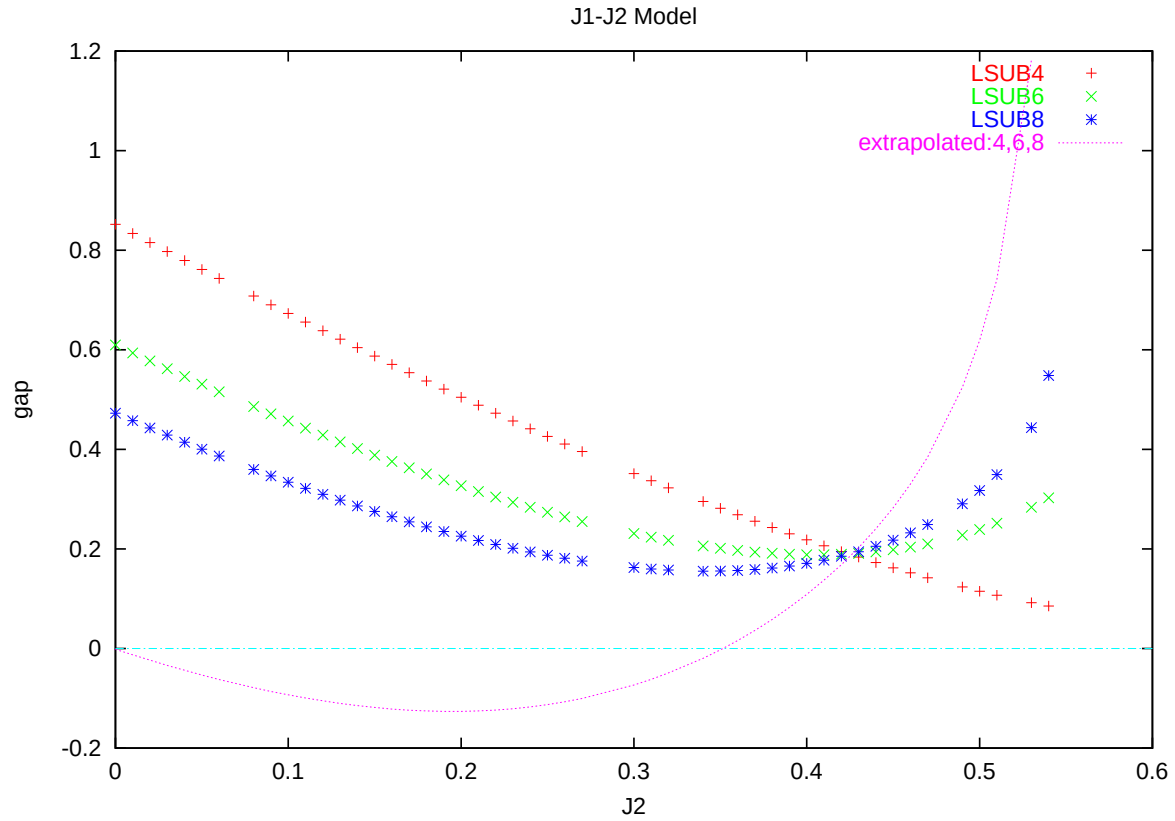

$$\text{extr1} \equiv a_0 + a_1(1/n) + a_2(1/n)^2$$

$$\text{extr2} \equiv a_0 + b_1(1/n)^{b_2}$$

- again: extr1 better at $J_2 = 1$,
  extr2 better at $J_2 = J_2^c$

# $J_1$–$J_2$ model: gap

- Néel ordered state $\leftrightarrow$ no gap
- quantum paramagnet $\leftrightarrow$ gap




number of confi gurations:

| LSUB$n$ | gs | ex |
|---|---|---|
| 4 | 7 | 6 |
| 6 | 75 | 91 |
| 8 | 1287 | 2011 |

- $\rightarrow$ Néel LRO disappears at $J_2^c \approx 0.34 \ldots 0.42$

# Conclusions: $J_1$–$J_2$ model

- already known: ground state (energy, magnetization)

  Bishop, Farnell, Parkinson PRB **58**, 6394

- new results:
  - magnetization: CCM-LSUB10 extrapolation for calculating $J_2^c$
  - spin stiffness
  - gap

- with all three measures:
  transition from Néel LRO to quantum paramagnet (magnetically disordered phase) can be described
  $\longrightarrow$ approximation of $J_2^c$

# Square lattice: magnetization

- CCM LSUB$n$ approximation with $n = \{2, 4, 6, 8, 10\}$ and extrapolated results
- $N_F$ – number of fundamental confi gurations
- $E_g/N$ – GS energy per spin
- $M$ – sublattice magnetisation

| | $N_F$ | $E_g/N$ | $M/M_{clas}$ |
|---|---|---|---|
| LSUB2 | 1 | $-0.64833$ | 0.84143 |
| LSUB4 | 7 | $-0.66366$ | 0.76480 |
| LSUB6 | 75 | $-0.66700$ | 0.72728 |
| LSUB8 | 1287 | $-0.66817$ | 0.70484 |
| LSUB10 | 29605 | $-0.66870$ | 0.68966 |
| Extrapolated CCM | – | $-0.66960$ | 0.610 |
| 3rd order SWT* | – | $-0.66999$ | 0.6138 |
| QMC** | – | $-0.669437(5)$ | 0.6140(6) |

* Hamer et al. PRB **46**, 6276 (1992); ** Sandvik PRB **56**, 11678 (1997)

# Square lattice: spin stiffness

- CCM:

| LSUB$n$ | number eqs. | stiffness $\rho_s$ |
|---|---|---|
| 2 | 3 | 0.2574 |
| 4 | 40 | 0.2310 |
| 6 | 828 | 0.2176 |
| 8 | 21124 | 0.2097 |
| extr1 | – | 0.1812 |

- comparison with other methods:

| method | $\rho_s$ |
|---|---|
| LSWT | 0.1912 |
| 2nd SWT | 0.1810 |
| 3rd SWT | 0.1747 |
| series exp. | 0.182 |
| exact diagon. | 0.183 |
| quantum Mone Carlo | 0.199 |

$\rightarrow$ CCM in *excellent agreement* with the best results obtained by other means

# Triangular lattice: spin stiffness

*parallel* stiffness, i.e., the spins are rotated by the twist $\theta$ *within* the plane of the system

- CCM:

| LSUB$n$ | number eqs. | stiffness $\rho_{s\|\|}$ |
|---|---|---|
| 2 | 3 | 0.1188 |
| 3 | 14 | 0.1075 |
| 4 | 67 | 0.0975 |
| 5 | 370 | 0.0924 |
| 6 | 2133 | 0.0869 |
| approx. | – | 0.0585 |

- comparison with other methods::

| method | $\rho_{s\|\|}$ |
|---|---|
| exact diagonalization | 0.05 |
| LSWT | 0.080 |
| Schwinger-boson approach | 0.088 |
| CCM | 0.060 |

$\rightarrow$ improved results by CCM (LSWT is to large)

# Conclusions

- CCM leads to quite accurate results for quantum spin systems
  (ground state and fi rst excitation)
- qualitativly correct description of GS order-disorder transitions
- no problems with frustration and incommensurate spiral phases
- higher spin $s > 1/2$ also possible

some further things to do in high-order CCM:

- calculation of correlation function
- dimerized state as CCM ground state