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

$$H = \sum_{i,j} J_{ij} s_i s_j$$

**ground state** HAFM on square and triangular lattice:
→ Néel ordered

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

*competition of bonds:*

- higher quantum fluctuations → suppression of long-range order, formation of *local singlets*; e.g., CaV$_4$O$_9$, SrCu$_2$(BO$_3$)$_2$
- *frustration* → my yield to PT to noncollinear (spiral) states in the classical model; quantum fluctuations – favor collinear order
→ 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 \(S\)

\[
|\Psi\rangle = e^S|\Phi\rangle, \quad S = \sum_{I \neq 0} S_I C_I^+; \quad \langle\tilde{\Psi}| = \langle\Phi|\tilde{S}e^{-S}, \quad \tilde{S} = 1 + \sum_{I \neq 0} \tilde{S}_I C_I
\]

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

\[
\frac{\partial \tilde{H}}{\partial \tilde{S}_I} = 0 \Leftrightarrow \langle\Phi|C_I e^{-S} H e^S|\Phi\rangle = 0, \Rightarrow \text{ket coefficients } S_I, \Rightarrow |\Psi\rangle, \\
\Rightarrow \quad E = \langle\Phi|e^{-S} H e^S|\Phi\rangle
\]

IV. bra-state equations (linear):

\[
\frac{\partial \tilde{H}}{\partial \tilde{S}_I} = 0, \Rightarrow \text{bra coefficients } \tilde{S}_I, \Rightarrow \langle\tilde{\Psi}|, \Rightarrow \tilde{A} = \langle\tilde{\Psi}|A|\Psi\rangle
\]
CCM – application on spin systems

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

$$\Rightarrow S = \sum_{i_1} S_{i_1} s_{i_1}^+ + \sum_{i_1 i_2} S_{i_1 i_2} s_{i_1}^+ s_{i_2}^+ + \sum_{i_1 i_2 i_3} S_{i_1 i_2 i_3} s_{i_1}^+ s_{i_2}^+ s_{i_3}^+ + \cdots$$

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 configurations
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:

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

- $\rho_s > 0 \rightarrow$ 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 $|\Phi\rangle$, → doing the CCM, → 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:

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

• 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

$$\epsilon_e \mathcal{X}^e_I = \langle \Phi | C_I e^{-S}[H, X^e] e^S | \Phi \rangle, \forall I \neq 0$$
CCM – Excited-State Formalism: application on spin systems

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

$$X^e = \sum_{i_1} x_{i_1} s_{i_1}^+ + \sum_{i_1 i_2} x_{i_1 i_2} s_{i_1}^+ s_{i_2}^+ + \sum_{i_1 i_2 i_3} x_{i_1 i_2 i_3} s_{i_1}^+ s_{i_2}^+ s_{i_3}^+ + \cdots$$

II. approximation of $X$:

- similar to the ground state
- but: choose configurations which change $s_T^z$ by ±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 ↔ dimerized paramagnetic phase with local singlets:
- \( J, J' \) different signs: frustration → 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 \textit{collinear} order

PRB 61, 14607 (2000); PRB 64, 0244331 (2001)
$J - J' \text{ model: new results with CMM}$

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

- influence of the Ising anisotropy $\Delta$

\[ s_i s_j \rightarrow s_i^x s_j^x + s_i^y s_j^y + \Delta s_i^z s_j^z \]

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

\[ \rightarrow \text{linear relation } J'_s(\Delta) \propto \alpha \Delta \text{ with } \alpha \approx 2.3 \ldots 3.0 \]


- 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

$J_1 - J_2$ 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 configuration (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
  → 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

\[ \begin{array}{c|c|c}
\text{LSUBn} & \text{gs} & \text{ex} \\
4 & 7 & 6 \\
6 & 75 & 91 \\
8 & 1287 & 2011 \\
\end{array} \]

- \( \rightarrow \) 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
  $\rightarrow$ 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 configurations
- \(E_g/N\) – GS energy per spin
- \(M\) – sublattice magnetisation

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

* Hamer et al. PRB 46, 6276 (1992); ** Sandvik PRB 56, 11678 (1997)
Square lattice: spin stiffness

<table>
<thead>
<tr>
<th>LSUBn</th>
<th>number eqs.</th>
<th>stiffness $\rho_s$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>3</td>
<td>0.2574</td>
</tr>
<tr>
<td>4</td>
<td>40</td>
<td>0.2310</td>
</tr>
<tr>
<td>6</td>
<td>828</td>
<td>0.2176</td>
</tr>
<tr>
<td>8</td>
<td>21124</td>
<td>0.2097</td>
</tr>
<tr>
<td>extr1</td>
<td>–</td>
<td>0.1812</td>
</tr>
</tbody>
</table>

- CCM:

- comparison with other methods:

- 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

<table>
<thead>
<tr>
<th>$\text{LSUB} n$</th>
<th>number eqs.</th>
<th>stiffness $\rho_s$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>3</td>
<td>0.1188</td>
</tr>
<tr>
<td>3</td>
<td>14</td>
<td>0.1075</td>
</tr>
<tr>
<td>4</td>
<td>67</td>
<td>0.0975</td>
</tr>
<tr>
<td>5</td>
<td>370</td>
<td>0.0924</td>
</tr>
<tr>
<td>6</td>
<td>2133</td>
<td>0.0869</td>
</tr>
<tr>
<td>approx.</td>
<td>–</td>
<td>0.0585</td>
</tr>
</tbody>
</table>

**CCM:**

- comparison with other methods:

  - exact diagonalization: 0.05
  - LSWT: 0.080
  - Schwinger-boson approach: 0.088
  - CCM: 0.060

→ improved results by CCM (LSWT is to large)
Conclusions

- CCM leads to quite accurate results for quantum spin systems (ground state and first excitation)
- Qualitatively 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