Coupled Cluster Theories of Quantum Magnetism

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Outline of Talk

• A very brief overview of the high-order CCM
• Comparison to results of other methods for various “Archimedean” lattices
• “Spiral” model states: example for an anisotropic square (“interpolating” square/triangular) model
• Specific examples of magnetic models:
  – The triangular lattice antiferromagnet in an external magnetic field
  – The spin-half $J_1$-$J_2$ Model on the square lattice
• Conclusions and future research
CCM Overview – Ground State

\[ |\Psi\rangle = e^S |\Phi\rangle \quad ; \quad \langle \widetilde{\Psi} | = \langle \Phi | \widetilde{S} e^{-S} \]

\[ S = \sum S_i C_i^+ \quad ; \quad \widetilde{S} = 1 + \sum \widetilde{S}_i C_i^- \]

\[ S.E. \Rightarrow E_g = \langle \Phi | e^{-S} H e^S | \Phi \rangle \quad \bar{H} = \langle \widetilde{\Psi} | H | \Psi \rangle \]

\[ \frac{\partial \bar{H}}{\partial \widetilde{S}_I} \equiv \langle \Phi | C_I^- e^{-s} H e^S | \Phi \rangle = 0 \quad \frac{\partial \bar{H}}{\partial S_I} \equiv \langle \Phi | \widetilde{S} e^{-s} [H, C_I^+] e^S | \Phi \rangle = 0 \]

A similar approach exists for the excited state – See Parkinson and Farnell, “An Introduction to Quantum Spin Systems” LNP 816 Chapter 10.
Approximation Schemes

• SUBm: All $m$-body or lower-order clusters.
• LSUBm: All clusters in a locale defined by $m$.
• SUBn-m: All $n$-body or lower-order clusters in a locale defined by $m$.

E.g., SUB4-4 for the $s=1/2$ and $s=1$ square-lattice ferrimagnet

We extrapolate these results in the limit, $m \to \infty$. 
CCM Flowchart

1. Define Fundamental CCM Clusters
   - Obtain Ground–State CCM Equations
     - Solve Ground–State CCM Equations
       - Ground– and Excited–State Expectation Values
   - Obtain Excited–State CCM Equations
     - Solve Excited–State CCM Equations
Archimedean Lattices

(a) Square
(b) Honeycomb
(c) CAVO
(d) SrCuBO
(e) Triangular
(f) Maple-Leaf
(g) Kagome
CCM results for unfrustrated lattices compared to some results of other approximate methods

<table>
<thead>
<tr>
<th>Model</th>
<th>Parameter</th>
<th>QMC</th>
<th>Series</th>
<th>ED</th>
<th>SWT</th>
<th>CCM</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Square HAF s=1/2</strong></td>
<td>E_g/bond</td>
<td>-0.334719(3)</td>
<td>-0.33465(5)</td>
<td>-0.335</td>
<td>-0.335233</td>
<td>-0.3348</td>
</tr>
<tr>
<td></td>
<td>Order Param &lt;s^z&gt;</td>
<td>0.3070(3)</td>
<td>0.307(1)</td>
<td>0.3173</td>
<td>0.3037</td>
<td>0.307</td>
</tr>
<tr>
<td></td>
<td>Gap</td>
<td>0</td>
<td>0</td>
<td>0.0247</td>
<td>0</td>
<td>-0.001</td>
</tr>
<tr>
<td></td>
<td>Spin Stiffness</td>
<td>0.175(2)</td>
<td>0.182</td>
<td>0.183</td>
<td>0.175</td>
<td>0.181</td>
</tr>
<tr>
<td></td>
<td>Mag. Suscept. χ</td>
<td>0.0669(7)</td>
<td>0.0659(10)</td>
<td></td>
<td>0.06426(1)</td>
<td>0.0700(6)</td>
</tr>
<tr>
<td></td>
<td>SW Velocity</td>
<td>2.28(1)</td>
<td></td>
<td></td>
<td>2.316 (1st order)</td>
<td>2.335 (SUB2)</td>
</tr>
<tr>
<td><strong>Square HAF s=1</strong></td>
<td>E_g/bond</td>
<td>-1.1640(1)</td>
<td></td>
<td>-1.1641</td>
<td>-1.1646</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Order Param &lt;s^z&gt;</td>
<td>0.8039(4)</td>
<td></td>
<td></td>
<td>0.8043</td>
<td>0.8049</td>
</tr>
<tr>
<td><strong>Honeycomb HAF s=1/2</strong></td>
<td>E_g/bond</td>
<td>-0.363</td>
<td>-0.3629</td>
<td>-0.3632</td>
<td>-0.365929 (2nd)</td>
<td>-0.363155</td>
</tr>
<tr>
<td></td>
<td>Order Param &lt;s^z&gt;</td>
<td>0.235</td>
<td>0.266</td>
<td>0.2788</td>
<td>0.2418 (2nd)</td>
<td>0.274066</td>
</tr>
<tr>
<td></td>
<td>Gap</td>
<td></td>
<td>0.0504</td>
<td>0</td>
<td>0.02</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Spin Stiffness</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>0.1379</td>
</tr>
<tr>
<td><strong>CAVO HAF s=1/2</strong></td>
<td>E_g/bond</td>
<td>-0.363</td>
<td>-0.3629</td>
<td>-0.3682</td>
<td>-0.3584 (linear)</td>
<td>-0.36888</td>
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<tr>
<td></td>
<td>Order Param &lt;s^z&gt;</td>
<td>0.178</td>
<td>0.2303</td>
<td>0.212 (linear)</td>
<td>0.204</td>
<td></td>
</tr>
</tbody>
</table>
CCM results for frustrated lattices compared to some results of other approximate methods

<table>
<thead>
<tr>
<th>Model</th>
<th>Parameter</th>
<th>Series</th>
<th>ED</th>
<th>SWT* (1st order)/Swinger Boson†</th>
<th>CCM</th>
</tr>
</thead>
<tbody>
<tr>
<td>Triangle</td>
<td>$E_G$/bond</td>
<td>-0.1842</td>
<td>-0.1842</td>
<td>-0.154*</td>
<td>-0.18147</td>
</tr>
<tr>
<td></td>
<td>Order Param $&lt;s^z&gt;$</td>
<td>0.20</td>
<td>0.193</td>
<td>0.2387*</td>
<td>0.189331</td>
</tr>
<tr>
<td></td>
<td>Spin Stiffness</td>
<td>0.05</td>
<td>0.08*</td>
<td>0.0564</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Mag. Suscept. $\chi$</td>
<td></td>
<td>0.0794*</td>
<td>0.065(23)</td>
<td></td>
</tr>
<tr>
<td>SrCuBO</td>
<td>$E_G$/bond</td>
<td>-0.231</td>
<td>-0.2310</td>
<td>0.231†</td>
<td>-0.2311</td>
</tr>
<tr>
<td></td>
<td>Order Param $&lt;s^z&gt;$</td>
<td>0.200</td>
<td>0.2280</td>
<td>0.203†</td>
<td>0.211</td>
</tr>
<tr>
<td>Kagome</td>
<td>$E_G$/bond</td>
<td>-0.2172</td>
<td></td>
<td>-0.2353*</td>
<td>-0.2126</td>
</tr>
<tr>
<td></td>
<td>Order Param $&lt;s^z&gt;$</td>
<td>~ 0</td>
<td></td>
<td></td>
<td>&lt; 0</td>
</tr>
<tr>
<td></td>
<td>Spin Stiffness</td>
<td></td>
<td></td>
<td></td>
<td>-0.023</td>
</tr>
</tbody>
</table>

See “Quantum Magnetism” LNP 645 (chapter 2) and “An Introduction to Quantum Spin Systems” LNP 816 (chapters 10 & 11) for more details about all of these approximate calculations. See also, “Series Expansions Methods for … Lattice Models” by Oitmaa et al. (Cambridge university Press, 2006).
“Spiral” model states: the interpolating square/triangular lattice model (AKA “anisotropic square”) (Bishop, Li, et al., PRB 79,174405 (2009))

\[ J_1 \quad J_2 \]

(a) Néel
(b) Spiral
(c) Striped

\[ J_{1'} = 0.0, \quad J_{1'} = 0.25, \quad J_{1'} = 0.5, \quad J_{1'} = 0.75, \quad J_{1'} = 0.8, \quad J_{1'} = 1.0, \quad J_{1'} = 1.2, \quad J_{1'} = 1.4 \]
Triangular-lattice antiferromagnets in an external magnetic field

Co\(^{2+}\) = spin-1/2 atoms  
Ni\(^{2+}\) = spin-1 atoms
Background

• Co\(^{2+}\) atoms in Ba\(_3\)CoSb\(_2\)O\(_9\) and Ni\(^{2+}\) atoms in Ba\(_3\)NiSb\(_2\)O\(_9\) form \(s=1/2\) and \(s=1\) a triangular lattice.

• Quantum spins interact via an antiferromagnetic Heisenberg exchange interaction.

• An interesting effect of “spin plateau” is seen as one imposes an external magnetic field of strength \(\lambda\).

• The relevant Hamiltonian is given by:

\[
H = J \sum s \cdot s + \lambda \sum s^z
\]
Spin Plateau

(see: Farnell, Richter, & Zinke, J. Phys.: Condens. Matt. 21, 406002 (2009))

$\text{Co}^{2+} = \text{spin-1/2 atoms}$

$\text{Ni}^{2+} = \text{spin-1 atoms}$
The $J_1$-$J_2$ Model on the Square Lattice

- Nearest and Next-Nearest Neighbour Bonds on the square lattice; $\langle ... \rangle$ indicates each bond counted once.

\[ H = J_1 \sum_{\langle i,j \rangle} S_i \cdot S_j + J_2 \sum_{\langle \{ i,k \} \rangle} S_i \cdot S_k \]
Background to the $J_1$-$J_2$ model

- Various quasi-2D materials are described by the $J_1$-$J_2$ model, e.g., $\text{Li}_2\text{VOSiO}_4$ and $\text{Li}_2\text{VOGeO}_4$ – $J_2/J_1$ in range 5 to 10. See later...
- It is a “canonical model” used to investigate quantum magnetic systems, especially for case of strong frustration
- Non-magnetic quantum phase (quantum paramagnet)
  - Does this phase survive for $T>0$?
- The nature of quantum phase is still not fully resolved
- Possible deconfined quantum criticality at quantum phase transitions
- No exact solutions for this 2D model – it is a good test of approximate techniques.
Ground-State Energy

CCM. R. Darradi et al. PRB 78, 214415 (2008)


Series Expansions, Sirker et al., PRB B 73, 184420 2006
Order Parameters

CCM. R. Darradi et al.
PRB 78, 214415 (2008)


Series Expansions,
Oitmaa et al. PRB 54 3022 (1996)
The “Spin Stiffness” - the response to a “twist” in local axes of spins, which so indicates *stability of ground state*

CCM. R. Darradi et al. PRB 78, 214415 (2008)


ED + LSWT, Einarsson, PRB 51, 6151 (1995)
Excitation Energy Gap

CCM: DJJF


Series: Kotov et al. PRB 60 14 613 (1999)

Gap opens at J2/1≈0.5. But is this result too large...
Higher LSUB\(m\) please!!

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Initial Results for the “Quantum Fidelity”

\[ F = \frac{\left\langle \Psi(J_2 / J_1) | \Psi(J_2 / J_1 + \delta J_2 / J_1) \right\rangle}{\sqrt{\left\langle \Psi(J_2 / J_1) | \Psi(J_2 / J_1) \right\rangle \left\langle \Psi(J_2 + \delta J_2 / J_1) | \Psi(J_2 / J_1 + \delta J_2 / J_1) \right\rangle}} \]

\[ \delta = 0.001 \] above
Sign Rule for Small $J_2/J_1$

\[ |\Psi\rangle = \sum I (-1)^{M_A} c_I |I\rangle \quad M_A = \sum_{i_A=1}^{N_A} s_{i_A}^z \quad c_I \geq 0 \forall I \]

Sites on A go over one sublattice →→→→→

“Hard” sign rule: rule above can be proven exactly at $J_2=0$ by noting that the above formulation results in a negative definite matrix formulation of the Schrödinger equation and so for which $c_I > 0$.

“Soft” sign rule: rule can’t be proven exactly (often due to frustration), although it is seen up to some value of $J_2$ numerically via ED and CCM results.

Weight of states: Sum over states $I$ for which the rule holds such that: weight=$\Sigma_I |c_I|^2$
Marshall-Peierls Sign Rule

CCM: DJJF


weight = $\sum_{i=1}^{N_M} |c_i|^2 / \sum_{i=1}^{N_F} |c_i|^2$

weight = $\sum_{i=1}^{N_M} |c_i|^2$
## Range of Paramagnetic Regime

<table>
<thead>
<tr>
<th>Method</th>
<th>$J_2^M$</th>
<th>$J_2^{c1}$</th>
<th>$J_2^{c2}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>ED$^1$</td>
<td>0.2-0.3</td>
<td>0.35</td>
<td>0.66</td>
</tr>
<tr>
<td>Series$^2$</td>
<td>--</td>
<td>0.38</td>
<td>0.60</td>
</tr>
<tr>
<td>Dimer Boson Model$^3$</td>
<td>--</td>
<td>0.38</td>
<td>0.62</td>
</tr>
<tr>
<td>CCM$^4$</td>
<td>0.2-0.3$^4$</td>
<td>0.44(±0.01)$^5$</td>
<td>0.59(±0.01)$^5$</td>
</tr>
</tbody>
</table>

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$^2$Sushkov et al. PRB 63, 104420 (2001)

$^3$Kotov et al. PRB 60 14 613 (1999)

$^4$Bishop, Farnell, Parkinson PRB 58 6394 (1998).

$^5$Darradi et al. PRB 78, 214415 (2008)
Nature of the paramagnetic regime

“Inverse” Magnetic Susceptibilities

CCM + ED: Darradi, PRB 78, 214415 (2008)

Series: Sirker PRB 73, 184420 (2006)

Taken from Sushkov, PRB 63, 104420 (2001)
Results for $J_1 < 0$

Richter et al. PRB 81, 174429 (2010)
Spin-Spin Correlation Functions

J₁<0: Results (thicker lines) indicate single PT point at J₂ ≈ -0.4J₁ (probably first-order)
J₁>0: Results (thinner lines) indicate PT points at J₂ ≈ 0.6J₁ (probably first-order)

See: Richter et al. PRB 81, 174429 (2010)
Quantum Phase Diagram at $T=0$

Phase diagram from a synthesis all of the results presented here.

Conclusions

• The CCM provides a useful tool in tackling (especially 2D) problems in quantum magnetism.
• It is **accurate**, **reliable**, and **flexible**.
• Can be used to detect phase transition point points, and possibly even their order.
Afterword and Thanks

• Final words in *The Theory Of Magnetism Made Simple* by DC Mattis:

  “I cannot resist pointing out the obvious: independently of the technical importance of magnetic substances – which cannot be denied – the *theory* of magnetism continues to lie at the core of *practically all* of contemporary theoretical physics. Its study continues to be a perpetual delight and inspiration.”

• Thanks to: WE-Hereaus Stiftung. All at the Physikszentrum, Bad Honnef.

• Also to: Prof. Raymond F. Bishop (Manchester), Prof. Johannes Richter (Magdeburg, Germany), Dr. Peggy Li (Manchester), Dr. John B. Parkinson (Manchester), Dr. Joerg Schulenburg (Magdeburg), Dr. Sven Krueger (Magdeburg), Dr. Klaus Gernoth (Manchester), Dr. Ronald Zinke (Magdeburg), Dr. Rachid Darradi (Technische Universität Braunschweig, Germany), and Prof. Charles Campbell (Minnesota, USA), *et (many more) al.*

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