NUMERICAL AND ANALYTICAL INVESTIGATION OF THE OPERATOR CONTENT OF ANISOTROPIC SPIN-1 CHAINS NEAR TRANSITION LINES

C. Degli Esposti Boschi

INFM
Unità di Ricerca di Bologna

in collaboration with:

F. Ortolani,
E. Ercolessi,
G. Morandi,
M. Roncaglia,
S. Pasini (doctorate)

Recent Progress and Prospects in Density-Matrix Renormalization,
Leiden, August 2-13, 2004
Outline

- Performance of the DMRG near Quantum Critical Points
- Crash-course in Conformal Field Theories
- Spin-1 Anisotropic Hamiltonians ($\Lambda$-$D$ Model)
- Implementation
- Locating the Critical Point and Identifying the Appropriate CFT
- Boundaries of the Haldane phase: $c = 1/2$ and $c = 1$ Transition Lines
- Off-Critical Theories
- Conclusions and Future Developments
Performance of the DMRG near Quantum Critical Points

➢ Quantum Phase Transition driven by a parameter $g$ ($T=0$)
\[ \Delta E(g = g_c) = 0 \]

➢ One would like to explore larger and larger sizes and keep a good accuracy in order to control the gap closure. However, close to critical points, the systems experiences fluctuations on very large scales. As a result of the diverging characteristic length...

➢ The spectrum of the density-matrix, $\{\rho\}$, becomes significantly broader. In general (including degeneracies):
\[ w_j \sim \exp[-C (\ln j)^p], \quad p > 1 \]  
Chan et al., J. Stat. Phys. 109, p. 289

For a class of integrable systems, the connection with the corner transfer matrix can be used to prove that:
\[ \rho_j \propto \exp(-\varepsilon j), \quad \varepsilon \propto 1/\ln L \]

at criticality

(Peschel's talk on reduced density matrices)
The minimum number of DMRG states, $M$, needed to go below a prescribed threshold with the sum of discarded weights:

$$W_M = 1 - P_M = \sum_{j > M} \rho_j$$

becomes larger in the vicinity of critical points. In other words, if $M$ is fixed there will be a regime where the gap (typically decreasing with size) is comparable with $W_M$.

The latter is a basic indicator of the accuracy:

$$\delta E \propto W_M$$

but only after a few finite-system iterations, $I$, are performed in order to get rid of the environment error.

---

Legeza & Fáth, PRB 53, p. 14349, fig. 5
There are various indications that the interplay between the DMRG truncation and criticality induces a (fake) crossover length $L_{\text{DMRG}}$.

- Andersson, Boman & Östlund, PRB 59, p. 10493: $L_{\text{DMRG}} \propto M^{1.3}$ for free hopping fermions (gapless)
- Nishino, Okunishi & Kikuchi, PLA 213, p. 69: 2D classical Ising and 3-states-Potts models at $T=T_c$
- Anisotropic $S=1$ Chains close to $c=1$ lines (cond-mat/0312707).

Infinite-system runs on very large systems are useful for a first insight, but a more precise and quantitative answer comes from finite-system iterations for not-too-large sizes, interpreted with powerful finite-size scaling (FSS) methods...

(Energy errors may grow with system's size)
Outline

- Performance of the DMRG near Quantum Critical Points
- Crash-course in Conformal Field Theories
- Spin-1 Anisotropic Hamiltonians ($\lambda-D$ Model)
- Implementation
- Locating the Critical Point and Identifying the Appropriate CFT
- Boundaries of the Haldane phase: $c = 1/2$ and $c = 1$ Transition Lines
- Off-Critical Theories
- Conclusions and Future Developments
A 'Crash-course' in Conformal Field Theories (CFT)

- Whenever the low-energy physics can be described by a continuum model in 1+1 dimensions (chains & ladders), we are led to consider the framework of CFT's, that encompasses the possible universality classes of 2D scale-invariant field theories.

- Conformal invariance in 2D is so strong because the associated Virasoro algebra is infinite-dimensional

\[
[L_m, L_n] = (m-n) L_{m+n} + \frac{c}{12} \delta_{m,-n} (m^3 - m), \quad m, n \in \mathbb{Z}
\]

and the states of the theory can be classified in terms of its irreducible representations (including a similar antiholomorphic part denoted by overbars).

Central term of the algebra (at the quantum level) The central charge \( c \) defines the structure of the theory...
**Minimal Models \((c < 1)\)**

- For unitary theories with \(c < 1\) only a set of discrete values is allowed:
  \[
c = 1 - 6/p(p+1), \quad p = 2, 3, \ldots
\]

- For a given \(p\) there is a finite number of eigenstates of \(L_0\)
  \[
  L_0 |\Delta\rangle = \Delta|\Delta\rangle
  \]
  \[
  \Delta = \left\{ \left[ \left( p+1 \right) r - ps \right]^2 - 1 \right\} / 4 p(p+1), \quad 1 \leq s \leq r \leq p-1
  \]
  and the whole Hilbert space is built by acting repeatedly on each primary state with negative-index generators:
  \[
  |\Delta; m, k\rangle = (L_{-m})^k |\Delta\rangle, \quad L_0 |\Delta; m, k\rangle = (\Delta + m k) |\Delta; m, k\rangle
  \]

- Most celebrated example:
  
  \(p=3, c=1/2 \rightarrow 2D\ Ising\ universality\ class\) \[
  \Delta = \overline{\Delta} = 0, \quad 1/16, \quad 1/2
  \]

  \(p=4, c=7/10\ Tricritical\ Ising,\ p=5, c=4/5\ 3\text{-states Potts}\)
Connection with Physical Observables

➢ Conformal mapping onto a infinite cylinder of circumference $L$ (space with periodic boundary conditions):

$$
\begin{align*}
H_{\text{Lattice}} & \Leftrightarrow u \frac{2\pi}{L} \left( L_0 + \frac{L_0}{12} - \frac{c}{12} \right) + L\epsilon_\infty, \\
Q & = \frac{2\pi}{L} (L_0 - \overline{L}_0)
\end{align*}
$$

Velocity (to be determined)

➢ In particular, the ground state (GS) energy density and the excitation gaps (eigenstates of $L_0, \overline{L}_0$) at finite $L$ scale as:

$$
\begin{align*}
\frac{E_{L}^{GS}}{L} & = \epsilon_\infty - \frac{\pi c u}{6L^2}, \\
\Delta E_{L}^d & = \frac{2\pi u}{L} \left( \Delta + \overline{\Delta} + mk + \overline{m}\overline{k} \right)
\end{align*}
$$

➢ $d$ is the scaling dimension that regulates the large-distance decay of the correlation functions of the operator $O$ associated to a given excited state $|\Delta, \overline{\Delta} ; m, k, \overline{m}, \overline{k} \rangle = O |\text{GS}\rangle$

$$
\langle \text{GS} | O(0,0) O(z, \overline{z}) | \text{GS} \rangle \sim z^{-2(\Delta + m k)} \overline{z}^{-2(\overline{\Delta} + \overline{m}\overline{k})} = r^{-2d} \quad \text{for} \quad z = \overline{z} = r
$$
Beyond Minimal Models

$c \geq 1$: Infinite # of Primary Fields

➢ Rational values of $c$: There are many constructions in which the Virasoro algebra is 'embedded' into a larger one, and it is possible to define the fields (and corresponding states) as 'primary' with respect to the irreducible representations of the new symmetry group $G$ (e.g. Sugawara construction for WZWN).

➢ (Very) roughly speaking, central charges can be summed or subtracted by taking tensor products and cosets of groups, respectively (Goddard-Kent-Olive construction).

➢ $c = 1$: Free bosonic field $\phi$. In 2D the correlation functions of $\phi$ have log divergences and it has to be compactified on a circle of radius $R_\phi$: $\Phi \equiv \Phi + 2\pi R_\phi$. By varying the radius one finds a continuum of universality classes (line of critical points) with scaling dimensions and exponents depending on $R_\phi$. The primary states ($G=U(1)$) are now topological excitations of $\Phi$. 
Outline

☑ Performance of the DMRG near Quantum Critical Points
☑ Crash-course in Conformal Field Theories
☐ Spin-1 Anisotropic Hamiltonians ($\lambda$-$D$ Model)
☐ Implementation
☐ Locating the Critical Point and Identifying the Appropriate CFT
☐ Boundaries of the Haldane phase: $c = 1/2$ and $c = 1$ Transition Lines
☐ Off-Critical Theories
☐ Conclusions and Future Developments
Spin-1 Anisotropic Hamiltonians: $\lambda-D$ Model and Applications

$$H = J \sum_{L \text{ sites}} \vec{S}_j \cdot \vec{S}_{j+1} + (\lambda - 1) S^z_j S^z_{j+1} + D(S_j)^2$$

- Ising-like ($\lambda$) and single-ion ($D$) anisotropies may drive the system out of the Haldane phase, where the GS is VBS-like.

- Theoretical (and experimental?) playground where both the conventional (finite) correlation length and the string-order can be varied in order to study the capability of the chain to maintain high levels of entanglement over large scales. (scenario put forth by F. Verstraete et al., PRL 92, p. 087201)

- Some compounds described by the model: 
  RbNiCl$_3$, Y$_2$BaNiO$_5$ (pure Haldane AFM's), so-called NENP and NENC (easy-plane AFM's with $D \approx 0.2$ and $D \approx 7.5$ resp.)
  CsNiFe$_3$ (FM with $\lambda = -1$, $D \approx 0.4$), CoCl$_2$ 2 H$_2$O (effective easy-axis Ising FM with large -ve $\lambda$ and $D \approx -5$).
Phases and String Order Parameters (SOP)

We have focused on:

➢ Borders of the Haldane phase (multicritical point in particular);
➢ Off-critical perturbations;
➢ Numerics and field-theoretical expressions of SOP's:

\[ O_S^\alpha \equiv - \lim \limits_{|j-k| \to \infty} \langle S_j^{\alpha} \exp \left( i \pi \sum \limits_{n=j+1}^{k-1} S_n^{\alpha} \right) S_k^{\alpha} \rangle \]

Fig. 1

DMRG data with PBC, \( M = 216, L = 100 \) and alg. extrapolations

\[ \lambda = 1 \]

\[ \beta = 0.244 \]

\[ 2\beta_S = 0.2496 \]

Bosonisation: Schulz, PRB 34, p. 6372
Exact Diagonalisation: Botet et al., PRB 28, p. 3914; Glaus & Schneider, PRB 30, p. 215; Chen et al, PRB 67, p. 104401
Outline

☑ Performance of the DMRG near Quantum Critical Points
☑ Crash-course in Conformal Field Theories
☑ Spin-1 Anisotropic Hamiltonians ($\lambda-D$ Model)
☐ Implementation
☐ Locating the Critical Point and Identifying the Appropriate CFT
☐ Boundaries of the Haldane phase: $c = 1/2$ and $c = 1$ Transition Lines
☐ Off-Critical Theories
☐ Conclusions and Future Developments
Implementation

Basically, we used original White’s algorithms with:

➢ Periodic Boundary Conditions (PBC), in order to (a) have a unique GS without adjusted spins at the edges, (b) eliminate the edge effects on rapidly-decaying (string) correlation functions and obtain a better estimate of the corresponding exponents;

➢ Superblock geometry: [Block][ ] | [Env. Block (refl.)][ ] (proved to be important with staggered fields). The blocks are always separated by a , and the correlation functions can be computed fixing one of the two points on it;

➢ 3 finite-system iterations to reduce the environment error;

\[ M^z = \sum_{j=0}^{L-1} S^z_j \] is the only good quantum number exploited...
Multi-target Calculation of Excited States
(Thick-restart Lanczos method)

➢ Equally-weighed density matrix on the block for \( N_t \) excited states + GS (in a given sector of \( M^z \)):

\[
\rho_{M^z} = \frac{1}{N_t} \sum_{b=0}^{N_t} \rho[\, |M^z, b\rangle] 
\]

➢ The results presented here are obtained with a code in which the states \( |M^z, b\rangle \) for the construction of \( \rho[\, |M^z, b\rangle] \) are determined using the so-called thick-restart variant of the Lanczos method, recently proposed by Wu & Simon (SIAM J. Matrix Anal. Appl. 22, p. 602).

➢ Features: Projection-based, not preconditioned, restarted (for the unconverged vectors). It is not difficult to implement it as an extension of an existing Lanczos routine, adding only one vector at each step thereby maintaining essentially a tridiagonal form of the projected Hamiltonian (except for one row and column). Initial motivation: test and exploit the stability in a DMRG program for quantum dots. For the moment we stick to it because it saves memory at the expenses of CPU-time (10-20% including re-orthogs.)
Outline

☑ Performance of the DMRG near Quantum Critical Points
☑ Crash-course in Conformal Field Theories
☑ Spin-1 Anisotropic Hamiltonians (\(\lambda - D\) Model)
☑ Implementation
□ Locating the Critical Point and Identifying the Appropriate CFT
□ Boundaries of the Haldane phase: \(c = 1/2\) and \(c = 1\) Transition Lines
□ Off-Critical Theories
□ Conclusions and Future Developments
Locating the Critical Point

Really determines the quality of the whole analysis

0. Use symmetries, dualities, etc. as much as possible! Otherwise...

1. Preliminary scan in various sectors of $M^x$, using a reasonable fit for $L \to \infty$.

2. Quantitative refinement using FSS or Phenomenological Renormalisation Group (PRG), that provides a series of $L$-dependent (pseudo)critical points via the formula:

$$\frac{(L+\delta L) \Delta E_{L+\delta L}(g_{pc}) - L \Delta E_L(g_{pc})}{\delta L} = 0$$

Sometimes the critical point gets mirrored...
Locating the Critical Point, $c=1$

This effect is likely to be related to the cause indicated by Kitazawa (JPA 30, p. L285), to explain the difficulties to obtain reliable numerical estimates of $c=1$ critical points. The first-order term in the expansion of the scaling function for $L \ll \xi$:

$$\Delta E_L \approx \frac{2\pi u}{L} \left( d_{\text{gap}} + C \left( \frac{L}{\xi} \right)^{1/\nu} \right) + \ldots$$

$(2-\nu^{-1})$ scal. dim. of gap-gener. term

vanishes and the intersections of the scaled gaps $L \Delta E_L$ are of parabolic type.

In this case twisted boundary conditions $S_{j+L}^z \equiv S_j^z$, $S_{j+L}^\pm \equiv S_{j+L}^\pm e^{\pm i \psi}$ are of great help. The levels from differently-twisted sectors have scaling dimensions depending on $\psi$ and they can be combined to cancel (part of) the effect of finite-size corrections.

3. Once the critical point has been identified, check that the scaled gap settles actually to a constant and that the finite-size $\beta$-function $\beta_L^{-1}(g_c) = (\partial \ln \Delta E_L / \partial g)_{g=g_c}$ scales to zero (gives and independent estimate of the exponent $\nu$).
Identifying the Appropriate CFT

- Estimate $\epsilon_\infty$ and $c u$ from finite-size GS energy densities;

- Find an independent estimate of $u$, using one of more levels whose scaling dimension is (supposed to be) known. Here one introduces an hypothesis on the type of the theory, to be checked self-consistently;

- Now $c$ can be computed, as well as the scaling dimensions from the slopes $d u$ from the plot $\Delta E/2\pi$ vs $1/L$. Their spectrum (values and multiplicities) provides a very stringent test of the hypothesis.
Outline

☑ Performance of the DMRG near Quantum Critical Points
☑ Crash-course in Conformal Field Theories
☑ Spin-1 Anisotropic Hamiltonians (λ-Δ Model)
☑ Implementation
☑ Locating the Critical Point and Identifying the Appropriate CFT
☐ Boundaries of the Haldane phase: $c = 1/2$ and $c = 1$ Transition Lines
☐ Off-Critical Theories
☐ Conclusions and Future Developments
Boundaries of the Haldane Phase: $c = 1/2$

- Recently, it has been suggested (cond-mat/0307266) that this case does not really belong to the 2D Ising universality, but the deviations are probably to be ascribed to the use of the infinite-system algorithm.

- The finite-size $\beta$-function is essentially the same in the three cases. The $c = 1/2$ line is not generated by the action of a marginal operator (forbidden).

<table>
<thead>
<tr>
<th>$\lambda_c, D_c$</th>
<th>$u$ [num]</th>
<th>$c$</th>
<th>$\nu^*$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0, 1.1856</td>
<td>2.676</td>
<td>0.4959</td>
<td>0.987</td>
</tr>
<tr>
<td>1, −0.315</td>
<td>2.65</td>
<td>0.498</td>
<td>1.003</td>
</tr>
<tr>
<td>0.5, −1.20</td>
<td>2.44</td>
<td>0.5008</td>
<td>1.023</td>
</tr>
</tbody>
</table>

$D = 0, \lambda = 1.1856, M = 243, L = 20-80, N_t = 8 + GS$

The states with $M^z \neq 0$ do not become critical.

*from $\beta$-function. Errors of some units in the last digit reported.
Boundaries of the Haldane Phase: $c = 1$

Two examples where the full low-lying spectra can be matched within a 3% in worst cases.

$\lambda = 1, D = 0.99$

$\lambda = 0.5, D = 0.65$

The slope of all the primary states depends on the point ($\rightarrow$ no Ginsparg's orbifold construction)

$[M = 405, \text{target states in the legends}]$
Nonlinear O(2) $\sigma$ Model as a $c = 1$ Theory

Starting from the large-$D$ phase, where the single-ion anisotropy favours planar order, we perform an Haldane-like mapping with the difference that the staggered part of the magnetisation is assumed to lie on the plane:

$$\bar{n}(x, \tau) = [\cos \theta(x, \tau), \sin \theta(x, \tau), 0]$$

Integrating out the field $\ell^z$ (at quadratic order) one arrives at the following Lagrangian density for $\Theta = \theta / u^{1/2}$, or for its dual field $\Phi$:

$$\mathcal{L}_{O(2)} = \frac{u}{2} \left[ (\partial_x \Theta)^2 + (\partial_x \Theta)^2 \right] = \frac{u}{2} \left[ (\partial_x \Phi)^2 + (\partial_x \Phi)^2 \right]$$

that provides a good quantitative description of the $c=1$ borders of the Haldane phase (EPJB 35, p. 465).

<table>
<thead>
<tr>
<th>$\lambda, D_c(\lambda)$</th>
<th>$u$ [num]</th>
<th>$u$ [O(2)]</th>
<th>$c$</th>
<th>$\nu^*$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.5, 0.65</td>
<td>2.197</td>
<td>2.07</td>
<td>1.008</td>
<td>2.38</td>
</tr>
<tr>
<td>1, 0.99</td>
<td>2.588</td>
<td>2.45</td>
<td>0.997</td>
<td>1.49</td>
</tr>
<tr>
<td>2.59, 2.30</td>
<td>4.04</td>
<td>3.43</td>
<td>0.99</td>
<td>0.870</td>
</tr>
<tr>
<td>3.20, 2.90</td>
<td>4.445</td>
<td>3.77</td>
<td>1.133</td>
<td>0.678</td>
</tr>
</tbody>
</table>

*from CFT formula: $\nu = 1/(2-K)$
Scaling Dims. of the pure Gaussian Model

\[ d_{m,n} = \left( \frac{m^2}{4K} + n^2 K \right) \]

Primary states are topological excitations: 
\( n \) winding # of \( \Theta \), \( m \) winding # of \( \Phi \).

\[ K \equiv \pi / u \]

\[ V_{m,n} = \exp \left[ i \left( \sqrt{4\pi K} n \Phi + \sqrt{\pi / K} m \Theta \right) \right] \]

Primary fields

\[ S^z(x) = \frac{\partial_x \Theta}{\sqrt{u}} \quad \Rightarrow \quad M^z = \int \! d\,x \, S^z(x) = \int \! d\,x \, \frac{\partial_x \Phi}{\sqrt{u}} = \frac{2\pi m R_\Phi}{\sqrt{u}} = m \]

For \( \frac{1}{2} < K < 2 \), the first excited states has \( (m=\pm 1, n=0) \) but the most relevant operator allowed by symmetries has \( (m=0, n=\pm 1) \) with scaling dimension \( K \). Interestingly enough, from FSS on the minima of \( O_S^z(x) \) at finite \( L \) we find a scaling exponent, \( \eta_{S^z} \), close to \( K/2 \), that is twice the scaling dimension of the so-called twist operator, which would be allowed with TBC \( (n=\pm 1/2) \). From the mapping onto O(2):

\[ O_S^z(x) \sim \exp \left[ i \sqrt{\pi K} \Phi(x) \right] \]

<table>
<thead>
<tr>
<th>( \lambda, D_c(\lambda) )</th>
<th>( K ) [num]</th>
<th>( \eta_{N\perp} ) (1/2K)</th>
<th>( \eta_{S\perp} ) (?)</th>
<th>( \eta_{S^z} ) (K/2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.5, 0.65</td>
<td>1.580</td>
<td>0.312 (0.316)</td>
<td>0.251</td>
<td>0.804 (0.790)</td>
</tr>
<tr>
<td>1, 0.99</td>
<td>1.328</td>
<td>0.374 (0.377)</td>
<td>0.2733</td>
<td>0.741 (0.664)</td>
</tr>
</tbody>
</table>
Outline

☑ Performance of the DMRG near Quantum Critical Points
☑ Crash-course in Conformal Field Theories
☑ Spin-1 Anisotropic Hamiltonians (\(\lambda-D\) Model)
☑ Implementation
☑ Locating the Critical Point and Identifying the Appropriate CFT
☑ Boundaries of the Haldane phase: \(c = 1/2\) and \(c = 1\) Transition Lines
☐ Off-Critical Theories
☐ Conclusions and Future Developments
Moving away from Critical Lines

Taking into account the most relevant operator we find a sine-Gordon model:

\[ \mathcal{L}_{SG} = \frac{\mu}{2} \left[ (\partial_x \Phi)^2 + (\partial_y \Phi)^2 \right] + \mu \cos \left( \sqrt{4\pi} K \Phi \right) \]

whose excitation spectrum changes qualitatively with \( K \): In addition to soliton and antisoliton states, one has other \( \text{int}[2/K-1] \) stable 'particles', with 'mass' \( \propto \mu^\nu \) (breathers).

\[ \Delta E_k = 2 \Delta E_{\text{soliton}} \sin \left[ \frac{k \pi K}{2(2 - K)} \right] \]

Near the \( c = 1/2 \) line the effective field-theoretical model is that of a massive Majorana fermion. Moving upwards one encounters line 2 within the Haldane phase, where excitations with \( M^x = 0 \) and \( M^z = \pm 1 \) have the same energy. The former is Majorana-like and the latter are soliton-like.

From fig. 1 of Chen et al., PRB 67, p. 104401

Botet et al., PRB 28, p. 3914
Looking for Breathers

In the same spirit of spin-1/2 systems with Dzyaloshinskii-Moriya interaction in external fields (Wang's talk, exp. Kenzelmann et al., PRL July 2004) or spin-Peierls compounds (e.g. Bouzerar et al., PRB 58, p. 3117)

- Critical point between the 'Free-Dirac' ($K=1$) and the multicritical point ($K=1/2$). Current estimate: $K=0.76$, $u=4.04$ (was $K=0.84$ in EPJB 35, p. 465 due to smaller $L$)

Preliminary evidence of the appearance of the 1st breather in the large-$D$ phase. From the ratio with the soliton gap we estimate $K=0.88$, $u=4.1$
Conclusions and Future Developments

➢ Our suggestion is that (if one has to choose) it is better to employ the computational resources to extract precise data with the finite-system algorithm for a suitable number of excited states, rather than 'pushing' $L$ only with infinite-system runs. The latter procedure may be necessary for a preliminary approach but the loss of accuracy may lead to ambiguous results, especially close to critical points where true scale invariance is hindered by the DMRG truncation.

➢ CFT provide a way to identify the underlying universality class and the associated exponents through the computation of the scaling dimensions of various finite-size excitation gaps.

➢ This program could benefit from:
  - Reliable FSS for slightly off-critical systems (Lüscher's theory);
  - TBC with the DMRG (to be tested against other types of BC's);
  - Most of all, take advantage of conserved quantities by selecting the quantum numbers of interest (like parity, momentum,...)
Thanks four your attention

A copy of this talk and more informations about the activity of the Condensed Matter Theory Group in Bologna are available at:

http://www.bo.infm.it/grp/morandi/home.html

or by email: desposti@bo.infm.it
General References

DMRG: Not needed here ...

CFT's & sine-Gordon:

➢ M. Henkel, Conformal Invariance and Critical Phenomena (Springer, 1999);
