Dimerization in antiferromagnetic $SU(2S+1)$ spin chains at $S > 1/2$

Michael Aizenman

Princeton Univ.

Talk based on a joint work with Hugo Duminil-Copin.

Incorporates insights from Aiz.– Nachtergaele '94,
D-C, Gagnebin, Harel, Manolescu, Tassion '16
and Gourab Ray – Yinon Spinka '19

Quantissima in the Serenissima
Venice, 21 Aug. 2019.

The talk will focus on one dimensional quantum spin chains with

$$\boxed{H = -(2S+1)\sum_x P^{(0)}_{x,x+1}}$$

$P^{(0)}_{x,y} \equiv \mathbb{I}[|\mathbf{S}_x + \mathbf{S}_y| = 0] =$ the orthogonal projection onto the singlet state.

The case $S = 1/2$ is the spin $1/2$ Heisenberg antiferromagnet, studied by Bethe '1931.

The extension to SU($2S+1$) invariant quantum spin chains was introduced by Affleck, and studied by Batchelor – Barber, and Klümper $\approx$'90,
Aiz. – Nachtergaele '94,
Nachtergaele – Ueltschi '17,
Aiz. – Duminil-Copin '19 (in prep).

Phenomena of interest:
frustration, dimerization, potential for non-unique grounds states.

Dilemma (A-N): slow decay of correlations, or symmetry breaking.

Applicable methods (range from hard calculations to soft power):

Bethe ansatz, loop representation (stochastic geometry), expansions, FKG inequality, relation to two-dimensional Q-state Potts models, stoch-topological arguments

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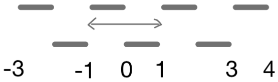
Dimerization (a naive, and potentially misleading, picture):

Bottom line $L = 3$, top $L = 4$



$\forall L$, the spin chain in $\Lambda(L) = (-L, L]$ consists of an even number of spins.
The pairing picture suggest that in the ground state for L even the expected energy of the $(0,1)$ term would be lower than that of the $(-1,0)$ term, and the reverse should be true for odd L.

More generally, this picture suggests that for finite L there will be local-mean-energy oscillations, with:

$$(-1)^L \left[\langle P^{(0)}_{2n-1,2n} \rangle_L - \langle P^{(0)}_{2n,2n+1} \rangle_L \right] \geq 0 .$$

A more nuanced picture:

i) Lower energy may be attained through the formation of larger coherent structures.

ii) These would naturally include even numbers of spins, but due to quantum tunneling these may intertwine.

iii) Cluster intertwining may prevent translation symmetry breaking (?!)

All that may initially sound vague, but can be understood trough the thermal state's $(d+1)$ functional integral representation, obtained through the canonical *Feynman-esque* construction.

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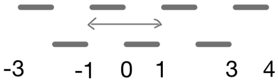

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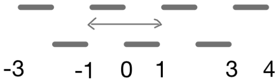

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Ground state expectation value functionals: $\langle F \rangle_L = \lim_{\beta\to\infty} \operatorname{tr} e^{-\beta H/2} F e^{-\beta H/2}$

For the infinite volume limit, based on the above observations, it is natural to consider separately the even and odd L:

$$\langle F \rangle_{ev} := \lim_{\substack{L\to\infty \\ L \text{ even}}} \langle F \rangle_L \quad \text{and} \quad \langle F \rangle_{odd} := \lim_{\substack{L\to\infty \\ L \text{ odd}}} \langle F \rangle_L \,,$$

The representation introduced in [AN], in line with Feynman's general prescription, allows to prove convergence in this two limits through an application of the FKG inequality. In each case the ground state's spin-spin correlations are of alternating sign (by a trivial argument).

The question on which we focus here is whether the two coincide.

Proposition (The AN'94 dichotomy) *For each S (integer or half integer) either*

1) the above two ground states coincide, in which case this ground state exhibits slowly decaying correlations, satisfying

$$\sum_{x\in\mathbb{Z}} |x| \, |\langle \sigma_0 \cdot \sigma_x \rangle| = \infty \,,$$

or else

2) dimerization: the system has two distinct ground states each of period 2, one being the shift of the other.

The case $S = 1/2$, which corresponds to the quantum Heisenberg anti-ferromagnet, was solved by Bethe by means of his famous ansatz. In this case there is a unique ground state and $\langle \sigma_0 \cdot \sigma_x \rangle \approx 1/|x-y|^\alpha$.

Our main result is that for all $S > 1/2$, regardless of the parity of $2S$, the second option holds.

Theorem (A – DC '19) *For all $S > 1/2$ the two ground states differ. The two states are related by a shift, but exhibit translation symmetry breaking. More specifically, they are of uneven energy density, and satisfy*

$$\langle P^{(0)}_{2n,2n+1} \rangle_{ev} - \langle P^{(0)}_{2n-1,2n} \rangle_{odd} \;=\; \alpha_S > 0. \tag{1}$$

for all n integer.

Previously dimerization was proved for $S \geq 8$

[Nachtergaele – Ueltschi '17]

Remark: Using the FKG inequality (applicable in the loop representation) the two can be shown to coincide: dimerization $\Leftrightarrow$ persistence of energy osc. Furthermore for even $L > 2|n|$:

$$\langle P^{(0)}_{2n,2n+1} \rangle_L - \langle P^{(0)}_{2n-1,2n} \rangle_L \;\searrow\; \alpha_S \quad (\text{as } L \nearrow). \tag{2}$$

The loop representation

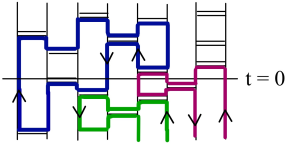
Feynman '53

Specific realizations (for distinct purposes):
Aiz. – Lieb '90, Conlon – Solovej '91, Toth '93, Aiz. – Nachtergaele '94.

$$e^{\beta \sum_{b \in \mathcal{E}(\Lambda)} K_b} = e^{\beta |\mathcal{E}|} \int_{\Omega(\Lambda,\beta)} \rho_0(d\omega)\, \mathcal{T} \left(\prod_{(b,t)\in\omega} K(b,t) \right)$$

$\Omega(\Lambda, \beta)$ – the set of countable subsets of $\mathcal{E} \times [0, \beta]$
$\rho_0(d\omega)$ – the probability measure under which ω forms a Poisson process over $\mathcal{E} \times [0, \beta]$, of intensity dt along each "vertical" line $\{b\} \times [0, \beta]$.

$\mathrm{tr}\, e^{-\beta H/2} F e^{-\beta H/2} \quad \Rightarrow$



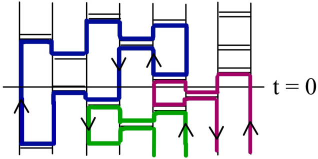
By this method, thermal expectation value functional are expressed in terms of an integral over histories of $\{\sigma_x^3\}$ (in "imaginary time"), i.e. configurations of $\sigma^3(x, t)$ defined over $[-L_1, L_2] \times [\beta/2, \beta/2]$.

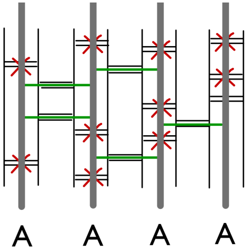
Each quantum operator F, on the Hilbert space associated with Λ, is represented by a specific action on this functional integral.

In the basis of the eigenstates of S^3, the Hamiltonian considered here is:

$$(2S+1)P^{(0)}_{x,y} = \sum_{\alpha,\beta=-S}^{S} (-1)^{\alpha-\beta} |\beta,-\beta\rangle\langle\alpha,-\alpha| \,. \tag{3}$$

The above construction yields a stochastic geometric representation of the finite volume thermal states. in terms of a system of random loops (AN'94).





$$\boxed{\mathrm{tr}\, \mathcal{T}\left(\prod_{(b,t)\in\omega} K(b,t)\right) = (2S+1)^{N(\omega)}}$$

$$\langle F\rangle_{\Lambda,\beta} = \int_{\Omega(\Lambda,\beta)} \mathbb{E}(F\,|\omega)\ \rho_S(d\omega)\,; \text{ with } \boxed{\rho_S(d\omega) = (2S+1)^{N(\omega)}\rho_S(d\omega)/\mathrm{Norm}}$$

$$\text{and} \qquad \mathbb{E}(F\,|\omega) := \mathrm{tr}\, F\,\mathcal{T}\left(\prod_{(b,t)\in\omega} K(b,t)\right)/(2S+1)^{N(\omega)} \,.$$

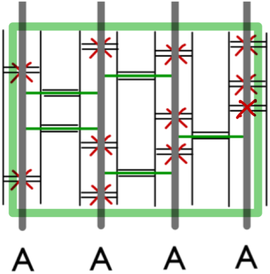
Duality: *A* domains are bounded by *B* domains, and vice versa.

A-biased partial order

bonds crossing *B* regions: $\nearrow$

bonds crossing *A* regions: $\searrow$

A favoring boundary conditions: $\Longrightarrow$



With respect to this order, for $Q \geq 1$ the measures $\boxed{\sqrt{Q}^{N(\omega)} \rho(d\omega)/\mathrm{Norm}}$ meet the conditions required for the Fortuin-Kasteleyn-Ginibre inequality.

Of relevance for us: $\boxed{\sqrt{Q} = (2S+1)}$.

This structure is reminiscent of the Q–state Potts model (and it can be obtained from the latter, taking a continuum limit.)

Useful implications: the convergence and monotonicity statements mentioned above.

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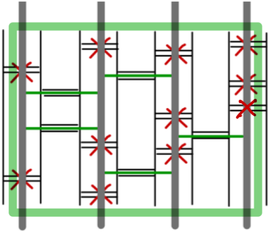

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Duality, FKG inequality, convergence, and energy oscillations

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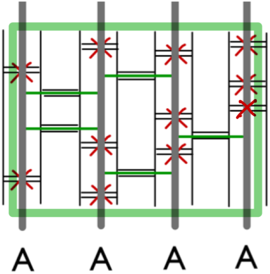

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The A–N dichotomy

Ask:

Is the number of loops encircling any given site (i) finite or (ii) infinite?

(The answer is almost surely constant w.r.t $\rho_S(d\omega)$.)

(i) $\Longrightarrow$ symmetry breaking: either A of B percolates, dimerization, etc.

(ii) $\Longrightarrow \sum_{x \in \mathbb{Z}} |x| \, |\langle \sigma_0 \cdot \sigma_x \rangle| = \infty$,

We now know that the answer changes at $Q = 4$, i.e. $S = 1/2$.

The harder question

What makes $Q = 4$ into a threshold value?

Two tracks to the answer:

I) An old hint (Baxter–Kelland–Wu '78):

Writing $\boxed{\sqrt{Q} \;=\; e^{\lambda} + e^{\lambda}}$ λ becomes real, and $\neq 0$, at $Q > 4$.

(**relevance to be explained in detail on the blackboard.)**

The challenge has been to develop an argument based on that.
This challenge was finally met in the very recent work of Ray – Spinka '19 (in the context of Q state Potts models on $\mathbb{Z}^2$.)

Their approach has now been extended to also cover the present quantum model. (**to be explained on the blackboard**)

An alternative track (which requires harder analysis, but yields more information):

II) Bethe ansatz analysis of the 6-vertex models, which is robust enough to handle also the model's 1–directional continuum limit. This was also recently accomplished, by DC, Gagnebin, Harel, Manolescu, and Tassion '16.

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Thank you for your attention.

Critical $Q = 3$ state Potts models

The power laws observed in the correlation functions at T_c are related to the Hausdorff dimensions of the critical clusters and of their boundaries.

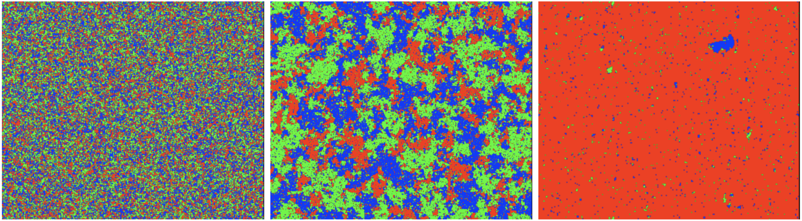

Figure 2: Simulations of three-state planar Potts model at subcritical, critical and supercritical temperatures.

Figure generated by V. Befara.