A Quantum Dimerization Phenomenon and the F-K Random Cluster Models

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Talk based on joint works with Bruno Nachtergaele ('94), Hugo Duminil-Copin and Simone Warzel ('19).

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Abstract (version 1)

Unlike classical antiferromagnets, quantum antiferromagnetic systems exhibit ground state frustration effects even in one dimension. A case in point is a quantum spin chain, with the interaction between neighboring S-spins given by the projection on the two-spins singlet state.

This 1D quantum system's ground state bears a close analogy to the self dual 2D Fortuin-Kasteleyn random cluster model, at $Q = (2S+1)^2$. The corresponding stochastic geometric representation has led to the dichotomy (Aiz-Nachtergale): for each S the ground state exhibits either

(i) slow decay of spin-spin correlations

(as in the Bethe solution of the Heisenberg $S = 1/2$ antiferromagnet) or else (ii) dimerization, manifested in translation symmetry breaking.

Drawing on the recent analysis of the phase transition of the FK models (by Duminil-Gagnebin-Harel-Manolescu-Tassion, and Ray-Spinka), we show that in the infinite volume limit for any $S > 1/2$ this $SU(2S+1)$ invariant quantum system has a pair of distinct ground states, each exhibiting spatial energy oscillations, and exponential decay of correlations.

(Joint work with H. Duminil-Copin and S. Warzel).

Equilibrium states and ground states of quantum systems can often be understood in terms of spontaneously emergent random geometric structures. This is also true of the equilibrium states of classical statistic mechanical system.

We shall discuss two quantum spin chains, exhibiting different physical phenomena, of a common mathematical scaffolding:

1. spin-S quantum spins with the $SU(2S+1)$ invariant A-F Hamiltonian

$$\boxed{H_{AF} = -(2S+1) \sum_{u \in \mathbb{Z}} P^{(0)}_{u,u+1}}$$

$P^{(0)}_{u,v} \equiv \mathbb{I}[|\mathbf{S}_u + \mathbf{S}_v| = 0]$ the orthog. projection onto the singlet state.

2. the quantum spin-$1/2$ spin chain with

$$\boxed{H_{XXZ} = \frac{1}{2} \sum_{u \in \mathbb{Z}} \left[(\sigma^x_u \sigma^x_{u+1} + \sigma^y_u \sigma^y_{u+1}) + \Delta(\sigma^z_u \sigma^z_{u+1} - 1) \right]} \quad \Delta = \cosh(\lambda) > 1$$

We prove that in the infinite volume limit:

(1) H_{AFF} for any $S > 1/2$ (but not $S = 1/2$) has a pair of distinct ground states, each gapped and exhibiting spatial energy oscillations.

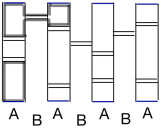
(2) H_{XXZ} at any $\Delta > 1$ (but not $\Delta = 1$) has a pair of ground states, with oscillatory magnetization but constant energy density.

Both (1) and (2) can be understood by studying the structure of a common loop system, associated also with the F-K Q-state random cluster model.

A flash from the theory of loop-soup measures

In the planar setup loops soups appear in percolation models as the separating lines between the connected clusters of a graph and of its dual

In that case $\boxed{N(\omega) \ = \ \#\{\text{finite connected clusters}\}}$



Random loop ensembles similar to the boundaries of our A/B regions appear also in of the self-dual Q-state Potts models, at $\boxed{\sqrt{Q} = (2S+1)}$.

[Translation symmetry breaking $\Leftrightarrow$ $Q > 4$]

Theorem: In the limit $\beta, L \to \infty$ the loop ensemble probability measure

$$\boxed{\mu_{L,\beta}(d\omega) = \int \rho_{L,\beta}(d\omega)\sqrt{Q}^{N_\ell(\omega)}/Z(L,\beta)}$$

decomposes into a superposition of two mutually singular measures $\mu = [\mu_A + \mu_B]/2$ which are not translation invariant, each being a shift of each other (by 1 lattice spacing).

- In μ_A the edges of ω are denser over the A edges than over B edges.
- The phase selection can be made through the A-wired, or B-wired, boundary conditions.
- The surface tension between the two phases is strictly positive.

[Yang, Baxter, Lieb,...,Duminil-Gagnebin-Harel-Manolescu-Tassion '16, Ray-Spinka'19,...]

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

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 random loop representation which was introduced in [AN] allows to prove convergence in these two limits (by means of the FKG inequality).

It also led to the following dichotomy which, based on topological arguments which this stochastic geometric representation enables.

Proposition (AN '94) *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, related by a one step shift.*

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 $\langle \sigma_0 \cdot \sigma_x \rangle \approx 1/|x-y|^{\alpha}$.

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

Theorem *For all $S > 1/2$ the two ground states of H_{AF} 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 $L > 2|n|$:

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

A $(d+1)$ dimensional functional integral representation

Feynman, Dyson, Ginibre ‘71, “Suzuki-Trotter”, .., Aiz.-Lieb ‘90, Conlon-Solovej ‘91, Toth ‘93, Aiz.- Nacht. ‘94.,..

Warmup: $\boxed{e^{\beta(H-1)} = \sum_n p_n H^n \equiv \mathbb{E}(H^N)}$ with $p_n = \frac{\beta^n}{n!} e^{-\beta}$ (the Poisson distribution)

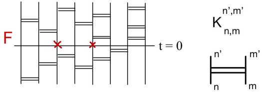
$$e^{\beta \sum_{b \in \mathcal{E}(\Lambda)} (K_b - 1)} = \int_{\Omega(\Lambda,\beta)} \rho(d\omega)\, \mathcal{T} \left(\prod_{(b,t)\in\omega} K(b,t) \right)$$

$\Omega(\Lambda,\beta)$ – the set of countable subsets of $\mathcal{E}(\Lambda) \times [0,\beta]$

$\rho(d\omega)$ – the probability measure under which ω forms a Poisson process over Ω, of intensity dt along each “vertical” line $\{b\} \times [0,\beta]$.

Hence:

$$\mathrm{tr}\, e^{-\beta H/2} F e^{-\beta H/2} = \int_{\Omega(\Lambda,\beta)} \rho(d\omega)\, \mathrm{tr}$$



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

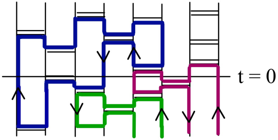
Each quantum operator F, on the Hilbert space associated with Λ, is represented by a specific action on this functional integral (typically at $t = 0$).

The loop representation for $H_{AF} = -\sum(2S+1)P^{(0)}_{u,u+1}$

In the basis of $\{S^z_u\}$: $\boxed{(2S+1)P^{(0)}_{u,v} = \sum_{m,m'=-S}^{S} (-1)^{m-m'} \, |m, -m\rangle\langle m', -m'|}$.

In this case, the signs can be changed to all positive by the gauge transformation $U = e^{i\pi\eta/2}$ at $\eta = \sum_u (-1)^u S^z_u$.

By these means, one gets a stochastic geometric representation of the thermal states in terms of a system of random loops (AN94):



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

with $S^z(u,t)$ restricted to $\pm m$ at $m \in [-S, S]$ constant, and $\pm$ flipping upon each "time reversal", as one travels along a loop.

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

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

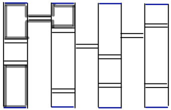
$H_{AF} \Longleftrightarrow$ loop ensemble

For a neatly stated relation of the H_{AF} system in terms of a random loop ensemble, it is convenient to start with the L-dimerized state

$$|\mathcal{D}_L\rangle\rangle := \otimes_{j=1}^{L} \left(\sum_{m_j=-S}^{S} e^{i\pi m_j} |m_j, -m_j\rangle_{-(L+1)+2j,-L+2j} \right) \quad ; \quad \| |\mathcal{D}_L\rangle\rangle \|^2 = (2S+1)^L$$

The rules described above yield

$$\boxed{\langle\langle \mathcal{D}_L | e^{-\beta H_{Aff}} | \mathcal{D}_L \rangle\rangle} = \int \rho_{L,\beta}(d\omega)(2S+1)^{N_\ell(\omega)} =: \boxed{Z(L,\beta)}$$



where $Z(L, \beta)$ is the partition function of a random loop ensemble based on the Poisson process of edges over $\Lambda(L, \beta) := \{-L+1, ..., L\} \times [-\beta/2.\beta/2]$ (of intensity dt), with $N_\ell(\omega)$ the number of loops of ω,

drawn with the "alternatively wired" boundary conditions.

Important: The resulting random loop measure as it appears near $u = 0$ depends on the parity of L.

LRO is manifest in the rate of dimerization: over A versus B edges.

$\Rightarrow$ Different physics in two projections of a common mathematical structure

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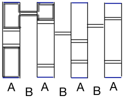
1) For $H_{AF} = -\sum(2S+1)P^{(0)}_{u,u+1}$, at $S > 1/2$:

$$\boxed{\langle\!\langle \mathcal{D}_L | e^{-\beta H_{\mathrm{Aff}}} | \mathcal{D}_L \rangle\!\rangle \;=\; Z(L,\beta)}$$



Two ground states: $\lim\limits_{\substack{L\to\infty \\ L \text{ even}}} \lim\limits_{\beta\to\infty} \dfrac{1}{Norm.} e^{-\beta H_{AF}} |\mathcal{D}_L\rangle\!\rangle$ & similar limit with L odd.

Broken symmetry: *translation invariance*. Manifested in: energy oscillation.

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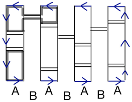
2) For $H_{XXZ} = H_{XY} - \sum_u \Delta \frac{1}{2} (\tau^z_u \tau^z_{u+1} - 1)$, $\Delta > 1$

$$\boxed{e^{\beta \sinh(\lambda)} \langle\!\langle -,+ | e^{-\beta \widetilde{H}_{XXZ}} | -,+ \rangle\!\rangle \;=\; Z_{\circlearrowleft,\lambda}(L,\beta)}$$



Two ground states: $\lim\limits_{L\to\infty} \lim\limits_{\beta\to\infty} \dfrac{1}{Norm.} e^{-\beta H_{XXZ}} |-,+\rangle\!\rangle$ & likewise with $|+,-\rangle\!\rangle$

Broken symmetry: *global spin flip*. Manifested in: Néel order.

Surprise: in this case there is no additional translation symmetry breaking i.e. both states are AV symmetric (& hence do not exhibit energy oscillations)!

The 4-edge (in lieu of 6-vertex) model

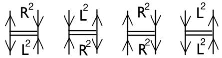
Back to our measures $\mu_{L,\beta}(d\omega) = \int \rho_{L,\beta}(d\omega)\sqrt{2S+1}^{N_\ell(\omega)}/Z(L,\beta)$:

As was done in the context of the random clusters of the Q-state Potts models (Baxter-Kelland-Wu '78), the factor $\sqrt{Q}^{N_\ell(\omega)}$ can be turned into a product of local weights.

For that we introduce what initially is a fictitious spin function $\tau(u,t)$, with values in $\{\uparrow,\downarrow\} = \{+1,-1\}$ flipping along each loop, and assign weight $e^{\pm\lambda/4}$ to each counterclockwise/ clockwise right turn

at λ satisfying $\boxed{\sqrt{Q} \;=\; e^{\lambda} + e^{-\lambda}}$ (= sum over two possible loop orientations).

The result is a system of random loops based on Poisson distributed edges, and a pseudo spin function, with 4 edge types (in the bulk):



a. b. c. d.

$W_a = 1, W_b = 1, W_c = e^{-\lambda}, W_d = e^{\lambda}$.

The loop ensemble and the H_{XXZ} operator

The variables τ (with values ± 1) were introduced in the context of H_{AF} as an auxiliary tool for the analysis of the stochastic geometry of it's thermal states. In terms of this model's spin variables $\tau(x,t)$ do not correspond to any local operator. However one may still ask about their induced distribution.

To find that, we find it convenient to view $\tau = \pm 1$ as the z component of a triplet $\boxed{(\tau^x_u, \tau^y_u, \tau_u)}$ with the algebra of the σ operators of spin $\frac{1}{2}$.

In this terminology, $W_a, ., W_d$ correspond to the interaction terms

$$\begin{aligned} K_{u,v} &= \frac{1}{2}\left(\tau^x_u\,\tau^x_v + \tau^y_u\,\tau^y_v\right) + e^{\lambda}(1+\tau^z_u)(1-\sigma^z_v)/4 + \ e^{-\lambda}(1-\tau^z_u)(1+\sigma^z_v)/4 \\ &= \frac{1}{2}\left[\left(\tau^x_u\,\tau^x_v + \tau^y_u\,\tau^y_v\right) \ + \cosh(\lambda)\left(1-\tau^z_u\tau^z_v\right)\right] + \frac{1}{2}\sinh(\lambda)(\tau^z_u - \tau^z_v) \end{aligned}$$

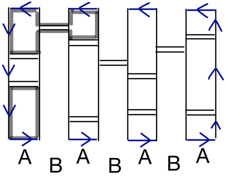
The sum over the edges may be recognized as the *spin*$\frac{1}{2}$ H_{XXZ} Hamiltonian, which is invariant under global (τ) spin flip, plus a boundary term:

$$\boxed{K = -H^{(\Delta)}_{XXZ} + \frac{1}{2}\sinh(\lambda)(\tau^z_L - \tau^z_{-L+1})} \qquad \text{(with } \Delta = \cosh(\lambda))$$

Loop ensemble $\Longleftrightarrow H_{XXZ}$

Towards an analog of the relation we found for H_{AF}, let us denote:

1) $|(-,+)_L\rangle\!\rangle := |-,+,...,-,+\rangle$
$= |\tau_u = (-1)^{x-L};\ u = -L+1,...,L\rangle$



2) $\widetilde{H}_{XXZ} := H_{XXZ} -$ [the XX and YY terms at the boundary edges]

One then finds

$$\boxed{e^{\beta\sinh(\lambda)}\,\langle\!\langle(-,+)_L|e^{-\beta\widetilde{H}_{XXZ}}|(-,+)_L\rangle\!\rangle} =$$

$$= \int_{\Lambda(L,\beta)} \rho(d\omega)\left(e^{\lambda}+e^{-\lambda}\right)^{N_\ell(\omega)^{int}} e^{\lambda N_\ell(\omega)^{bnd}} =: \boxed{Z_{\circlearrowleft,\lambda}(L,\beta)}$$

with $Z_{\circlearrowleft,\lambda}$ the partition function of the (ω,τ) ensemble, based on the above Poisson process of edges over $\Lambda(L,\beta) := \{-L+1,...,L\}\times[-\beta/2.\beta/2]$ restricted to configurations for which all the boundary-touching loops are of positive helicity.

A surprising symmetry

Let $\quad \mu_{\beta,L;\lambda}(d\omega\, d\tau) = \mathbb{1}[(\tau,\omega) \text{ consistent}] \prod_{\ell} e^{\gamma(\ell)\lambda} \rho_{L,\beta}(d\omega)/Z(L,\beta;\lambda)$

with ℓ ranging over the loops of ω, and $\gamma(\ell) = \pm 1$ the helicity of τ along ℓ [$= (-1)$ for the clockwise orientatation].

and let $\boxed{\mu_{\beta,L;\lambda}(d\omega)}$ & $\boxed{\mu_{\beta,L;\lambda}(d\tau)}$ be the restrictions of this probability measure to functions of just ω and τ, correspondingly. Consider the event:

$$\mathcal{A}_{L,\beta;\circlearrowleft} = \{(\omega,\tau) \,:\, \gamma(\ell) = +1 \ \forall \ell \text{ touching } \partial\Lambda(L\beta)\}.$$

Theorem 2: For any $\beta, L < \infty$, the conditional distribution of the process τ, conditioned on $+$ helicity all along the boundary is an even function of λ. I.e. the $\pm\lambda$ measures, conditioned on $\mathcal{A}_{\cdot\cdot\cdot}$, are equal:

$$\boxed{\mu_{\beta,L;\lambda}(d\tau \,|\, \mathcal{A}_{L,\beta;\circlearrowleft}) \;=\; \mu_{\beta,L;-\lambda}(d\tau \,|\, \mathcal{A}_{L,\beta;\circlearrowleft})\,.}$$

The statement echoes an observation about lattice loop models which appears implicitly in Galzman-Peled '18, and which Ray-Spinka '19 employed for a novel proof of symmetry breaking in the rand. cluster models at $Q > 4$.

This hidden symmetry, combined with the A-N criterion, allows:

- a short & topological proof of the translation symmetry breaking in the two ground states of H_{AF} (bypassing the Bethe ansatz calculation)
- proof that the two ground states of H_{XXZ} have the AV symmetry.

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Special cases of the S-spin H_{AF} spin chain:

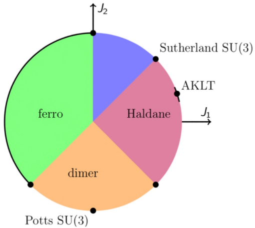
$S = \frac{1}{2}$: it is the Heisenberg antiferromag.

$S = 1$: it is the bi-quadratic Hamiltonian

$$H = \sum_{u \in \mathbb{Z}} J_1 \mathbf{S}_u \cdot \mathbf{S}_{u+1} + J_2 \left(\mathbf{S}_u \cdot \mathbf{S}_{u+1}\right)^2$$

the latter corresponds to the lowest point on the wheel

(fig. courtesy of Bach.-Nacht.)



Summary:

Lessons from classical probabilistic models produce insights on interesting quantum phenomena:

1. frustration in quantum system
2. conditions under which it may lead to non-uniqueness of the ground state, and symmetry breaking
3. a more nuanced understanding of:
   - dimerization
   - the Néel phase [and the AV symmetry, shift $\circ$ flip]
4. a stoch.-geom. / topological dichotomy

   slow decay of correlations, or translation symmetry breaking
5. topological indices (of relevance for "topological states", cf. B-N).

Rigorous proofs can be obtained through non-computational qualitative analysis (loop representation, monotonicity arguments, and inequalities such as FKG) where Bethe ansatz calculations are less than fully transparent.

In the converse direction, integrable probability has benefitted from ideas originating in quantum physics.

Quantum and Classical - best together.

Thank you for your attention.