

GRAPHICAL REPRESENTATIONS FOR QUANTUM SPIN SYSTEMS

Daniel Ueltschi
University of Warwick

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1. INTRODUCTION

The study of quantum spin systems is difficult. Linear algebra, group theory, and Functional analysis provide the main mathematical tools. Graphical or probabilistic representations give a totally different viewpoint and allow to use the intuition from classical statistical mechanics and the tools of probability theory.

Their origin goes back to Feynman's description of the quantum Bose gas in terms of interacting Brownian trajectories (1953). In 1969 Ginibre proved the occurrence of phase transitions in quantum perturbations of classical models, using "space-time configurations" and a Peirls argument. The quantum spin $\frac{1}{2}$ Heisenberg Ferromagnet was described using random transpositions by Powers (1976) and independently by Tóth (1993). Tóth used it to find a bound for the free energy (this was motivated by an earlier work of Conlon and Solovay, 1991; optimal results have been just proposed by Correggi, Giuliani, and Seiringer, 2014).

Another loop representation was proposed by Aizenman and Nachtergaele for the quantum spin $\frac{1}{2}$ Heisenberg antiferromagnet (1994). This allowed them to relate the quantum chain to the 2D Potts model and random cluster models. Nachtergaele proposed an extension to spin 1 systems shortly afterwards. Marada and Kawashima introduced it anew in 2001.

It was recently noticed that the representations of Tóth and Aizenman-Nachtergaele can be combined so as to include the spin $\frac{1}{2}$ quantum XY (or XXZ) model (Ueltrichi, 2013). This representation also provides a simpler alternative to Nachtergaele's for the spin 1 model, but only in a reduced area of the phase diagram. It has been useful in the study of the quantum spin nematic phase of the spin 1 model with $SU(2)$ -invariant nearest-neighbor interactions.

These notes describe in details the representation for the spin $\frac{1}{2}$ quantum Heisenberg ferromagnet, XY, and antiferromagnet.

2. RANDOM LOOP MODELS

The Poisson point process plays an essential rôle. It can be introduced in many different ways, including abstract nonsense involving measures on spaces of measures. We choose a more pedestrian and intuitive approach.

In words, the Poisson point process on $[0,1]$ describes the occurrence of events that are independent of one another. Let $\lambda > 0$ be the intensity of the process. Let us discretize the interval $[0,1]$ by considering the set $\{\frac{1}{n}, \frac{2}{n}, \dots, 1\}$, with $\frac{\lambda}{n} < 1$. We consider the probability distribution on subsets of $\{\frac{1}{n}, \dots, 1\}$, where the probability of the subset ω is

$$P_n(\omega) = \left(\frac{\lambda}{n}\right)^{|\omega|} \left(1 - \frac{\lambda}{n}\right)^{n-|\omega|}.$$

The interpretation is that each point of the form $\frac{i}{n}$, $1 \leq i \leq n$, occurs with probability $\frac{\lambda}{n}$. As $n \rightarrow \infty$, this process converges to the Poisson point process on $[0,1]$ with intensity λ .

The total number of events varies and is a Poisson random variable with parameter λ :

$$P(|\omega| = k) = \frac{\lambda^k}{k!} e^{-\lambda}, \quad k \in \mathbb{N}_0.$$

Exercise: (a) Check that the moment generating function (Laplace transform) of a Poisson random variable X is given by

$$E(e^{tX}) = \exp\{\lambda(e^t - 1)\}$$

(b) Find the moment generating function of $|w|$, and check that

$$\lim_{n \rightarrow \infty} E_n(e^{t|w|}) = \exp\{\lambda(e^t - 1)\}$$

(c) Find $E(X)$ and $E_n(|w|)$. Moment gen. Fcts may help.

Integration with respect to Poisson point process can also be defined by a limit. Let $F = (F_k)$ be a collection of smooth functions $F_k: [0, 1]^k \rightarrow \mathbb{R}$ (with $F_0 = 1$ by definition). Then

$$\begin{aligned} E(F) &= \lim_{n \rightarrow \infty} \sum_w \left(\frac{\lambda}{n}\right)^{|w|} \left(1 - \frac{\lambda}{n}\right)^{n-|w|} F_w(w) \\ &= \lim_{n \rightarrow \infty} \sum_{k \geq 0} \left(\frac{\lambda}{n}\right)^k \left(1 - \frac{\lambda}{n}\right)^{n-k} \sum_{w, |w|=k} F_k(w) \\ &= \sum_{k \geq 0} \lambda^k e^{-\lambda} \int_{0 < t_1 < \dots < t_k < 1} dt_1 \dots dt_k F_k(t_1, \dots, t_k) \end{aligned}$$

The exchange of limit and sum can be justified by dominated convergence. The latter expression is concrete and practical.

Next, we describe the model of random loops. Let (Λ, \mathcal{E}) be an arbitrary finite graph, with Λ the set of vertices and \mathcal{E} the set of edges. Let $\beta > 0$ and $u \in [0, 1]$ be two parameters. To each edge $\{x, y\} \in \mathcal{E}$ is associated the interval $[0, \beta]$ and a Poisson point process on this interval. There occur two kinds of events:

- crosses \times occur with intensity u
- double bars $=$ occur with intensity $1-u$.

(This process can be defined by generalizing the Poisson point process above to two kinds of events, or by considering two separate, independent processes.) We let ρ denote the measure of independent Poisson processes at each edge of \mathcal{E} . Let w denote realizations of this probability measure. It contains finitely many objects with probability 1.

Exercise: Check that $|w|$ is a Poisson random variable with parameter $\beta|\mathcal{E}|$.

Let $\mathcal{L}(w)$ denote the set of loops of the realization w . Their definition is intuitive and extremely cumbersome to write down mathematically, so we content ourselves with pictures:

3. RELATIONS BETWEEN RANDOM LOOPS & QUANTUM SPINS

We consider a spin $\frac{1}{2}$ model. The Hilbert space is $\mathcal{H}_\Lambda = \bigotimes_{x \in \Lambda} \mathbb{C}^2$.
The Hamiltonian is

$$H_\Lambda^{(u)} = -2 \sum_{\{x,y\} \in \mathcal{E}} \left(S_x^1 S_y^1 + (2u-1) S_x^2 S_y^2 + S_x^3 S_y^3 - \frac{1}{4} \right)$$

The case $u=1$ corresponds to the Heisenberg Ferromagnet;
the case $u=\frac{1}{2}$ corresponds to the XY model; and the case $u=0$ is unitarily equivalent to the Heisenberg antiFerromagnet when the lattice is bipartite.

Exercise: Find the unitary operator U such that

$$U H_\Lambda^{AF} U^{-1} = H_\Lambda^{(u)}$$

Here are precise relations between random loops and quantum spins.

Theorem

(a) Partition Functions: $Z(u, \beta) = \int 2^{|\mathcal{E}(u)|} p(dw) = \text{Tr} e^{-\beta H_\Lambda^{(u)}}$

(b) Correlations in spin directions 1 and 3:

$$\langle S_x^1 S_y^1 \rangle = \langle S_x^3 S_y^3 \rangle = \frac{1}{4} P(x \leftrightarrow y)$$

↑ quantum Gibbs state ↑ random loops

(c) Correlations in spin direction 2:

$$\langle S_x^2 S_y^2 \rangle = \frac{1}{4} [P(x \not\leftrightarrow y) - P(\overline{x \leftrightarrow y})]$$

We prove this theorem by writing the Hamiltonian in terms of suitable interaction operators T_{xy} and Q_{xy} introduced below, and by using a "Poisson expansion" of the Gibbs operator $e^{-\beta H_\Lambda^{(u)}}$, see the lemma below.

Let T_{xy} be the transposition operator on $\mathbb{C}^2 \otimes \mathbb{C}^2$:

$$T_{xy} |a, b\rangle = |b, a\rangle, \quad a, b = \pm \frac{1}{2}$$

Let Q_{xy} be the operator in $\mathbb{C}^2 \otimes \mathbb{C}^2$ with the following matrix elements:

$$\langle a, b | Q_{xy} |c, d\rangle = \delta_{a,b} \delta_{c,d}, \quad a, b, c, d = \pm \frac{1}{2}$$

Exercise: Show that

$$(a) \vec{S}_x \cdot \vec{S}_y = \frac{1}{2} T_{xy} - \frac{1}{4}$$

$$(b) S_x^1 S_y^1 - S_x^2 S_y^2 + S_x^3 S_y^3 = \frac{1}{2} Q_{xy} - \frac{1}{4}$$

Once the exercise has been completed, we can express the Hamiltonian $H_\Lambda^{(u)}$ in terms of T_{xy} and Q_{xy} :

$$H_\Lambda^{(u)} = - \sum_{\{x,y\} \in \mathcal{E}} \left(u T_{xy} + (1-u) Q_{xy} - 1 \right).$$

This is the perfect expression for a Feynman-Kac type of expansion.

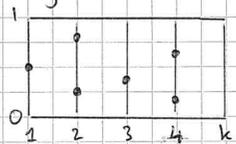
The following lemma goes back at least to Aizenman - Nachtergaele (1994).

Lemma

Let A_1, \dots, A_k be bounded operators, and ρ a Poisson point process on $\{1, \dots, k\} \times [0, 1]$ of intensity 1. Then

$$\exp \left\{ \sum_{j=1}^k (A_j - 1) \right\} = \int \rho(dw) \prod_{(j,t) \in w}^* A_j$$

In the lemma, the product \prod^* is over the events of w in increasing times.



This realization gives the product $A_4 A_2 A_3 A_1 A_4 A_2$

Proof: We start with the Poisson process. We have

$$\begin{aligned} \int \rho(dw) \prod_{(j,t) \in w}^* A_j &= \lim_{n \rightarrow \infty} \sum_{m=0}^n \sum_{\substack{(j_1, t_1), \dots, (j_m, t_m) \\ t_1 < t_2 < \dots < t_m}} \left(\frac{1}{n}\right)^m \left(1 - \frac{1}{n}\right)^{kn-m} \prod_{i=1}^m A_{j_i} \\ &= \lim_{n \rightarrow \infty} \prod_{i=1}^n \left(1 + \frac{1}{n} \sum_{j=1}^k (A_j - 1)\right) \\ &= \lim_{n \rightarrow \infty} \left(1 + \frac{1}{n} \sum_{j=1}^k (A_j - 1)\right)^n \\ &\stackrel{\text{ Trotter }}{=} \exp \left\{ \sum_{j=1}^k (A_j - 1) \right\}. \quad \square \end{aligned}$$

Proof of the Theorem: We start with (a), the partition function.

Given a realization w of the Poisson point process on $E \times [0, \beta]$, let $m = |w|$ denote the total number of crosses and double bars.

From the lemma above, we have

$$\begin{aligned} e^{-\beta H_n^{(w)}} &= \exp \left\{ \sum_{(x,y) \in E} (u T_{xy} + (1-u) Q_{xy} - 1) \right\} \\ &= \int \rho(dw) \prod_{(x,y,t) \in w}^* \begin{cases} T_{xy} & \text{if event is a cross} \\ Q_{xy} & \text{if event is a double bar} \end{cases} \end{aligned}$$

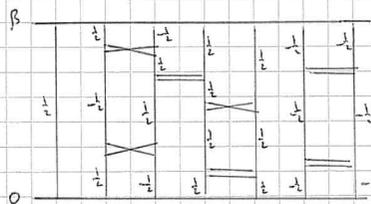
We actually used a straightforward generalization of the lemma with two Poisson processes of intensities u and $1-u$. Using a basis of classical spin configurations, $|\sigma\rangle$ with $\sigma \in \{-\frac{1}{2}, \frac{1}{2}\}^m$, we get

$$\begin{aligned} \text{Tr} e^{-\beta H_n^{(w)}} &= \int \rho(dw) \sum_{\sigma^1, \dots, \sigma^m} \langle \sigma^1 | R_{x_1 y_1} | \sigma^2 \rangle \langle \sigma^2 | R_{x_2 y_2} | \sigma^3 \rangle \\ &\quad \dots \langle \sigma^m | R_{x_m y_m} | \sigma^1 \rangle, \end{aligned}$$

where $R_{x_i y_i}$ is either $T_{x_i y_i}$ or $Q_{x_i y_i}$. Observe that the product of matrices elements is zero, unless $\sigma_z^i = \sigma_z^{i+1}$ for all $z \neq x_i, y_i$, and the constraints at x_i, y_i are as follows:

$$\begin{aligned} T_{x_i y_i}: & \begin{array}{ccc} \sigma_{x_i}^{i+1} = \sigma_{y_i}^i & & \sigma_{y_i}^{i+1} = \sigma_{x_i}^i \\ \sigma_{x_i}^i & \times & \sigma_{y_i}^i \end{array} \\ Q_{x_i y_i}: & \begin{array}{ccc} \sigma_{x_i}^{i+1} & & \sigma_{y_i}^{i+1} = \sigma_{x_i}^{i+1} \\ \sigma_{x_i}^i & = & \sigma_{y_i}^i = \sigma_{x_i}^i \end{array} \end{aligned}$$

Let us introduce "space-time configurations", which are piecewise constant functions $\sigma: [0, \beta] \rightarrow \{-\frac{1}{2}, \frac{1}{2}\}^{\uparrow}$.
 Given w , let $\Sigma(w)$ be the set of space-time configurations such that σ_{xt} is constant along any loop.



Example of a realization w and a compatible space-time configuration.

Then it is possible to write the equation above as

$$\text{Tr } e^{-\beta H_N^{(w)}} = \int p(dw) \sum_{\sigma \in \Sigma(w)} 1$$

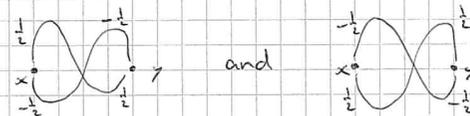
There are two possibilities per loop, so the sum gives $2^{|\Sigma(w)|}$.

This proves (a).

For (b), we expand as before and we get

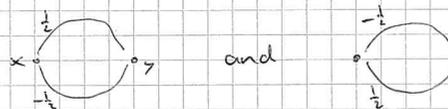
$$\begin{aligned} \text{Tr } S_x^z S_y^z e^{-\beta H_N^{(w)}} &= \int p(dw) \sum_{\sigma \in \Sigma(w)} \sigma_{x0} \sigma_{y0} \\ &= \int p(dw) \underbrace{1_{x \leftrightarrow y}(w)}_{= \frac{1}{4}} \sum_{\sigma \in \Sigma(w)} \sigma_{x0} \sigma_{y0} + \int p(dw) \underbrace{1_{x \not\leftrightarrow y}(w)}_{= 0} \sum_{\sigma \in \Sigma(w)} \sigma_{x0} \sigma_{y0} \\ &= \frac{1}{4} P(x \leftrightarrow y). \end{aligned}$$

The proof of (c) is similar, but the operators $S_x^z S_y^z$ force spin flips at $(x,0)$ and $(y,0)$. If w does not connect x and y , there are no compatible configurations and we get 0. If $x \leftrightarrow y$, these are the two possibilities:



In both cases, we get the factor $\langle -\frac{1}{2} | S_x^z | \frac{1}{2} \rangle \langle \frac{1}{2} | S_y^z | -\frac{1}{2} \rangle = \frac{-i^2}{4} = \frac{1}{4}$.

If $x \not\leftrightarrow y$, the two possibilities are



In both cases, the factor is $\frac{i^2}{4} = -\frac{1}{4}$. Hence the difference of probabilities in (c). \square

4. LENGTHS OF LOOPS & PHASE TRANSITIONS

Quantum spin systems undergo phase transitions that are associated with long-range correlations. It is natural to expect a transition in the random loop model as well, that involves one or many long loops. Rather unexpectedly, the loop models have a universal behavior that can be described explicitly, at least heuristically.

A convenient expression for the length of the loops turns out to be the sum of the lengths of their vertical components. In the following, we denote

- L_x , the length of the loop that contains $(x, 0) \in \Lambda \times [0, \beta]$.
- $L^{(1)}, L^{(2)}, \dots$, the lengths of the loops in decreasing order.

Notice that $0 < L_x, L^{(i)} \leq \beta|\Lambda|$ and $\sum_{i \geq 1} L^{(i)} = \beta|\Lambda|$.

Theorem

(a) Length of loops & magnetic susceptibility:

$$\mathbb{E} \left(\sum_{x \in \Lambda} L_x \right) = \frac{4}{\beta} \frac{\partial^2}{\partial h^2} \log \text{Tr} e^{-\beta H_{\Lambda}^{(h)} + \beta h \sum_{x \in \Lambda} S_x^z} \Big|_{h=0}$$

(b) Length of loops & spontaneous magnetization: There exists K s.t.

$$4\beta \sum_{x, y \in \Lambda} \langle S_x^z S_y^z \rangle - K\beta \sqrt{|\Lambda|} \leq \sqrt{\mathbb{E} \left(\sum_{x \in \Lambda} L_x \right)} \leq \mathbb{E} \left(\sum_{x \in \Lambda} L_x \right) \leq 4\beta \sum_{x, y \in \Lambda} \langle S_x^z S_y^z \rangle$$

Exercise: Suppose that (Λ, \mathbb{E}) is a cube in \mathbb{Z}^d with periodic boundary conditions. Use translation invariance to simplify the claims (a) and (b). The result makes more sense!

The proof of this theorem can be found in Ueltschi (2013). For (a), it involves the Duhamel two-point function and Schwinger correlations, that have natural loop counterparts. The upper bound in (b) is not hard and involves convexity properties of the Duhamel two-point function. The lower bound is much harder and it relies on the Falk-Bruch inequality.

Next, we consider the joint distribution of the lengths of the loops. Recall that a partition of the interval $[0, m]$, $m \in \mathbb{R}_+$, is a sequence $(a^{(1)}, a^{(2)}, \dots)$ of decreasing positive numbers such that $\sum_{i \geq 1} a^{(i)} = m$. Then $(\frac{L^{(1)}}{\beta|\Lambda|}, \frac{L^{(2)}}{\beta|\Lambda|}, \dots)$ is a random partition of $[0, 1]$, $\mathcal{P}(\Lambda)$.

The infinite-volume limit is a bit subtle and it needs a careful definition. It turns out that almost all loops are either macroscopic (their length is of order $|\Lambda|$) or microscopic (their length is of order 1). There are no mesoscopic loops. Precisely, we expect that there exists

$m(\beta) \in [0, 1)$ such that

$$\lim_{k \rightarrow \infty} \lim_{\Lambda \rightarrow \mathbb{Z}^d} \sum_{i: L^{(i)} < k} \frac{L^{(i)}(\omega)}{\beta |\Lambda|} = 1 - m(\beta)$$

$$\lim_{k \rightarrow \infty} \lim_{\Lambda \rightarrow \mathbb{Z}^d} \sum_{i=1}^k \frac{L^{(i)}(\omega)}{\beta |\Lambda|} = m(\beta)$$

For almost all realization ω . This is expected for $d \geq 3$.

Further, the joint distribution of macroscopic loops is given by a Poisson-Dirichlet distribution. This distribution is best defined using the closely related Griffiths-Engen-McCloskey distribution. Recall that a Beta(θ) random variable satisfies $\mathbb{P}(X > s) = (1-s)^\theta$ for $s \in [0, 1]$. Given i.i.d. Beta(θ) r.v.s X_1, X_2, \dots , consider the sequence $(X_1, (1-X_1)X_2, (1-X_1)(1-X_2)X_3, \dots)$

This sequence is a random partition of $[0, 1]$ and it is distributed according to $\text{GEM}(\theta)$. A little thought shows that this is the "stick breaking" construction. Notice its inherent scale invariance. Rearranging in decreasing order, we get $\text{PD}(\theta)$.

The conjecture is that

- if $u = 0$ or 1 , macroscopic loops satisfy $\text{PD}(u)$
- if $u \in (0, 1)$, " " " " $\text{PD}(1)$

This conjecture is based on an effective coagulation-fragmentation process, see Goldschmidt, U, Windridge (2011) for $u = 0, 1$ and U (2013) for $u \in (0, 1)$. It has been checked numerically in other, related models. See Grosskinsky, Lovisolo, U (2012) and Nahum, Chalker, et al (2013).

The distributions on partitions may look rather abstract, but here is a calculation which is fairly doable, and is all that we need. The probability that two random numbers X, Y , chosen uniformly in $[0, 1]$, belong to the same element of the random partition is

$$\begin{aligned} \mathbb{P}_{\text{PD}(\theta)}(X, Y \in \text{same el.}) &= \mathbb{P}_{\text{GEM}(\theta)}(X, Y \in \text{same el.}) \\ &= \sum_{k \geq 1} \mathbb{P}_{\text{GEM}(\theta)}(X, Y \in k\text{-th el.}) \\ &= \sum_{k \geq 1} \mathbb{E}_{\text{GEM}(\theta)} \int_0^1 dx \int_0^1 dy \mathbb{1}_{x \in k\text{-th el.}} \mathbb{1}_{y \in k\text{-th el.}} \\ &= \sum_{k \geq 1} \mathbb{E}_{\text{GEM}(\theta)} \left((1-X_1)^2 \dots (1-X_{k-1})^2 X_k^2 \right) \\ &= \sum_{k \geq 1} \left(\underbrace{\mathbb{E}_{\text{Beta}(\theta)} (1-X)^2}_{\frac{\theta}{\theta+2}} \right)^{k-1} \left(\underbrace{\mathbb{E}_{\text{Beta}(\theta)} X^2}_{\frac{2}{(\theta+1)(\theta+2)}} \right) = \frac{1}{\theta+1} \end{aligned}$$

We use this result in order to calculate long-range correlation functions. For $\|x-y\| \gg 1$, we have

$$\begin{aligned} \langle S_x^3 S_y^3 \rangle &= \frac{1}{4} P(x, y \in \text{same loop}) \\ &= \frac{1}{4} P(x, y \in \text{long loops}) \cdot \underbrace{P(x, y \in \text{same loop} \mid x, y \in \text{long loops})}_{= P_{PD}(x, y \in \text{same el.})} \\ &= \frac{1}{4} m(\beta)^2 \cdot \begin{cases} \frac{1}{2+1} & \text{if } u=0, 1 \\ \frac{1}{1+1} & \text{if } u \in (0, 1) \end{cases} \\ &= \begin{cases} \frac{1}{12} m(\beta)^2 & \text{if } u=0, 1 \\ \frac{1}{8} m(\beta)^2 & \text{if } u \in (0, 1) \end{cases} \end{aligned}$$

At low temperatures and for $d \geq 3$, the Heisenberg ferromagnet is expected to have pure states with spontaneous magnetization. That is, with $\vec{a} \in S^2$ (i.e. $\vec{a} \in \mathbb{R}^3$ with $\|\vec{a}\|=1$), the following should be a pure state:

$$\langle \cdot \rangle_{\vec{a}} = \lim_{h \rightarrow 0^+} \lim_{L \rightarrow \mathbb{Z}^d} \langle \cdot \rangle_{H_h^{(L)} - h \sum_{x \in \Lambda} \vec{a} \cdot \vec{S}_x}$$

where $\langle \cdot \rangle_H = \frac{1}{\text{Tr}_e e^{-\beta H}} \text{Tr}_e e^{-\beta H}$. Further, the Gibbs state obtained as the infinite-volume limit of $\langle \cdot \rangle_{H_h^{(L)}}$, call it $\langle \cdot \rangle$, should satisfy

$$\langle \cdot \rangle = \frac{1}{4\pi} \int_{S^2} \langle \cdot \rangle_{\vec{a}} d\vec{a}$$

We can check that this is compatible with the calculation above.

We have

$$\begin{aligned} \langle S_x^3 S_y^3 \rangle &= \frac{1}{3} \langle \vec{S}_x \cdot \vec{S}_y \rangle = \frac{1}{3} \frac{1}{4\pi} \int_{S^2} \langle \vec{S}_x \cdot \vec{S}_y \rangle_{\vec{a}} d\vec{a} \\ &= \frac{1}{3} \langle \vec{S}_x \cdot \vec{S}_y \rangle_{\vec{e}_3} = \frac{1}{3} \sum_{i=1}^3 \langle S_x^i \rangle_{\vec{e}_3} \langle S_y^i \rangle_{\vec{e}_3} \end{aligned}$$

We used the fact that $\vec{S}_x \cdot \vec{S}_y$ is rotation-invariant, so its expectation with respect to any pure state is the same. Then we used the clustering property of pure states, i.e. factorization when $\|x-y\| \gg 1$. Next, we use

$$\langle S_x^i \rangle_{\vec{e}_3} = \langle S_x^i \rangle_{\vec{e}_3} = 0 \quad (\text{this follows by rotation-invar. around } \vec{e}_3)$$

$$\langle S_x^3 \rangle_{\vec{e}_3} = \frac{1}{2} m(\beta) \quad (\text{can be seen using loop representation})$$

We obtain that for $\|x-y\| \gg 1$,

$$\langle S_x^3 S_y^3 \rangle = \frac{1}{3} \left(\frac{1}{2} m(\beta) \right)^2 = \frac{1}{12} m(\beta)^2$$

This is compatible with the result above!

Exercise: Do the same calculation in the case $u \in (0, 1)$. Pure states are expected to have spontaneous magnetization in the 1-3 plane.

The ideas above have recently been useful to better understand the quantum nematic phase of spin 1 systems, see U (2014).