A STOCHASTIC GEOMETRIC APPROACH TO QUANTUM SPIN SYSTEMS

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Abstract. We review some stochastic geometric models that arise from the study of certain quantum spin systems. In these models the fundamental properties of the ground states or equilibrium states of the quantum systems can be given a simple stochastic geometric interpretation. One thus obtains a new class of challenging stochastic geometric problems.

Key words: Stochastic geometry, percolation, FKG inequalities, quantum spin systems, Heisenberg model, dimerization, Néel order.

1. Introduction

Stochastic geometric methods have been very successful in the analysis of classical lattice systems. Techniques from percolation theory, correlation inequalities etc. have allowed for a tremendous progress in our understanding of these systems (see e.g. the contributions of Grimmett and Newman in this volume [14, 22]). There is no direct analogue of this technology for quantum lattice systems and progress of our understanding of the latter has been much slower. This is true at all levels: numerical, theoretical, as well as mathematical. Restricting our attention to rigorous work we find that a lot of it is based on indirect applications of 'classical techniques', made possible by representing the system (typically ferromagnetic) in space–time [13, 24]. Illustrious exceptions are given by the work of Lieb, Schulz, and Mattis [21] and e.g. [9]. One can hardly expect that for all quantum spin Hamiltonians H, $e^{-\beta H}$ would admit such a path-integral type representation with a non-negative measure. What we found is that for a wide class of interactions, including some well-known antiferromagnetic ones, one can in fact construct such a representation, on which the powerful techniques available for classical systems (probability measures) can then be brought to bear.

In this note I would like to show what kind of stochastic geometric models arise in this way starting from quantum spin Hamiltonians, and I will discuss what the basic issues are. In [6] we have obtained some interesting results for a particular family of one-dimensional models. For an application of a similar stochastic geometric representation to some random models see [5] and the contribution of Klein [18] in this volume. For some other models that are frequently discussed in the physics literature, the best problems remain open and we will briefly mention some of these.

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2. Poisson Integrals and the Stochastic Geometric Representation

For simplicity I will only treat one-dimensional quantum spin chains with nearest neighbour interactions. For higher-dimensional models with possibly also non-nearest neighbour interactions, a stochastic geometric representation is obtained by a straightforward generalization. I will also not describe the most general nearest neighbour interactions that can be treated, but only discuss some simple and typical examples. For a more general discussion the reader is referred to [6].

Let the Hamiltonian of a quantum spin chain of length $2L + 2$ be of the form

$$H_L = -\sum_{x=-L}^{L} J_x (h_{x,x+1} - 1) \tag{1}$$

where the J_x are positve real constants and $h_{x,x+1}$ is a hermitian operator acting on the Hilbert space of the pair of sites $\{x, x+1\}$. We assume that the state space of one site is a fixed finite-dimensional Hilbert space and that the $h_{x,x+1}$ are all copies of one hermitian matrix h. Note that, because of the presence of the coupling constants J_x, this does not imply that we only treat translation invariant models. We now show that under some assumptions on h one can derive a stochastic geometric representation for $e^{-\beta H_L}$. One starts from the following Poisson integral formula:

$$e^{-\beta H_L} = \int \rho^J_{L,\beta}(d\omega) K(\omega) \tag{2}$$

where

- $\rho^J_{L,\beta}(d\omega)$ is the probability measure of a product of independent Poisson processes, one for each bond $\{x, x+1\}$ in the chain, running over the time interval $[0, \beta]$, and with rates J_x. For the time being we draw the configurations ω for this process as in Figure 1,
- $K(\omega)$ is a product of operators $h_{x,x+1}$, one for each bond occurring in ω and ordered according to the times at which they occur.

An important quantity is the partition function $\mathcal{Z}_{L,\beta} = \operatorname{Tr} e^{-\beta H}$, which by (2) and linearity of the trace is given by

$$\mathcal{Z}_{L,\beta} = \int \rho^J_{L,\beta}(d\omega) \operatorname{Tr} K(\omega). \tag{3}$$

We have found that for a quite large class of interactions h the following is true:

- $\operatorname{Tr} K(\omega) > 0$ for all ω and this number can be computed in terms of relatively simple geometric properties of ω,
- the diagonal matrix elements of the operators $K(\omega)$ are all non-negative in a certain tensor product basis of the Hilbert space of the system.

Let us consider some elementary examples of this before we proceed. Recall that h is a self-adjoint operator on the (finite-dimensional) Hilbert space $V \otimes V$ of two sites.

2.1. Example 1

Let h be the operator which interchanges the states of the two sites, i.e., $h\phi \otimes \psi = \psi \otimes \phi$ for any two vectors $\phi, \psi \in V$. In any basis of V the matrix elements are 0

Fig. 1. A typical configuration of the multiple Poisson process $\rho^J_{L,\beta}(d\omega)$.

or 1 and a fortiori non-negative. $K(\omega)$ represents a permutation $\pi(\omega)$ of the sites of the chain and its trace is easily seen to be $p^{\#\text{ cycles in }\pi(\omega)}$, where $p = \dim V$. The number of cycles in ω becomes a geometric property of the configuration if we replace the Poisson-'beeps' by two horizontal lines that cross each other as in Figure 2. With the convention of periodic boundary conditions in the vertical direction the number of cycles in the permutation $\pi(\omega)$ is then equal to the number of loops in ω, which we will frequently denote by $l(\omega)$.

With $p = 2$ this interaction is equivalent to the usual spin $\frac{1}{2}$ Heisenberg ferromagnet.

2.2. Example 2

Also the spin $\frac{1}{2}$ Heisenberg antiferromagnetic interaction has a simple stochastic geometric interpretation. The appropriate choice for h is the operator:

$$h = \sum_{\alpha,\beta} (-1)^{\alpha-\beta} |\alpha, -\alpha\rangle\langle\alpha, -\alpha| \tag{4}$$

where $\{|\alpha\rangle\}$ is a basis of V given by the eigenvectors of the third component S^3 of the spin with eigenvalues α. For the spin $\frac{1}{2}$ case $\dim V = 2$ but the same expression defines an interesting interaction for any finite dimension (any magnitude of the spin) and was proposed by Affleck [1] (also see [7, 19]). The interaction is proportional to the projection operator onto the singlet vector for a pair of spins

Fig. 2. A typical configuration of the multiple Poisson process $\rho^{J}_{L,\beta}(d\omega)$ decorated for the ferromagnetic models of Example 1.

and hence antiferromagnetic. It can be shown that the diagonal matrix elements of the corresponding $K(\omega)$ are non-negative and there is again a simple formula for the trace. Each Poisson-'beep' is now replaced by two parallel horizontal lines as shown in Figure 3. Again this turns ω into a configuration of loops (assuming periodic boundary conditions in the vertical direction) and $\operatorname{Tr} K(\omega) = p^{l(\omega)}$.

The examples given above are not the most general ones that can be treated but they are in some sense the two basic ones. Unlike the their classical analogues quantum ferro- and antiferromagnets behave in a very different way and it is therefore not a surprise that they lead to two very different stochastic geometric models (of course one can turn the argument around and say that it is no surprise now that they behave very differently because they have very different stochastic geometric representations).

We complete the stochastic geometric picture by establishing the relation between expectation values of observables for the quantum spin system on the one hand and probabilities of events (or more generally expectations of random variables) in a probability measure describing the stochastic geometric model on the other hand. From (2) it follows that for for any local observable A for the quantum spin chain

$$\langle A \rangle_{L,\beta} \equiv \frac{\operatorname{Tr} A e^{-\beta H_L}}{\operatorname{Tr} e^{-\beta H_L}} = \int \mu(d\omega) E_\omega(A) \tag{5}$$

Fig. 3. A typical configuration of the multiple Poisson process $\rho^J_{L,\beta}(d\omega)$ decorated for the antiferromagnetic models of Example 2.

where

$$\mu(d\omega) = \frac{1}{\mathcal{Z}^J_{L,\beta}} \rho^J_{L,\beta}(d\omega) \operatorname{Tr} K(\omega) \tag{6}$$

and

$$E_\omega(A) = \frac{\operatorname{Tr} AK(\omega)}{\operatorname{Tr} K(\omega)}. \tag{7}$$

$\mu(d\omega)$ is a probability measure on the configurations ω and for A fixed $E_\omega(A)$ is a random variable. We found that for many important observables A this random variable can in fact be given a simple geometric interpretation. Take e.g. $A = S^3_x S^3_y$. One then finds:

$$E_\omega(S^3_x S^3_y) = \begin{cases} C(S)\mathbf{I}[(x,0) \text{ and } (y,0) \text{ are on the same loop}] & \text{for Ex. 1} \\ (-1)^{|x-y|} C(S)\mathbf{I}[(x,0) \text{ and } (y,0) \text{ are on the same loop}] & \text{for Ex. 2} \end{cases} \tag{8}$$

with

$$C(S) = \frac{1}{2S+1} \sum_{m=-S}^{S} m^2 = \frac{1}{3} S(S+1) \tag{9}$$

and where $(x,t) \in [-L, L+1] \times [0, \beta]$ denotes a space-time point and $\mathbf{I}[\ \cdot\ ]$ denotes the indicator function of the event described between the brackets. Hence, the

Fig. 4. The configurations ω for the antiferromagnetic models of Example 2 can be viewed as a partition of the plane into connected clusters. By labeling the vertical strips $n < x < n+1$ alternatingly A and B, the relation with a random cluster model becomes evident.

spin–spin correlation is proportional to the probability, with respect to the effective probability measure $\mu(d\omega)$ on the space of loop configurations, that two sites are on the same loop of ω:

$$\langle S_x^3 S_y^3 \rangle = \begin{cases} C(S)\mathrm{Prob}_\mu((x,0) \text{ and } (y,0) \text{ are on the same loop}) & \text{for Ex. 1} \\ (-1)^{|x-y|}C(S)\mathrm{Prob}_\mu((x,0) \text{ and } (y,0) \text{ are on the same loop}) & \text{for Ex. 2.} \end{cases} \tag{10}$$

Now, we give a brief account of the main questions one would like to answer about the stochastic geometric models of Example 1 and 2 and some generalizations of these.

3. Discussion of Results and Open Problems

Example 2, in the limit $L, \beta \to \infty$, was treated in quite some detail in [6], mainly for the case of translation invariant or staggered (period 2) coupling constants J_x. In that work an important rôle was played by the FKG structure [11] of the measure $\mu(d\omega)$. The relevant order structure on the space of configurations ω takes into account the antiferromagnetic nature of the model in the following way. The space-time of the quantum spin chain is embedded in $\mathbb{R}^2$ and can be partitioned into vertical strips of width 1 which we label alternatingly A and B, with the strip $0 < x < 1$

getting the label A, as in Figure 4. The Poisson 'beeps' occurring in a strip with label A (B) are called A-bonds (B-bonds). A partial order on the configurations ω is defined by: $\omega' \preceq \omega$ if the set of A-bonds in ω *is contained in* the set of A-bonds in ω' and the set of B-bonds in ω *contains* the set of B-bonds in ω'. We consider the loops in ω as the boundaries of a collection of connected subsets (connected clusters) of the plane. Each such connected set consists of the vertical strips $n < x < n+1$ connected by horizontal bridges. All strips in a given cluster are either of the A or of the B type. Let $C_A(\omega)$ denote the number of connected clusters of type A and $C_B(\omega)$ the number of clusters of type B. With these definitions one then has the following obvious properties: $N_A(\omega)$ and $C_A(\omega)$ are decreasing functions of ω and $N_B(\omega)$ and $C_B(\omega)$ are increasing, where $N_C(\omega)$ denotes the number of bonds in ω which occur in the strips of type C, $C = A$ or B. The measure $\mu(d\omega)$ thus becomes a random cluster model. It was shown in [6] that this random cluster model is actually the FK representation [4, 10] of a certain two-dimensional Potts model (with the number of states per site $q = p^2$). Crucial in the derivation of this equivalence are the following two relations:

$$l(\omega) = C_A(\omega) + C_B(\omega) + \text{constant} \tag{11}$$

$$C_A(\omega) - C_B(\omega) - N_A(\omega) + N_B(\omega) = \text{constant} \tag{12}$$

The first equation follows from the fact that each loop is the 'outer' boundary of a connected cluster (of either type A or type B). The second relation is a version of a well-known formula due to Euler. The work of Burton and Keane [8] and Gandolfi, Keane, and Russo [12] on two-dimensional correlated percolation models provides us with some important a priori information about the possible geometries of the connected clusters, in particular that the A- and B-clusters cannot percolate simultaneously. This immediately shows that all loops are finite μ-almost surely. By (9) this corresponds to absence of Néel order for the quantum spin chains. Further analysis leads to a proof of the Affleck–Lieb dichotomy for the class of models under consideration [3]. We refer the reader to [6] for more details and other results.

The two-dimensional version of Example 2 (loops in three dimensions) it is expected that in the $\lim_{\text{volume}\to\infty} \lim_{\beta\to\infty}$, and for $p = 2$ (the spin $\frac{1}{2}$ model), Néel order does occur (for $p \geq 3$ this has been shown by a different method in [9, 16]). Invoking a result from Kohma and Tasaki [20], a proof of this conjecture would follow from

$$\lim_{|x-y|\to\infty} \text{Prob}_\mu((x,0) \text{ and } (y,0) \text{ are on the same loop}) > 0. \tag{13}$$

To find interesting phenomena in Example 1, we have to consider β large but finite and the dimension of the lattice three or higher. The aim would then also be to prove (12). This would imply long-range order in the Heisenberg ferromagnet at low temperatures and in high enough dimensions and solve an outstanding open problem that has challenged many of the best mathematical physicists in the past decades.

Finally I would like to mention a random loop model that arises from the spin-1 Heisenberg antiferromagnetic chain. More generally we would like to study the

Fig. 5. (a)–(b) The diagrams representing the two terms in the interaction of the spin-1 antiferromagnetic chain with Hamiltonian (13). (c) The two lines in each vertical segment of ω are parallel or crossing with equal probabilities.

Fig. 6. A decorated configuration ω^* of random loops for the model (14). The dotted blobs are Bernoulli variables that with probability $\frac{1}{2}$ attain the value 'parallel' and with probability $\frac{1}{2}$ the value 'crossed'.

spin-1 chain ($p = 3$) with Hamiltonian

$$H = \sum_x \alpha \mathbf{S}_x \cdot \mathbf{S}_{x+1} + (\alpha - 1)(\mathbf{S}_x \cdot \mathbf{S}_{x+1})^2. \tag{14}$$

The stochastic geometric representation discussed below covers the range $\alpha \in [0, 1]$. Note that $\alpha = 0$ is a special case of Example 2. A different stochastic geometric representation for the $\alpha = 1$ case and related models was used in [17, 23].

The probability measure $\mu(d\omega)$ for this model is of the form

$$\mu(d\omega) = \rho^{\alpha}_{L,\beta}\rho^{1-\alpha}_{L,\beta}(d\omega)\frac{1}{2^{X(\omega)}}\sum_{\omega^*\sim\omega} q^{l(\omega^*)} \tag{15}$$

with $q = 2$ and where ω now contains two types of horizontal bonds generated with rates α and $1-\alpha$ respectively. Bonds of the first type are replaced by the diagram shown in Figure 5(a), the bonds of the second type by the diagram of Figure 5(b). ω^* is a configuration of loops obtained from ω by the following decoration procedure: each vertical segment between bonds in ω is drawn as a double line, which, independently for each segment, can either be parallel or crossing with equal probabilities (see Figure 5(c)). The result is illustrated in Figure 6. $l(\omega^*)$ denotes the number of loops in ω^* and $X(\omega)$ is the number of vertical segments in ω (so, $2^{X(\omega)}$ is the number of distinct ω^*'s obtained from ω).

The main conjecture about this model is that the loop connectivity decays exponentially fast except at the point $\alpha = \frac{1}{2}$ [2, 15], i.e., for all $\alpha \neq \frac{1}{2}$ there exist $C > 0$, $\xi < \infty$ such that

$$\mathrm{Prob}_{\mu}((x,t) \text{ and } (y,s) \text{ are on the same loop}) \leq Ce^{-\|(x,t)-(y,s)\|/\xi}. \tag{16}$$

The best constant ξ for which (15) holds should diverge as $\alpha \to \frac{1}{2}$, indicating the point of transition between the Haldane-phase with a unique ground state ($\alpha > \frac{1}{2}$) and the dimerized phase in which the translation symmetry of the chain is spontaneously broken ($\alpha < \frac{1}{2}$).

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