Prob. Theory and Math. Stat., Vol. 1, pp. 000 –000
B. Grigelionis et al. (Eds.)
1994 VSP/TEV

QUASI-STATE DECOMPOSITIONS FOR QUANTUM SPIN SYTEMS

Bruno Nachtergaele*

Department of Physics, Princeton University,
P.O. Box 708, Princeton, NJ 08544-0708, USA
E-mail: bxn@math.princeton.edu

ABSTRACT

I discuss the concept of quasi-state decompositions for ground states and equilibrium states of quantum spin systems. Some recent results on the ground states of a class of one-dimensional quantum spin models are summarized and new work in progress is presented. I also outline some challenging open problems and conjectures.

INTRODUCTION

The aim of this contribution is threefold. First I would like to review the notion of quasi-state decomposition as it was developed and used in (Aizenman and Nachtergaele, 1993a). I then show how interesting quasi-state decompositions for the ground states of a class quantum spin models can be obtained using a Poisson integral representation of the Gibbs kernel $e^{-\beta H}$. Secondly I will try to give a short review of the results we have recently obtained using quasi-state decompostions. These results mainly concern a class of one-dimensional quantum spin Hamiltonians introduced by Affleck (Affleck, 1985). The third and last part is devoted to a discussion of work in progress and some open problems in the subject as well as some stimulating conjectures.

2. QUASI-STATE DECOMPOSITIONS AND POISSON INTEGRAL REPRESENTATIONS

A quantum system is determined by a C*-algebra of observables $\mathcal{A}$ and a one-parameter group of automorphisms of $\mathcal{A}$ representing the dynamics. Here we are mainly interested in quantum spin systems defined on a finite lattice Γ for which $\mathcal{A} \equiv \mathcal{A}_\Gamma = \bigotimes_{x\in\Gamma} \mathcal{A}_{\{x\}}$ with $\mathcal{A}_{\{x\}} \cong M(d,\mathbb{C})$ (the complex $d\times d$ matrices), for all $x\in\Gamma$. Often Γ is a subset of an infinite lattice (e.g. $\mathbb{Z}^\nu$) and one is then interested in properties of the system as Γ tends to the full lattice (the thermodynamic limit). The dynamics is usually defined in terms of a Hamiltionian $H = H^* \in \mathcal{A}$ and we will give several examples of interesting Hamiltonians below. A state of the system is a normalized positive linear functional of $\mathcal{A}$. A class of physically interesting states are the equilibrium states: for any $\beta \geq 0$ one defines a state ω_β by

$$\omega_\beta(A) = \frac{\mathrm{Tr}\, A e^{-\beta H}}{\mathrm{Tr}\, e^{-\beta H}} \tag{2.1}$$

for all $A\in\mathcal{A}$. In this paper by ground state we always mean a state which is a limiting point of (2.1) as $\beta\to\infty$, possibly under specified boundary conditions. In most examples discussed here (2.1) will converge to a unique limit for finite systems and the thermodynamic limit will be taken afterwards.

It has been remarked many times that analyzing the structure of equilibrium states and ground states of a quantum system poses extra difficulties as compared to the situation in classical equilibrium statistical mechanics where the states are probability measures. Sure enough these probability measures can be highly non-trivial as well, but the fact that there is an underlying configuration space which can be visualized in a concrete way helps a lot in understanding their behaviour.

The aim of this section is to explain how at least for some quantum spin models one can obtain a pictorial representation of the ground states and equilibrium states which resembles somewhat the

* Partially supported by NSF Grants No. PHY92–14654 and PHY90–19433 A02.

situation for classical systems. More precisely we will derive a decomposition of ω_β of the form

$$\omega_\beta(A) = \int \mu(\mathrm{d}\omega) E_\omega(A) \tag{2.2}$$

where $\mu(\mathrm{d}\omega)$ is a probability measure on a space of configurations ω, and for each ω, E_ω is a linear functional of $\mathcal{A}_\Gamma$. Of course such an integral decomposition will only be useful if the structure of the E_ω is considerably simpler than ω_β itself and if we are able to analyse the measure $\mu(\mathrm{d}\omega)$. Below we show that for a certain class of Hamiltonians there is a quasi-state decomposition to which one can give a stochastic geometric interpretation. The resulting stochastic geometric model has proved to be rather helpful in revealing structural properties of the states (see Section 3 and 4).
The linear functionals E_ω will in general not be states and for infinite systems they are in general only defined on a dense subalgebra of the form

$$\mathcal{A}_{\mathrm{loc}} = \bigcup_{\Lambda\subset\Gamma} \mathcal{A}_\Lambda \tag{2.3}$$

where the union is over finite subsets Λ of Γ. Implicit in (2.3) is the natural embedding of $\mathcal{A}_\Lambda$ in $\mathcal{A}_{\Lambda'}$ for $\Lambda \subset \Lambda'$. Although the E_ω are typically not positive and not even bounded, they will be states of an abelian subalgebra of $\mathcal{A}$. We therefore call these functionals *quasi-states*.

2.1. *Poisson integral representations*

In this subsection we consider a quantum spin model defined on a finite set of sites Γ, which is completely arbitrary at this point. The set of "bonds", denoted by $\mathcal{B}$, is a collection of subsets of Γ. Soon we will specialize to the case where the bonds $b \in \mathcal{B}$ are pairs of sites and in the case of antiferromagnetic models it will be important that Γ be given a bipartite struture: $\Gamma = \Gamma_A \cup \Gamma_B$, $\Gamma_A \cap \Gamma_B = \emptyset$. Γ_A and Γ_B are called the A- and the B-sublattice respectively. In that situation a bond $b = \{x,y\} \in \mathcal{B}$ will be called *ferromagnetic* if x and y belong to the same sublattice and *antiferromagnetic* if x and y belong to different sublattices. We denote the set of ferromagnetic bonds by $\mathcal{B}_F$ and the set of antiferromagnetic bonds by $\mathcal{B}_{AF}$.
A complex Hilbert space $\mathcal{H}_x$ is associated with each site $x \in \Gamma$. Although this is not necessary for most of what follows, we will assume that all $\mathcal{H}_x$ have the same finite dimension d: $\mathcal{H}_x \cong \mathbb{C}^d$. A spin S system has $d = 2S+1$, $S = \frac{1}{2}, 1, \frac{3}{2}, \ldots$. The observables at site x are the elements of $\mathcal{B}(\mathcal{H}_x) \cong M(d,\mathbb{C})$. The Hilbertspace of the system is then $\mathcal{H}_\Gamma = \bigotimes_{x\in\Gamma} \mathcal{H}_x$ and the algebra of observables is $\mathcal{A}_\Gamma = \bigotimes_{x\in\Gamma} M(d,\mathbb{C})$. Physically important observables are usually expressed in terms of the spin matrices S^1, S^2, S^3 which are the generators of the d-dimensional irreducible unitary representation of SU(2). They satisfy the commutation relations

$$[S^\alpha, S^\beta] = i \sum_\gamma \varepsilon_{\alpha\beta\gamma} S^\gamma \tag{2.4}$$

where $\alpha, \beta, \gamma \in \{1,2,3\}$ and $\varepsilon_{\alpha\beta\gamma}$ is the completely antisymmetric tensor with $\varepsilon_{123} = 1$. One often combines the three spin matrices into a vector $\mathbf{S} = (S^1, S^2, S^3)$. The magnitude of this "spin-vector" is related to S by $\mathbf{S}\cdot\mathbf{S} = S(S+1)\mathbb{1}$.
A quantum spin modeled is defined by its Hamiltonian $H = H^* \in \mathcal{A}_\Gamma$ which we write in the form

$$H = -\sum_{b\in\mathcal{B}} J_b(h_b - 1) \tag{2.5}$$

with $h_b \in \mathcal{A}_b \cong \bigotimes_{x\in b} M(d,\mathbb{C})$, and we assume $J_b > 0$ for all $b \in \mathcal{B}$.
To obtain a quasi-state decomposition of ω_β, we start from the following Poisson integral formula:

$$e^{-\beta H} = \int \rho_\beta^J(d\omega) K(\omega) \tag{2.6}$$

where:
• $\rho_\beta^J(d\omega)$ is the probability measure of a product of independent Poisson processes, one for each bond $b \in \mathcal{B}$, running over the time interval $[0,\beta]$, and with rates J_b. For the time being we draw the configurations ω for this process as in Figure 1 (for evident reasons the figures are drawn for the simplest case of a one-dimensional system: $\Gamma = [a,b] \in \mathbb{Z}$ and $\mathcal{B} = \{\{x,x+1\} \mid a \leq x \leq b-1\}$.

• $K(\omega)$ is a product of operators h_b, one for each bond occurring in ω and ordered according to the times at which they occur: $K(\omega) = \prod^* h_{b_1} h_{b_2} \cdots h_{b_n}$ if ω is the set of time-indexed bonds $\{(b_1, t_1), (b_2, t_2), \ldots, (b_n, t_n)\}$ with $t_1 < t_2 < \cdots < t_n$.

An important quantity is the partition function $\mathcal{Z}_\beta = \operatorname{Tr} e^{-\beta H}$, which by (2.6) and linearity of the trace is given by:

$$\mathcal{Z}_\beta = \int \rho_\beta^J(d\omega)\ \operatorname{Tr} K(\omega) \tag{2.7}$$

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. For a more detailed discussion of these examples we refer to (Aizenman and Nachtergaele, 1993a).

Figure 1. A typical configuration of the Poisson process $\rho_\beta^J(d\omega)$.

Example 1

Let h be the operator which interchanges the states of the two sites, i.e. $h\varphi \otimes \psi = \psi \otimes \varphi$ for any two vectors $\varphi, \psi \in \mathbb{C}^d$. In any basis of $\mathbb{C}^d$ the matrix elements are 0 or 1 and a fortiori non-negative. $K(\omega)$ represents a permutation $\pi(\omega)$ of the sites in Γ, and its trace is easily seen to be $d^{\#\text{ cycles in } \pi(\omega)}$. 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 $d = 2$ this interaction is equivalent to the usual spin 1/2 Heisenberg ferromagnet: $h_{\{x,y\}} = \frac{1}{2} + \frac{1}{2}\boldsymbol{\sigma}_x \cdot \boldsymbol{\sigma}_y$, where $\boldsymbol{\sigma}$ is the vector with as its components the three canonical Pauli-matrices.

Figure 2. A typical configuration of the Poisson process $\rho^J_\beta(d\omega)$ decorated for the ferromagnetic models of Example 1.

Example 2

For the second example (which includes the spin 1/2 Heisenberg antiferromagnet) we require Γ to be bipartite and all bonds are assumed to be antiferromagnetic in the sense of above (so, $\mathcal{B} = \mathcal{B}_{AF}$). We consider the interaction h defined by

$$h = \sum_{m,m'} (-1)^{m-m'} |m, -m\rangle\langle m', -m'| \tag{2.8}$$

where $\{|m\rangle\}$ is a basis of $\mathbb{C}^d$ given by the eigenvectors of the third component S^3 of the spin with eigenvalues m. In the case $d = 2$ this is the interaction for the standard Heisenberg antiferromagnet ($h = \frac{1}{2} - \frac{1}{2}\boldsymbol{\sigma}_x \cdot \boldsymbol{\sigma}_y$)but the same expressions define an interesting interaction for any finite dimension (any magnitude of the spin) and was first studied by Affleck (Affleck, 1985) and later in (Affleck, 1990; Klümper, 1990; Batchelor and Barber, 1990). The interaction is proportional to the projection operator onto the singlet vector for a pair of spins and hence antiferromagnetic. It can be shown that the diagonal matrix elements of the corresponding $K(\omega)$ (but not the off-diagonal ones) 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 $\mathrm{Tr}\, K(\omega) = d^{l(\omega)}$.

The examples given above are not the most general ones that can be treated but they are in some sense the two basic ones as will become clear at the end of this section. Unlike 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.

We complete the quasi-state decomposition of ω_β 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 the probability measure describing the stochastic geometric model on the other hand. From (2.6) it follows that for any local observable A for the quantum spin chain

$$\omega_\beta(A) \equiv \frac{\mathrm{Tr}\, A e^{-\beta H}}{\mathrm{Tr}\, e^{-\beta H}} = \int \mu(d\omega) E_\omega(A) \tag{2.9}$$

where

$$\mu(d\omega) = (\mathcal{Z}_\beta)^{-1} \rho^J_\beta(d\omega)\, \mathrm{Tr}\, K(\omega) \tag{2.10}$$

and

$$E_\omega(A) = \frac{\operatorname{Tr} AK(\omega)}{\operatorname{Tr} K(\omega)} \tag{2.11}$$

$\mu(d\omega)$ 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. $A = S_x^3 S_y^3$. One then finds:

$$E_\omega(S_x^3 S_y^3) = \begin{cases} C(S)\mathbf{I}[(x,0) \text{ and } (y,0) \text{ are on the same loop }] & \text{for Example 1} \\ (-1)^{|x-y|} C(S)\mathbf{I}[(x,0) \text{ and } (y,0) \text{ are on the same loop }] & \text{for Example 2} \end{cases} \tag{2.12}$$

with $C(S) = (\sum_{m=-S}^{S} m^2)/(2S+1) = S(S+1)/3$ and where $(x,t) \in \Gamma \times [0,\beta]$ denotes a space-time point. $\mathbf{I}[\ \cdot\ ]$ denotes the indicator function of the event described between the brackets. Hence, the 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:

$$\langle S_x^3 S_y^3 \rangle = \begin{cases} C(S)\mathrm{Prob}_\mu((x,0) \text{ and } (y,0) \text{ are on the same loop}) & \text{for Example 1} \\ (-1)^{|x-y|} C(S)\mathrm{Prob}_\mu((x,0) \text{ and } (y,0) \text{ are on the same loop}) & \text{for Example 2} \end{cases} \tag{2.13}$$

For ω fixed (2.11) defines a functional of the algebra of observables which is a state on a certain abelian subalgebra (see (2.20)). We therefore call (2.9) a quasi-state decomposition of the state ω_β.

Figure 3. A typical configuration of the Poisson process $\rho_\beta^J(d\omega)$ decorated for the antiferromagnetic models of Example 2.

Examples 1 and 2 can be combined in order to obtain a quasi-state decomposition for a class of models with mixed ferro- and antiferromagnetic interactions.
In the statement of the following theorem some extra notation is used: for any configuration $\sigma = (\sigma_x)_{x\in\Gamma}$ we denote by $|\sigma\rangle$ the vector in $\mathcal{H}_\Gamma$ given by

$$|\sigma\rangle = \bigotimes_{x\in\Gamma} |\sigma_x\rangle \tag{2.14}$$

where $|\sigma_x\rangle$ is the eigenvector of S_x^3 belonging to the eigenvalue $\sigma_x \in \{-S, -S+1, \ldots, S\}$. $\sigma(t) = (\sigma_x(t))_{x\in\Gamma}$ is a piecewise constant function on $\Gamma \times [0,\beta]$ taking values in $\{-S, -S+1, \ldots, S\}$. A configuration of the Poisson process becomes a configuration of loops if we draw the ferromagnetic bonds as in Example 1 (Figure 2) and the antiferomagnetic ones as in Example 2 (Figure 3). As before, $l(\omega)$ denotes the number of loops in ω. We call $\sigma(t)$ *consistent* with a configuration of loops

ω if the discontinuities only occur at the time-indexed bonds in ω (but ω need not be discontinuous at a bond) and if in addition for each time-indexed bond $b = (\{x,y\},t) \in \mathcal{B} \times [0,\beta]$:

$$\sigma_x(t^-) = \begin{cases} \sigma_y(t^+) & \text{if } \{x,y\} \text{ is a ferromagnetic bond} \\ -\sigma_y(t^-) & \text{if } \{x,y\} \text{ is an antiferromagnetic bond} \end{cases} \tag{2.15}$$

$$\sigma_x(t^+) = \begin{cases} \sigma_y(t^-) & \text{if } \{x,y\} \text{ is a ferromagnetic bond} \\ -\sigma_y(t^+) & \text{if } \{x,y\} \text{ is an antiferromagnetic bond} \end{cases} \tag{2.16}$$

THEOREM 2.1. *For a Hamiltonian H of the form (2.5) and such that h_b is the interaction of Example 1 if $b \in \mathcal{B}_F$ and h_b is the interaction of Example 2 if $b \in \mathcal{B}_{AF}$ we have the following relations:*
i)

$$\langle \sigma' \mid e^{-\beta H} \mid \sigma \rangle = sign(\sigma', \sigma) \int \rho_\beta^J(\mathrm{d}\omega) \sum_{\sigma \text{ consistent with } \omega} \mathbf{I}[\sigma(\beta) = \sigma', \sigma(0) = \sigma] \tag{2.17}$$

where $sign(\sigma', \sigma) = (-1)^{N_{AF}(\pi)}$ with $N_{AF}(\pi)$ denoting the number of transpositions $t_{x,y}$ with $\{x,y\} \in \mathcal{B}_{AF}$ in any permutation π of the sites in Γ such that $\sigma'_x = \sigma_{\pi(x)}$ (the sign is well-defined because of the bipartite structure of the model).
ii) the partition function is given by:

$$\mathcal{Z}_\beta = \mathrm{Tr}\, e^{-\beta H} = \int \rho_{[0,\beta]}^J(\mathrm{d}\omega)\, (2S+1)^{l(\omega)} \tag{2.18}$$

iii) the equilibrium expectation values of observables which are functions of the operators S_x^3 can be expressed as

$$\frac{\mathrm{Tr}\, f((S_x^3)_{x\in\Gamma}) e^{-\beta H}}{\mathcal{Z}_\beta} = \int \mu(\mathrm{d}\omega)\, E_\omega(f) \tag{2.19}$$

where $\mu(\mathrm{d}\omega) = \mathcal{Z}_\beta^{-1} \rho_{[0,\beta]}(\mathrm{d}\omega)\, (2S+1)^{l(\omega)}$ and the expectation functional $E_\omega(f)$ is obtained by averaging, with equal weights, over all the spin configurations consistent with ω:

$$E_\omega(f) = \frac{1}{(2S+1)^{l(\omega)}} \sum_{\sigma \text{ consistent with } \omega} f(\sigma(t=0)) \tag{2.20}$$

2.2. *Quasi-state decompositions for more general models*

We now show that the method yielding the quasi-state decompositions of Theorem 2.1 can be extended, with little effort, to a much larger class of Hamiltonians of the form

$$H = -\sum_{b\in\mathcal{B}} h_b = \sum_{\{x,y\}\in\mathcal{B}} \sum_{k=0}^{2s} \tilde{J}_k(x,y)(\mathbf{S}_x \cdot \mathbf{S}_y)^k \tag{2.21}$$

It is in fact useful to think of the bonds here as a pair $\{x,y\}$ of sites together with a label $k \in \{1, 2S\}$. So, for a nearest neighbour model, we now have $2S$ bonds associated with each pair of nearest neighbour sites and also $2S$ independent Poisson processes with rates $J_k(x,y) > 0$. The $J_k(x,y)$ are not the same as the $\tilde{J}_k(x,y)$ because it will be necessary to reorganize the $2S$ interaction terms in (2.21) as follows:

$$\sum_{k=0}^{2s} \tilde{J}_k(x,y)(\mathbf{S}_x \cdot \mathbf{S}_y)^k = -\sum_{k=0}^{2s} J_k(x,y) Q_k(\mathbf{S}_x \cdot \mathbf{S}_y) \tag{2.22}$$

where Q_k are particular polynomials of degree k to be specified below. Hence the J_k will be related to the $\tilde{J}_k$ by a linear transformation.
The most straigthforward way to obtain a stochastic geometric representation for a quite extensive class of spin S Hamiltonians of the form (2.21) is by representing them as a spin $1/2$ system. To this end we introduce the (up to a phase) unique isometry $V^{(S)} : \mathbb{C}^{2S+1} \to (\mathbb{C}^2)^{\otimes 2S}$, which intertwines the spin S representation of SU(2) with $2S$ copies of the spin $1/2$ representation:

$$V^{(S)} D^{(S)}(g) = (D^{(1/2)}(g))^{\otimes 2S} V^{(S)}\,, \qquad g \in \mathrm{SU}(2) \tag{2.23}$$

$V^{(S)}$ satisfies: $V^{(S)*}V^{(S)} = \mathbb{1}$ and $V^{(S)}V^{(S)*} = P^{(S)}$ where $P^{(S)}$ is the orthogonal projection onto the spin S states in the $2S$-fold tensor product of the spin $1/2$ states. The spin S states coincide with the states that are symmetric under permutations of the $2S$ factors in $(\mathbb{C}^2)^{\otimes 2S}$, and hence $P^{(S)}$ can be expressed as

$$P^{(S)} \bigotimes_{i=1}^{2S} \varphi_i = \frac{1}{(2S)!} \sum_\pi \bigotimes_{i=1}^{2S} \varphi_{\pi(i)} \ , \qquad \varphi_i \in \mathbb{C}^2 \tag{2.24}$$

It follows by differentation of the intertwining property (2.23) that the spin S operators $S^\alpha, \alpha = 1, 2, 3$, can be expressed in terms of $2S$ copies of the Pauli matrices (for $S = \frac{1}{2}$, $S^\alpha = \frac{1}{2}\sigma^\alpha$):

$$V^{(S)} S^\alpha = \tfrac{1}{2} \sum_i^{2S} \sigma^\alpha V^{(S)} \tag{2.25}$$

We can now define a class of Hamiltomians H for a spin S system on a lattice Γ by representing it as a spin $1/2$ model on the extended lattice $\tilde{\Gamma} = \Gamma \times \{1, \ldots, 2S\}$. With each $x \in \Gamma$ we associate a set of $2S$ sites of the form (x, k) in $\tilde{\Gamma}$. The set of bonds $\tilde{\mathcal{B}}$ is constructed as follows. For $k = 1, \ldots, 2S$ and $b = \{x, y\} \in \mathcal{B}$ we define $b_k = \{(x, 1), (y, 1), \ldots, (x, k), (y, k)\}$. Then $\tilde{\mathcal{B}} = \{b_k \mid b \in \mathcal{B}, 1 \le k \le 2S\}$. The interactions $\tilde{h}_{b_k}$ are defined by

$$\tilde{h}_{b_k} = \prod_{l=1}^{k} h_{(x,l),(y,l)} \tag{2.26}$$

where $h_{(x,l),(y,l)}$ is one of the following two operators, depending on whether b is a ferro- or antiferromagnetic bond:

$$h_{(x,l),(y,l)} = \begin{cases} \frac{1}{2} + \frac{1}{2}\boldsymbol{\sigma}_{(x,l)} \cdot \boldsymbol{\sigma}_{(y,l)} & \text{if } b \text{ is ferromagnetic} \\ \frac{1}{2} - \frac{1}{2}\boldsymbol{\sigma}_{(x,l)} \cdot \boldsymbol{\sigma}_{(y,l)} & \text{if } b \text{ is antiferromagnetic} \end{cases} \tag{2.27}$$

It is then straightforward to derive (as an extension of Theorem 2.1) a quasi-state decomposition and the corresponding stochastic geometric representation for a Hamiltonian of the form

$$H = -V^* \left(\sum_{b \in \mathcal{B}} \sum_{k=1}^{2S} J_k \tilde{h}_{b_k} \right) V \tag{2.28}$$

where $V = \bigotimes_{x \in \Gamma} V_x^{(S)}$. We will describe to resulting stochastic geometric representation in detail below. But first we address the question of how to express a Hamiltonian of the form (2.28) in terms of the spin S matrices. In particular what are the polynomials Q_k appearing in (2.22). That (2.28) is equivalent with (2.22) for some particualar choice of the polynomials Q_k follows directly form the SU(2) invariance which one can check using the intertwining relation (2.23). Explicit knowledge of the Q_k is important if one wants to check whether some particular Hamiltonian (e.g. one that is discussed in the physics literature) has a stochastic geometric representation of the kind developed here or not.
So, we are looking for two sets of polynomials $\{Q_k^F\}$ and $\{Q_k^{AF}\}$ of degree $\le 2S$ such that

$$Q_k^F(\mathbf{S}_x \cdot \mathbf{S}_y) = V^* \prod_{l=1}^{k} t_{(x,l),(y,l)} V \tag{2.29}$$

$$Q_k^{AF}(\mathbf{S}_x \cdot \mathbf{S}_y) = V^* \prod_{l=1}^{k} p_{(x,l),(y,l)} V \tag{2.30}$$

where

$$t_{(x,l),(y,l)} = \tfrac{1}{2} + \tfrac{1}{2}\boldsymbol{\sigma}_{(x,l)} \cdot \boldsymbol{\sigma}_{(y,l)} \tag{2.31}$$

$$p_{(x,l),(y,l)} = \tfrac{1}{2} - \tfrac{1}{2}\boldsymbol{\sigma}_{(x,l)} \cdot \boldsymbol{\sigma}_{(y,l)} \tag{2.32}$$

The sites x and y in (3.29)-(3.30) just indicate any two distinct sites and play further no role. We therefore omit these indices in the discussion that follows. We also denote by V and P the tensor products of the isometry $V^{(S)}$ and the projection $P^{(S)}$ over the relevant sites.

The following two lemma's will be useful.

LEMMA 2.2. *For any $k, l, k', l' \in \{1, \ldots 2S\}, k \neq k', l \neq l'$ the following relations hold:*

$$
\begin{aligned}
t_{k,l}^2 &= \mathbb{1} & p_{k,l}^2 &= 2p_{k,l} \\
Pt_{k,l}t_{k',l} &= Pt_{k,l} & Pp_{k,l}p_{k',l} &= Pp_{k,l} \\
Pt_{k,l}t_{k',l}t_{k,l'} &= Pt_{k,l} & Pp_{k,l}p_{k',l}p_{k,l'} &= Pp_{k,l}p_{k',l'} \\
Pt_{k,l}P &= \frac{1}{(2s)^2}\sum_{i,j=1}^{2s} Pt_{i,j} & Pp_{k,l}P &= \frac{1}{(2s)^2}\sum_{i,j} Pp_{i,j}
\end{aligned}
$$

Proof :. The set of relations for the t's follows directly from (2.24) and the fact that $t_{k,l}$ is the transposition interchanging the k th factor of the $2S$-fold tensor product associated with the first site and the l th factor of the $2S$-fold tensor product associated with the second site. The relations for the p's follow from the relations for the t's by using

$$p_{k,l} = \mathbb{1} - t_{k,l} \tag{2.33}$$

which in turn follows directly from (2.31-32).

■

LEMMA 2.3. *The operators $Q_k^F \equiv Q_k^F(\mathbf{S}_0 \cdot \mathbf{S}_1)$ and $Q_k^{AF} \equiv Q_k^{AF}(\mathbf{S}_0 \cdot \mathbf{S}_1)$ defined in (2.29-30) satisfy the recursion relations*

$$(2S-k)^2 Q_{k+1}^F = \{(2S)^2 Q_1^F - 2k(2S-k)\}Q_k^F - k^2 Q_{k-1}^F \tag{2.34}$$

$$(2S-k)^2 Q_{k+1}^{AF} = \{(2S)^2 Q_1^{AF} - 2k(4S-k+1)\}Q_k^{AF} \tag{2.35}$$

for $1 \leq k \leq 2S-1$ and

$$
\begin{aligned}
Q_0^F &= \mathbb{1} & Q_0^{AF} &= \mathbb{1} \\
Q_1^F &= \frac{1}{2}\mathbb{1} + \frac{1}{2S^2}\mathbf{S}_0 \cdot \mathbf{S}_1 & Q_1^{AF} &= \frac{1}{2}\mathbb{1} - \frac{1}{2S^2}\mathbf{S}_0 \cdot \mathbf{S}_1
\end{aligned}
\tag{2.36}
$$

Proof :. We derive the recursion relation for the ferromagnetic case. The relation for the antiferromagnetic operators can be derived in a similar way. We use the formulas of Lemma 2.2 and the properties of V and P.

$$
\begin{aligned}
Q_1^F Q_k^F &= V^* t_{1,1} V^* V t_{1,1} \cdots t_{k,k} V \\
&= \frac{1}{(2S)^2}\sum_{i,j=1}^{2S} V^* P t_{i,j} t_{1,1} \cdots t_{k,k} V
\end{aligned}
\tag{2.37}
$$

The $(2S)^2$ terms in the RHS of the last equality can be taken together into three groups of terms which are equal: $(2S-k)^2$ terms where $i > k$ and $j > k$, k^2 terms where $i \leq k$ and $j \leq k$, and the rest which are $2(k-1)(2S-k+1)$ terms where either $i \leq k < j$ or $j \leq k < i$. The result is:

$$
\begin{aligned}
Q_1^F Q_k^F = &\frac{(2S-k)^2}{(2S)^2} V^* t_{i_1,j_1} t_{i_2,j_2} \cdots t_{i_{k+1},j_{k+1}} V \\
&+ \frac{2k(2S-k+1)}{(2S)^2} V^* t_{i_1,j_1} \cdots t_{i_k,j_k} V \\
&+ \frac{k^2}{(2S)^2} V^* t_{i_1,j_1} \cdots t_{i_{k-1},j_{k-1}} V
\end{aligned}
\tag{2.38}
$$

where $\{i_1, i_2, \ldots, i_{k+1}\}$ and $\{j_1, j_2, \ldots, j_{k+1}\}$ are two sets of distinct indices taken from $\{1, \ldots, 2S\}$. This proves the recursion relation for the Q_k^F. The recursion realtion for the Q_k^{AF} is derived in the same way with one small difference: when $i, j \leq k$ the cases $i = j$ and $i \neq j$ lead to different terms due to the relations of Lemma 2.2.

For $k = 0$ one has $Q_0^F = Q_0^{AF} = V^* V = \mathbb{1}$. For $k = 1$ we use the relations (2.25) and (3.31-32):

$$
\begin{aligned}
Q_1^F &= V^* t_{1,1} V = V^* P \frac{1}{(2S)^2} \sum_{i,j} t_{i,j} V \\
&= \tfrac{1}{2} V^* V + \frac{1}{2S^2} V^* (\tfrac{1}{2} \sum_i \boldsymbol{\sigma}_i) \cdot (\tfrac{1}{2} \sum_j \boldsymbol{\sigma}_j) V \\
&= \frac{1}{2} \mathbb{1} + \frac{1}{2S^2} \mathbf{S}_0 \cdot \mathbf{S}_1
\end{aligned}
\tag{2.39}
$$

and $Q_1^{AF} = \mathbb{1} - Q_1^F$ by (2.33).

■

In particular this lemma shows that Q_k^F and Q_k^{AF} are two complete independent families of rotation invariant operators on $\mathbb{C}^{2S+1} \otimes \mathbb{C}^{2S+1}$ because the recursion relations imply that the they are polynomials of degree k in the Heisenberg interaction $\mathbf{S}_0 \cdot \mathbf{S}_1$. The recursion relation can also be used to obtain explicit expressions for the polynomials Q_k^F and Q_k^{AF}. For $S = 1$ one finds:

$$
\begin{aligned}
Q_0^F &= \mathbb{1} & Q_0^{AF} &= \mathbb{1} \\
Q_1^F &= \tfrac{1}{2} + \tfrac{1}{2} \mathbf{S}_0 \cdot \mathbf{S}_1 & Q_1^{AF} &= \tfrac{1}{2} - \tfrac{1}{2} \mathbf{S}_0 \cdot \mathbf{S}_1 \\
Q_2^F &= -\mathbb{1} + \mathbf{S}_0 \cdot \mathbf{S}_1 + (\mathbf{S}_0 \cdot \mathbf{S}_1)^2 & Q_2^{AF} &= -\mathbb{1} + (\mathbf{S}_0 \cdot \mathbf{S}_1)^2
\end{aligned}
\tag{2.40}
$$

For later reference we also give here a general formula for the Q_k^{AF}:

$$
Q_k^{AF}(z) = 2^k \left[\frac{(2S-k)!}{(2S)!} \right]^2 \prod_{l=2S-k+1}^{2S} (z_l - z) \tag{2.41}
$$

where $z_l = \frac{1}{2} l(l+1) - S(S+1)$ are the eigenvalues of $\mathbf{S}_0 \cdot \mathbf{S}_1$. From (2.41) it immediately follows that $Q_k^{AF}(\mathbf{S}_0 \cdot \mathbf{S}_1)$ is of the form

$$
Q_k^{AF}(\mathbf{S}_0 \cdot \mathbf{S}_1) = \sum_{l=0}^{2S-k} a_{kl} P^{(l)} \tag{2.42}
$$

where $P^{(l)}$ is the orthogonal projection onto the states of total spin l in the tensor product of two spin S's. One can in fact easily determine the a_{kl} by computing the eigenvalue $Q_k^{AF}(\mathbf{S}_0 \cdot \mathbf{S}_1)$ takes on a state of total spin l:

$$
a_{kl} = 2^k \left[\frac{(2S-k)!}{(2S)!} \right]^2 \prod_{m=2S-k+1}^{2S} (z_m - z_l) \tag{2.43}
$$

It follows immediately that $a_{kl} = 0$ if $l > 2S - k$ and that $a_{kl} > 0$ if $l \leq 2S - k$. From this observation it also follows that the class of integer spin antiferromagnetic Valence Bond Solid (VBS) chains studied in (Arovas et al., 1988) and (Fannes et al., 1989, 1992) do not alow for a stochastic geometric representation of the kind discussed here; the measure μ would not be non-negative. On the other hand the interactions of VBS models are tuned such that exact cancelations in the measures occur, ie., positive and negative constributions in the measure cancel each other in such a way that some types of fluctuations are greatly reduced. The simplest non-trivial example of a VBS model is the AKLT chain, introduced in (Affleck et al., 1988). For this model one can derive an extremely simple quasi-state decomposition for its unique ground state which reveals beautifully the structure of the state (Nachtergaele, 1993b).

We now proceed to describe the stochastic geometric representation which is the result of the discussion above. We consider a spin S model on a lattice Γ with Hamiltonian

$$
H = -\sum_{\{x,y\} \in \mathcal{B}_F} \sum_{k=0}^{2S} J_{b,k}(x,y) Q_k^F(\mathbf{S}_x \cdot \mathbf{S}_y) - \sum_{\{x,y\} \in \mathcal{B}_{AF}} \sum_{k=0}^{2S} J_{b,k}(x,y) Q_k^{AF}(\mathbf{S}_x \cdot \mathbf{S}_y) \tag{2.44}
$$

It is assumed that the lattice has a bipartite structure in the sense discussed in Section 2.1. Let $\rho(\mathrm{d}\omega)$ denote the Poisson process on $\tilde{\mathcal{B}}$ as defined in Section 2. As in Examples 1 and 2 of Section 2 $\mathrm{Tr}\, K(\omega)$ can be computed in a geometric way. One proceeds as follows. Because V is an isometry and the cyclicity of the trace it is obvious that

$$\begin{aligned} \mathrm{Tr}\, K(\omega) &= \mathrm{Tr}_{\mathcal{H}_\Gamma} \prod\nolimits^*_{b_k \in \omega} V^* \tilde{h}_{b_k} V \\ &= \mathrm{Tr}_{\mathcal{H}_{\tilde{\Gamma}}} P \tilde{K}(\omega) \end{aligned} \tag{2.45}$$

where the $\tilde{h}_{b_k}$ are defined in (2.26), $\prod^*$ denotes a time-ordered product, and

$$\tilde{K}(\omega) = \prod\nolimits^*_{b_k \in \omega} (\tilde{h}_{b_k} P) \tag{2.46}$$

If there would be no projection operators P in (2.46), it would immedately follow from Theorem 2.1 that $\mathrm{Tr}\, K(\omega) = 2^{l(\omega)}$. At each site of the original lattice Γ there would then be $2S$ vertical lines, one for each site in $\tilde{\Gamma}$. Each lines carries a spin-$\frac{1}{2}$ degree of freedom. The time indexed bonds b_k are graphically represented by the diagrams shown in Figure 4.

Figure 4. The diagrams representing the interactions Q_k^F and Q_k^{AF}. The shaded boxes represent the permutations π_v of the lines in each vertical segment: the index i_1 at the top of the leftmost line indicates that this line is identified with the line number i_1 under the shaded box etc.

The projection operators P reflect the fact that only states which are symmetric under permutations of the $2S$ factors are relevant. ¿From (2.24) it is quite obvious how the inserted projection operators can be incorporated into the stochastic geometric representation. It is sufficient to average over all permutations of the lines between any two time-indexed bonds, i.e. we introduce a random permutation at each vertical segment in ω. By a *vertical segment* v in ω we mean a maximal time interval at a site $x \in \Gamma$ such that no bond $b_k = (\{x, y\}, k)$ occurs in ω during that time interval. For each ω we define $\nu_\omega(\mathrm{d}\pi)$ to be the uniform probability measure on configurations $(\pi_v)_{v \in \omega}$ of permutations π_v of the set of $2S$ lines running through the segment v. It is then obvious that

$$\mathrm{Tr}\, \tilde{K}(\omega) = \int \nu_\omega(\mathrm{d}\pi) 2^{l((\omega,\pi))} \tag{2.47¬}$$

It is convenient to define $\tilde{\rho}^J_\beta(\mathrm{d}\tilde{\omega}) = \rho^J_\beta(\mathrm{d}\omega)\nu_\omega(\mathrm{d}\pi)$ with $\tilde{\omega} = (\omega, \pi)$.

THEOREM 2.4. *For a Hamiltonian H of the form (2.44) with all $J_k(x, y) \geq 0$ for $1 \leq k \leq 2S$. Without loss of generality we may assume that $J_0(x, y) = 0$. Then:*
i)

$$\langle \sigma' \mid e^{-\beta H} \mid \sigma \rangle = \int \rho^J_\beta(\mathrm{d}\tilde{\omega}) \sum_{\tilde{\sigma} \text{ consistent with } \tilde{\omega}} sign(\tilde{\sigma}', \tilde{\sigma}) \mathbf{I}[\sum_{k=1}^{2S} \tilde{\sigma}(\beta) = \sigma', \sum_{k=1}^{2S} \tilde{\sigma}(0) = \sigma] \tag{2.48}$$

where $\tilde\sigma = (\tilde\sigma_{(x,k)})$, $\tilde\sigma_{(x,k)} \in \{-\frac{1}{2}, \frac{1}{2}\}$ and $\sigma = (\sigma_x)$, $\sigma_x \in \{-S, S+1, \ldots, S\}$, and sign$(\tilde\sigma', \tilde\sigma)$ is the sign defined in Theorem 2.1 (note that this sign depends only on σ and σ'.)
ii) the partition function is given by:

$$\mathcal{Z}_\beta = \mathrm{Tr}\, e^{-\beta H} = \int \tilde\rho^J_\beta(\mathrm{d}\tilde\omega)\, 2^{l(\tilde\omega)} \tag{2.49}$$

iii) the equilibrium expectation values of observables which are functions of the operators S^3_x can be expressed as

$$\frac{\mathrm{Tr}\, f((S^3_x)_{x\in\Gamma})e^{-\beta H}}{\mathcal{Z}_\beta} = \int \mu(\mathrm{d}\tilde\omega)\, E_{\tilde\omega}(f) \tag{2.50}$$

where $\mu(\mathrm{d}\tilde\omega) = \mathcal{Z}_\beta^{-1}\tilde\rho^J_\beta(\mathrm{d}\tilde\omega)\, 2^{l(\tilde\omega)}$ and the expectation functional $E_{\tilde\omega}(f)$ is obtained by averaging, with equal weights, over all the spin configurations consistent with ω:

$$E_{\tilde\omega}(f) = \frac{1}{2^{l(\tilde\omega)}} \sum_{\sigma \text{ consistent with } \tilde\omega} f(\sum_{k=1}^{2S} \tilde\sigma(t=0)) \tag{2.51}$$

iv) For a general local observable A one has

$$\omega_\beta(A) = \int \tilde\rho(\mathrm{d}\tilde\omega) E_{\tilde\omega}(A) \tag{2.52}$$

with

$$E_{(\omega,\pi)}(A) = 2^{-l((\omega,\pi))}\, \mathrm{Tr}_{\tilde\Gamma}\, VAV^* {\prod}^*_{b_k, v\in\omega} \tilde h_{b_k} \pi_v \tag{2.53}$$

There is a special case of the models (2.44) for which the stochastic geometric picture simplifies a lot. They are models on a bipartite lattice with only antiferromagnetic bonds ($\mathcal{B}_F = \emptyset$) and for which only $J_{2S} > 0$ and all other coupling constants vanish. Then only the diagram D^{AF}_{2S} appears and the $2S$ lines belonging to one site always act in unison, and therefore can equally well be drawn as one line. Therefore we will refer to this special cases as the *single-line* models as oppposed to the general *multi-line* models. The integral over the permutation variables π_ω can be carried out explicitely and one finds

$$\int \nu_\omega(\mathrm{d}\pi) 2^{l((\omega,\pi))} = (2S+1)^{l(\omega)} \tag{2.54}$$

where $l(\omega)$ is now the number of loops in the configuration ω drawn with a single line at each site and with the diagram D^{AF}_1 at each of the time-indexed bonds as if it were a spin-$\frac{1}{2}$ antiferromagnet. Up to trivial constants the Hamiltonians of this model is given by

$$H = -\sum_{b\in\mathcal{B}_{AF}} P^{(0)}_b \tag{2.55}$$

where $P^{(0)}_b$ denotes the orthogonal projection onto the singlet state at the bond b. In fact $(2S+1)P^{(0)}_b$ is identical to the interaction h given in Example 2 (2.8), and the quasi-state decomposition for these models can be derived directly—without reference to the general multi-line models—as was done in (Aizenman and Nachtergaele, 1993a).

3. MAIN RESULTS FOR THE ONE-DIMENSIONAL SINGLE-LINE MODELS

In this section we only consider one-dimensional single-line models, i.e. $\Gamma = [-L, L] \subset \mathbb{Z}$ and the Hamiltonian is

$$H = -\sum_{x=-L}^{L} J_x P^{(0)}_{x,x+1} \tag{3.1}$$

where all J_x are strictly positive and we will mostly assume that J_x is independent of x or alternatingly takes on two different values. For the proofs of the theorems in this section and further details see (Aizenman and Nachtergaele, 1993a).
One is mainly interested in properties of the ground states of (3.1) in the thermodynamic limit ($L \to \infty$). The existence of some specific thermodynamic limits is guaranteed by Theorem 0 of our study.

THEOREM 3.0. *For each $L \geq 0$ the Hamiltonian H_L has a unique ground state ψ_L and if $J_x = J_{x+2}$ for all x, the following two limits exist for all local observables A (finite algebraic combinations of the spin matrices $S^i_x, i = 1, 2, 3$ and $x \in \mathbb{Z}$):*

$$\langle A \rangle_{\text{even}} = \lim_{\substack{L\to\infty \\ L \text{ even}}} \frac{\langle \psi_L \mid A\psi_L \rangle}{\langle \psi_L \mid \psi_L \rangle} \quad , \qquad \langle A \rangle_{\text{odd}} = \lim_{\substack{L\to\infty \\ L \text{ odd}}} \frac{\langle \psi_L \mid A\psi_L \rangle}{\langle \psi_L \mid \psi_L \rangle} \tag{3.2}$$

A priori it is not obvious whether $\langle\cdot\rangle_{\text{even}}$ and $\langle\cdot\rangle_{\text{odd}}$ represent pure phases or not, and also these two limits are not necessarily distinct.
Our main results are the following:

a) Long range order
The interaction $-P^{(0)}$ is obviously antiferromagnetic in nature: it favours states where nearest neighbour spins are antiparallel. It is therefore natural to ask whether the ground states posses long-range antiferromagnetic order in the sense that

$$\langle S^3_0 S^3_x \rangle \sim (-1)^x m^2 \qquad \text{for } x \text{ large} \tag{3.3}$$

with $m \neq 0$. This kind of behaviour is called Néel order. Ignoring the quantum fluctuations such a state could be pictorially represented by

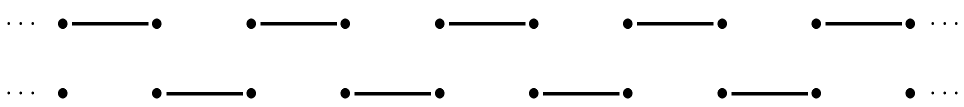
$$\cdots \uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow \cdots$$

It turns out that Néel order does not occur in the models with Hamiltonian (3.1). Absence of Néel order is in fact expected to hold for any one-dimensional quantum antiferromagnet based on the very general argument of (Mermin and Wagner, 1966). So far a rigorous proof of the general statement has not been found but for the family of models under consideration here we have the following theorem.

THEOREM 3.1. *The infinite volume ground states described in (3.2) do not have Néel order:*

$$\lim_{x\to\infty} \langle S^3_0 S^3_x \rangle_{\text{even(odd)}} = 0$$

The interaction $-P^{(0)}$ could however give rise to another type of long-range order. Although for a chain of length ≥ 3 there is no state in which all nearest neighbour pairs of spins are exactly in the singlet state, there are two states in which half of the nearest neighbour pairs do form a singlet: all the spins at an even site could form a singlet with their nearest neighbour on the right or, alternatively, with their nearest neighbour on the left. This leads to two states of periodicity 2 with respect to lattice translations. Pictorially these two states would look as follows:



This kind of long-range order is called dimerization for obvious reasons. Again we are ignoring the quantum fluctuations and one can actually not expect that these are the true ground states. Also in cases where there is only a preference of the spins at even sites to form singlet states with their left or right neighbours, we call the state (partially) dimerized.
The stochastic geometric representation permits us to prove the following result related to the Affleck-Lieb dichotomy (Affleck and Lieb, 1986).

THEOREM 3.2. *For the ground states of the translation invariant model (3.1) ($J_x \equiv J$), one of the following holds:*
i) either the translation symmetry is spontaneously broken in the infinite volume ground states
ii) or the spin-spin correlation function decays slowly (non-exponential) with

$$\sum_x |x \langle S^3_0 S^3_x \rangle| = +\infty$$

In the first case, the symmetry breaking is manifested in the non-invariance of the pair correlation:

$$\langle \mathbf{S}_0 \cdot \mathbf{S}_1 \rangle_{\text{even}} \neq \langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle_{\text{even}} = \langle \mathbf{S}_0 \cdot \mathbf{S}_1 \rangle_{\text{odd}}$$

The stochastic geometric representation in fact gives us a detailed picture of the correlations in the dimerized phase. We find the following behaviour: in the state where the spins on the even sites are more correlated with their neighbours to the right one finds that with probability 1 some spins on the left half-infinite chain $(-\infty, x]$ form a singlet with some spins on the right half-infinite chain $[x+1, +\infty)$, for each even x. In the same state this probability is < 1 for odd x.

b) Decay of correlations

Theorems 3.1 and 3.2 do not specify how fast $\langle S_0^3 S_x^3 \rangle$ converges to zero as $x \to \infty$. The decay rate by itself is interesting information and in particular one would like to show that the decay is exponentially fast (existence of a finite correlation length) in the cases where the translation symmetry is broken. More generally one can consider the truncated correlation function of any two local observables A and B. For any local observable C we denote by C_x the observable obtained by translating C over x and let supp$C$ be the smallest interval $[a, b]$ in the chain such that C is localized in $[a+1, b-1]$. We have an estimate for the truncated correlation function

$$|\langle A\,; B_x \rangle| = \langle A B_x \rangle - \langle A \rangle \langle B_x \rangle \tag{3.4}$$

in terms of the truncated two-point function $\tau(x; y)$ of an associated two-dimensional Potts model. For the translation invariant case the Potts model is at its self-dual point and for the staggered model it can be taken to be in the high temperature phase. The precise definition of this Potts model is given in (Aizenman and Nachtergaele, 1993a). The comparison theorem reads as follows.

THEOREM 3.3. *Let $\langle \cdot \rangle$ denote the expectation in the ground state of a finite chain containing an even number of sites, or in one of the limiting states $\langle \cdot \rangle_{\rm even}$ or $\langle \cdot \rangle_{\rm odd}$. Then, for any pair of local observables A and B of the quantum spin chain there are constants C_A and C_B such that*

$$|\langle A\,; B_x \rangle| \leq C_A C_B \sum_{\substack{y \in {\rm supp} A \\ z \in {\rm supp} B_x}} \tau(y\,; z)$$

In this theorem supp$A$ is roughly equal to the set of sites in the lattice on which the observable A acts non-trivially.

c) The spectral gap

One says that the system has a spectral gap of magnitude at least $\gamma > 0$ in an infinite volume ground state $\langle \cdot \rangle$ if for any local observable A the following inequality holds

$$\lim_{L \to \infty} \langle A^* [H_L, A] \rangle \geq \gamma (\langle A^* A \rangle - |\langle A \rangle|^2) \tag{3.5}$$

This is equivalent to the GNS Hamiltonian having a spectral gap separating the ground state from the rest of the spectrum. It is therefore obvious that the existence of a spectral gap would also follow from an estimate of the type

$$|\langle A e^{-tH} B \rangle| \leq C_A C_B e^{-\gamma t} \tag{3.6}$$

One can actually prove the analogue of Theorem 3.3 for the observable B being translated in imaginary time instead of in space and this implies the following theorem.

THEOREM 3.4. *Whenever the two-dimensional Potts model associated with the quantum spin chain has an exponentially decaying truncated two-point function there is a spectral gap in the ground states $\langle \cdot \rangle_{\rm even}$ and $\langle \cdot \rangle_{\rm odd}$.*

4. RESULTS, OPEN PROBLEMS, AND CONJECTURES FOR THE MULTI-LINE MODELS

Also here we retrict ouselves to one-dimensional models. Some important questions related to higher dimensional models were briefly discussed in (Nachtergaele, 1993a). We will also only consider translation invariant models, i.e. the coupling constants J_k do not depend on the position in the chain. So, the Hamiltonians under investigation here are

$$H = -\sum_{x=-L}^{L-1} \sum_{k=0}^{2S} J_k Q_k^{AF} (\mathbf{S}_x \cdot \mathbf{S}_{x+1}) \tag{4.1}$$

where Q_k^{AF} is the polynomial of degree k defined in (2.41) and we assume that $J_k \geq 0$ for $1 \leq k \leq 2S$.

4.1. *The excess spin operator*

In the stochastic geometric picture of the ground state provided by the Poisson integral representation of Section 2, it is rather clear intuitively that the quantity

$$\hat{S}_x^\alpha = \sum_{y>x} S_y^\alpha$$

might indeed make sense when the spin-spin correlations have sufficient decay. We call these quantities the excess spin operators. We would like to give meaning to this infinite sum in such a way that the associated random variable satisfies

$$E_{\tilde{\omega}}(\hat{S}_x^\alpha) = \sum_{\substack{\text{loops } \gamma \text{ in } \omega \\ \text{intersecting both } (-\infty,x] \text{and } (x,+\infty)}} \sum_{(y,k) \text{on } \gamma} \tfrac{1}{2}\sigma^\alpha_{(y,k)} \tag{4.2}$$

A crucial property then is that the total third component of the spin (or any component for that matter) on the collection of sites where a given loop intersects the $t=0$ axis, is always identically zero. So, therefore only these loops that intersect both $(-\infty,x]$ and $[x+1,+\infty)$, appear in the sum (4.2). Because of (2.51) decay of the spin-spin correlation function translates directly into a restriction on the typical size of the loops in a configuration ω.
We define local approximants $\hat{S}_x^\alpha(\varepsilon)$ for the excess spin as follows:

$$\hat{S}_x^\alpha(\varepsilon) = \sum_{y>x} e^{-\varepsilon|y-x|} S_y^\alpha \tag{4.3}$$

for $\varepsilon > 0$, $x \in \mathbb{Z}$, and $\alpha = 1,2,3$. The $\hat{S}_x^\alpha(\varepsilon)$ are bounded self-adjoint operators and generate one-parameter unitary groups, although they are not representations of SU(2). For all $g \in$ SU(2) we will denote by $\mathbf{g}$ the vector in $\mathbb{R}^3$ such that in any strongly continuous unitary representation U, $U(g) = \exp i\mathbf{g}\cdot\hat{\mathbf{S}}$, where $\hat{\mathbf{S}}$ denotes the vector of generators of the representation.
For any state $\langle\cdot\rangle$ of the infinite spin chain there is a (up to unitary equivalence) unique Hilbert space $\mathcal{H}_{\rm GNS}$, a vector $\Omega \in \mathcal{H}_{\rm GNS}$ and a representation π of the algebra of observables $\mathcal{A}_{\mathbb{Z}}$ on $\mathcal{H}_{\rm GNS}$ such that

$$\langle A\rangle = \langle\Omega \mid \pi(A)\Omega\rangle \tag{4.4}$$

for all $A \in \mathcal{A}_{\mathbb{Z}}$. This is called the GNS representation of the state (Bratteli and Robinson, 1981). A natural dense subspace of $\mathcal{H}_{\rm GNS}$ is defined by

$$\mathcal{H}_{\rm loc} = \{\pi(A)\Omega \mid A \in \mathcal{A}_{\rm loc}\} \tag{4.5}$$

where $\mathcal{A}_{\rm loc}$ is the subalgebra of $\mathcal{A}$ formed by all finite combinations of the operators S_x^α.

Theorem 4.1. *Let $\langle\cdot\rangle$ be a ground state of a Hamiltonian of the form (4.1) and denote by $\mathcal{H}_{\rm GNS}$ its GNS Hilbert space. If*

$$\sum_x |x^3\langle S_0^\alpha S_x^\alpha\rangle| < +\infty, \quad \textit{or for the single-line models:} \quad \sum_x |x\langle S_0^\alpha S_x^\alpha\rangle| < +\infty \tag{4.6}$$

then, for every $x \in \mathbb{Z}$ there is a strongly continous unitary representation U_x of SU(2) defined by the limit

$$U_x(g)\psi = \lim_{\varepsilon\downarrow 0} e^{i\mathbf{g}\cdot\pi(\hat{\mathbf{S}}_x(\varepsilon))}\psi \tag{4.7}$$

for all $\psi \in \mathcal{H}_{GNS}$ with the following properties:
i) $U_x(g)$ commutes with $\mathcal{A}_{(-\infty,x]}$
ii) $U_{x-1}(g) = e^{i\mathbf{g}\cdot\pi(\mathbf{S}_x)}U_x(g)$
iii) The domain of the generators of U_x contains $\mathcal{H}_{\rm loc}$.

The proof of this theorem will be given in (Aizenman and Nachtergaele, 1993b).

COROLLARY 4.2. *There are well-defined self-adjoint generators $\hat{S}_x^\alpha$ of the representation U_x which are strong limits of the local approximants (4.3) and they have a common domain for all $\alpha = 1, 2, 3$ and $x \in \mathbb{Z}$. On this domain, which contains $\mathcal{H}_{\mathrm{loc}}$, one has the relation*

$$\hat{S}_{x-1}^\alpha = \pi(S_x^\alpha) + \hat{S}_x^\alpha \tag{4.8}$$

For situations where the excess spin operators exists one can then apply the following theorem to prove that sufficient decay of correlations in a ground state of a quantum spin chain with a Hamiltonian of the form (4.1) and $S = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \ldots$, necessarily exhibits breaking of the translation invariance.

THEOREM 4.3. *Let ω be a pure state of the spin S chain with halfintegral S, which is invariant under even translations and such that the operators $\hat{S}_x^\alpha$ exist and have the properties stated in Theorem 4.1 and Corollary 4.2, then ω is not invariant under odd translations.*

Proof :. As $\hat{S}_x^\alpha$ is self-adjoint the following spectral projection is well-defined:

$$P_x \equiv \text{ projection onto subspace where } \hat{S}_x^\alpha \in \mathbb{Z} + \tfrac{1}{2} \tag{4.9}$$

(4.8) and the $SU(2)$-commutation relations of the excess spin operators imply that the $\hat{S}_x^\alpha$ have spectrum $\subset \frac{1}{2}\mathbb{Z}$ and that

$$P_{x-1} = \mathbb{1} - P_x = P_{x+1} \tag{4.10}$$

and hence P_x commutes with any local observable: $P_x \in \mathcal{A}'_{(-\infty,x+2k]}$ for all $k \in \mathbb{Z}$. In an irreducible representation of the observable algebra this means that P_x is a multiple of the identity and because it is a projection we conclude that $P_x = \lambda_x \mathbb{1}$ with $\lambda_x \in \{0, 1\}$. By (4.10) this implies

$$\omega(P_x) = \begin{cases} 1 & \text{for } x \text{ even (odd)} \\ 0 & \text{for } x \text{ odd (even)} \end{cases} \tag{4.11}$$

and therefore ω is not invariant under translations over an odd distance.

■

4.2. *A topological index as order parameter*

The configurations of loops in the plane that occur in the Poisson integral representation of the quantum spin chains (4.1) have interesting topological properties which we expect to be of determining importance for the behaviour of their ground states. We will be considering configurations of loops in the infinite plane, which corresponds to studying the bulk of the quantum spin chain in the ground state. Afterwards we also make a remark about topological effects in finite and half-infinite chains.
A possible configuration of loops $\tilde{\omega}$ for a spin-1 chain is shown in Figure 5, and in general we consider configuartions which are constructed using the diagrams D_k^{AF}, $k = 0, \ldots, 2S$. Obviously one can construct configurations out of these diagrams that contain infinite lines. Such configurations are excluded from the considerations in this section. More precisely we impose the following condition.

CONDITION 4.4. *Let $\tilde{\omega}$ be a loop configuration for a spin-S chain. $\tilde{\omega}$ satisfies the Condition if all loops are finite and any point (x, t) in the plane is surrounded by only a finite number of loops. The set of all configurations satisfying this condition will be denoted by Ω_0. The probability measure $\mu(\mathrm{d}\tilde{\omega})$ satisfies the Condition if* $\mathrm{Prob}_\mu(\Omega_0) = 1$.

Here, by "surrounded by a loop", we mean that any continuous path connecting (x, t) to infinity must necessarily intersect that loop.
In a translation invariant ground state of the quantum spin chain Condition 4.4 will be satisfied if there is suffcient deacy of the spin-spin correlation function, e.g. Condition 4.4 is satisfied if

$$\sum_x |x\, \omega(\mathbf{S}_0 \cdot \mathbf{S}_x)| < \infty \tag{4.12}$$

Figure 5. A typical configuration of loops $\tilde{\omega}$ for a spin 1 antiferromagnetic chain. The loops are shown with the canonical orientation with respect to x which is used in the definition of the canonical winding number (4.13).

In fact (4.12) implies that the average number of loops surrounding any given point is finite:

$$\begin{aligned}\sum_{x\geq 0}|x\,\omega(S_0^3S_x^3)| &= \sum_{x\leq 0, y>0}|\omega(S_0^3S_x^3)| \\ &\geq \tfrac{1}{4}\sum_{x\leq 0,y>0}\text{Prob}(x \text{ is connected by a loop to } y) \\ &\geq \tfrac{1}{4}\mathbb{E}(\text{ connected pairs } x\leq 0, y>0) \\ &\geq \tfrac{1}{4}\mathbb{E}(\text{ loops } \gamma \text{ surrounding } (\tfrac{1}{2},0))\end{aligned}$$

Let $\tilde{\omega}$ be a configuration for which Condition 4.4 is satisfied. For any $(x,t)\in\mathbb{R}^2$ such that (x,t) does not belong to a loop in $\tilde{\omega}$, we define the canonical orientation of the loops $\gamma\in\tilde{\omega}$ as the one for which the vertical lines located at $z\in\mathbb{Z}$ are oriented in the positive time direction if $\text{sign}(x-z)(-1)^{[x-z]}=1$ ($[a]$ denotes the integral part of a), and in the negative time direction if $\text{sign}(x-z)(-1)^{[x-z]}=-1$ (see Figure 5). We then define the *canonical winding number* $w_{(x,t)}(\tilde{\omega})$ of $\tilde{\omega}$ with respect to (x,t) by

$$w_{(x,t)}(\tilde{\omega}) = \sum_{\gamma\in\tilde{\omega}}\frac{1}{2\pi}\int_\gamma d\theta_{(x,t)} \tag{4.13}$$

where θ is defined in Figure 5. By Condition 4.4 only a finite number of terms in the sum are non-vanishing and of course $w_{(x,t)}(\tilde{\omega})$ is an integer. The following crucial properties, which are straightforward to derive from the definition of the canonical winding number, show that the value of the winding number is actually a property of $\tilde{\omega}$, i.e. it does not depend upon the point (x,t) with respect to which it is computed, except for a trival dependence on the parity of x:

$$w_{(x,t)}(\tilde{\omega}) = w_{(x,s)}(\tilde{\omega}) \equiv A_x(\tilde{\omega}) \tag{4.14}$$

and

$$A_{x+1}(\tilde{\omega}) = 2S - A_x(\tilde{\omega}) \tag{4.15}$$

for all $x\in\mathbb{R}\setminus\mathbb{Z}$ and $s,t\in\mathbb{R}$.
What we have found is an index $A_0(\tilde{\omega})$ which takes on integer values and which characterizes a global topological property of $\tilde{\omega}$. It follows that for any $\mathbb{Z}$-ergodic probability measure $\mu(d\tilde{\omega})$ on Ω_0, $A_0(\tilde{\omega})$ will take a fixed value with probability 1 with respect to $\mu(d\tilde{\omega})$. We claim that the dimerization transition observed in certain antiferromagnetic quantum spin chains can be

interpreted as a transition between phases with a different value for the index $A_0(\tilde{\omega})$. It can be shown that for each integer z there are indeed $\tilde{\omega} \in \Omega_0$ for which $A_0(\tilde{\omega}) = z$, with the exception of the case $s = \frac{1}{2}$, where $A_0(\tilde{\omega})$ can only be 0 or 1. But we expect that only relatively small values will occur in the ground states of the Hamiltonians (4.1) although we have not been able to prove this so far. A second important open problem is to show that the winding number, which under certain conditions on the decay of spin-spin correlations is certainly measurable with respect to $\mu(\mathrm{d}\tilde{\omega})$, is also observable for the quantum spin chain. It is indeed not trivial that there exists an observable $A \in \mathcal{A}$ of the quantum spin chain of which the expectation value $\omega(A)$ would be equal to (or determine uniquely) the value of the topological index A_0 in the probability measure $\mu(\mathrm{d}\tilde{\omega})$ related to ω by (2.52) (with $\beta = +\infty$).
My main interest in the problems mentioned in the previous paragraph stems from the implications they have for the general structure of the ground state phase diagram of antiferromagnetic quantum spin chains. (Affleck and Haldane, 1987) make an thorough analyis of that phase diagram on the basis of an identifaction of the low-energy spectrum of spin chains with certain conformal quantum field theories. Their (non-rigorous) arguments lead to some very interesting predictions which we can summarize as follows. For the parameters in the Hamiltonian taking values in the complement of some submanifold of less than maximal dimension one expects that: i) for the half-integer spin antiferromagnetic chains the ground states either exhibit one of a finite number of possible types of dimerization, in which case they have exponential decay and a spectral gap, or the ground state is unique and translation invariant with slow (non-exponential) decay of correlations and no spectral gap; ii) for the integer spin antiferromagnetic chains there also is a finite number of possible types of dimerization and there is also a translation invariant phase but one with exponential decay and a spectral gap (the so-called Haldane-phase). So, apart from special choices of the coupling constants where one is on the boundary between two or more different phases, one expects that the integer spin chains always have expontential decay and a spectral gap where for the half-integer spin chains a gapless translation invariant phase exists. Our Theorem 4.3 (combined with Theorem 4.1 and Corollary 4.3) shows that for half-integer spin chains with antiferromagnetic interactions of the form (4.1) indeed there is no translation invariant phse with rapid decay of correlations. We believe that the different possible phases can be characterized by the value of the index A_0. Note that (4.15) has no translation invariant solutions for half integer S but that there is a translation invariant solution $A_x \equiv S$ for integer S. It follows that the gapless translation invariant phase for half-integer spin chains must have a slowly decaying spin-spin correlation function so as to make (4.6) divergent.
The existence of the excess spin operators also allows for a natural interpretation of the "exotic" edge states in finite and half-infinite integer spin chains. It was observed in Electron Spin Resonance experiments on the quasi-one dimensional compound NENP (Hagiwara et al., 1990,1992; Hagiwara and Katsumata, 1992) that the edges interact with a magnetic moment near to it as if they carry spin 1/2, although the system in all other respects seems to be modelled very well by a spin 1 antiferromagnetic chain. It was noted in (Hagiwara et al., 1990) that if the ground state of this system resembles the one of the AKLT model (for which the exact ground state is given in (Affleck et al., 1987,1988)), the spin 1/2 nature of the edge states could be easily explained. Our proof of the existence of the excess spin operator is valid for a quite general class of Hamiltonians. If one assumes that it is correct that a unique translation invariant ground state for a spin 1 chain implies that the index A_x is identically equal to 1 (or equal to S for higher integer spin), it follows that the excess spin is half-integral and that the edge states should have half-integral spin as well.

Acknowledgement. The research discussed in this paper was carried out in collaboration with Michael Aizenman.

REFERENCES

Affleck, I. (1985). Large-n limit of SU(n) quantum "spin" chains. *Phys. Rev. Lett.* **54**, 966–969.

Affleck, I. (1990). Exact results on the dimerization transition in SU(n) antiferromagnetic chains. *J. Phys. C: Condens. Matter* **2**, 405–415.

Affleck, I and Haldane, F.D.M. (1987). Critical theory of quantum spin chains. *Phys. Rev.* **B36**, 5291–5300.

Affleck, I., Kennedy, T., Lieb, E.H., and Tasaki, H. (1987). Rigorous results on valence-bond ground states in antiferromagnets. *Phys. Rev. Lett.* **59**, 799–802.

Affleck, I., Kennedy, T., Lieb, E.H., and Tasaki, H. (1988). Valence bond solid states in isotropic quantum antiferromagnets. *Comm. Math. Phys.* **115**, 477–528.

Affleck, I. and Lieb, E.H. (1986). A proof of part of Haldane's conjecture on quantum spin chains *Lett. Math. Phys.* **12**, 57–69.

Aizenman, M. and Nachtergaele, B. (1993a). Geometric aspects of quantum spin states. to appear in Comm. Math. Phys.

Aizenman, M. and Nachtergaele, B. (1993b). Geometric aspects of quantum spin states II. in preparation.

Arovas, D.P., Auerbach, A., and Haldane, F,D.M. (1988). Exenteded Heisenberg models of antiferromagnetism: analogies to the fractional quantum Hall effect *Phys. Rev. Lett.* **60**, 531–534.

Batchelor, M.T. and Barber, M. (1990). Spin-s quantum chains and Temperley-Lieb algebras. *J. Phys. A: Math. Gen.* **23**, L15–L21.

Bratteli, O. and Robinson, D.W. (1979). *Operator algebras and quantum statistical mechanics I.* Springer, New York-Heidelberg-Berlin.

Fannes, M., Nachtergaele, B., and Werner, R.F. (1989). Exact Antiferromagnetic Ground States for Quantum Chains. *Europhys. Lett.* **10**, 633-637.

Fannes, M., Nachtergaele, B., and Werner, R.F. (1992). Finitely correlated states for quantum spin chains. *Comm. Math. Phys.* **144**, 443–490.

Hagiwara, M., Katsumata, K., Renard, J.P., and Affleck, I., Halperin, B.I. (1990). Observation of $S = \frac{1}{2}$ degrees of freedom in an $S = 1$ linear chain Heisenberg antiferromagnet. *Phys. Rev. Lett.* **65**, 3181–3184.

Hagiwara, M. and Katsumata, K. (1992). Observation of $S = \frac{1}{2}$ degrees of freedom in an undoped $S = 1$ linear chain Heisenberg antiferromagnet. *J. Phys. Soc. Japan.* **61**, 1481–1484.

Hagiwara, M., Katsumata, K., Affleck, I., Halperin, B.I., and Renard, J.P. (1992). Hyperfine structure due to the $S = \frac{1}{2}$ degrees of freedom in an $S = 1$ linear chain antiferromagnet. *J. Mag. Mag. Materials* **104-107**, 839–840.

Haldane, F.D.M. (1983). Continuum dynamics of the 1-D Heisenberg antiferromagnet: identification with the O(3) nonlinear sigma model. *Phys.Lett.* **93A**, 464–468.

Klümper, A. (1990). The spectra of q-state vertex models and related antiferromagnetic quantum spin chains. *J.Phys. A: Math. Gen.* **23**, 809–823.

Mermin, N.D. and Wagner, H. (1966). Absence of ferromagnetism or antiferromagnetism in one- or two-dimensional isotropic Heisenberg models. *Phys. Rev. Lett.* **17**, 1133-1136.

Nachtergaele, B. (1993a). A stochastic geometric approach to quantum spin systems. Probability theory of spatial disorder and phase transition. G.R. Grimmett (Ed). Kluwer (to be published, 1994).

Nachtergaele, B. (1993b). A note on quasi-state decompositions of finitely correlated states. unpublished.