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Entropy estimates for finitely correlated states

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ABSTRACT. – We study in this paper the Rényi entropy densities of integer order for the class of finitely correlated states on a quantum spin chain, and obtain in this way explicit lower bounds for the usual entropy density. We apply this technique to obtain good bounds on the entropy density of a certain state on a spin-3/2 chain. This state is a ground state of a translation invariant nearest neighbour SU (2)-invariant interaction, which is thus shown to posses a residual entropy as $T \to 0$. Breaking the translation symmetry by adding a small SU (2)-invariant interaction of period two removes the ground state degeneracy, and produces a non-zero spectral gap above the ground state.

RÉSUMÉ. – Nous étudions la densité d'entropie de Rényi pour une classe d'états, dit à correlations finies, d'une chaine de spins quantiques. Grâce à ce résultat nous obtenons des bornes inférieures pour la densité d'entropie usuelle. En particulier nous appliquons cette technique à l'étude d'un état fondamental d'un modèle à spin 3/2. L'hamiltonien correspondant est défini par une interaction à plus proches voisins, invariante sous SU(2) et sous les translations. Nous montrons que cet état est à densité d'entropie non nulle ce qui démontre que le modèle a une entropie résiduelle et ne satisfait donc pas à la Troisième Loi de la Thermodynamique. La forte dégénérescence de l'état fondamental est levée en introduisant une petite perturbation de période deux sur la chaine, toutefois invariante sous SU(2). Cette perturbation introduit un «gap» dans le spectre de l'hamiltonien, gap qui tend vers zéro quand la perturbation tend vers zéro.

1. INTRODUCTION

In this paper we will consider the class of finitely correlated states on a quantum spin chain. These translation invariant states were introduced in [1] and extensively studied in [6]. The characteristic property of these states is that their correlation functions are described in terms of finite dimensional spaces. It is shown in [6] that the finitely correlated states coincide with (generalized) valence bond states [4]. Moreover, the pure exponential clustering states among them can be obtained as the unique ground states of translation invariant, finite range Hamiltonians and these Hamiltonians have a non-zero spectral gap.

The special properties of finitely correlated states makes them easy to handle in applications. For example, the computation of their correlation functions reduces to computing the powers of a finite matrix. Nevertheless, the class of finitely correlated states is still convex and weakly dense in the set of translation invariant states on the chain. This makes them good candidates for trial states in variational computations. However, in order to use them in the Gibbs variational principle for finite-temperature equilibrium states, one would need a way of computing the mean entropy of finitely correlated states.

Our main objective in this paper is to obtain information about the mean entropy of finitely correlated states. In Section 2 we will study the integer order Rényi entropy densities for finitely correlated states and use our results to gain control over the usual von Neumann entropy. As an application we will construct in Section 3 a translation invariant, nearest neighbour, anti-ferromagnetic SU(2) invariant Hamiltonian for a spin-3/2 chain with highly degenerate ground state. Using the results of Section 2 we will in fact show that this ground state has non-zero mean entropy, thereby producing an example of a quantum Hamiltonian with residual entropy. This is counter to general expectations about half-integral spin chains formulated by Affleck and Lieb [3] in their discussion of Haldane's Conjecture [10]. We also show that the addition of an arbitrarily small "staggered" interaction destroys the degeneracy of the ground state and produces a gap.

Our notations for quantum spin chains are as follows. The algebra of observables for a single site will be taken as the algebra $\mathcal{M}_d$ of the complex $d \times d$ matrices. The algebra of observables localized in the finite volume $\Lambda \subset \mathbb{Z}$ is then given by $\mathcal{A}_\Lambda = \bigotimes_{i \in \Lambda} \mathcal{A}_i$, where $\mathcal{A}_i$ is a copy of $\mathcal{M}_d$. As usual if $\Lambda_1 \subset \Lambda_2 \subset \mathbb{Z}$, $\mathcal{A}_{\Lambda_1}$ is identified as a subalgebra of $\mathcal{A}_{\Lambda_2}$ by tensoring with unit matrices on the sites $i \in \Lambda_2 \setminus \Lambda_1$. The algebra $\mathcal{A}_\mathbb{Z}$ of the infinite chain is then the C*-inductive limit of the $\mathcal{A}_\Lambda$, Λ finite. The group $\mathbb{Z}$ acts on $\mathcal{A}_\mathbb{Z}$ as a group of translation automorphisms $\{ \tau_a \mid a \in \mathbb{Z} \}$ where τ_a maps $\mathcal{A}_\Lambda$ onto $\mathcal{A}_{\Lambda + a}$. Any one-site symmetry, given by a unitary $U \in \mathcal{M}_d$, defines an automorphism of $\mathcal{A}_\mathbb{Z}$: on any local element $X \in \mathcal{A}_\Lambda$ it is given by $\alpha_U(X) = (\otimes_\Lambda U^*) X (\otimes_\Lambda U)$. A state ω on $\mathcal{A}_\mathbb{Z}$ is a normalized positive linear functional on $\mathcal{A}_\mathbb{Z}$. ω is called translation invariant if $\omega \circ \tau_a = \omega$ for all $a \in \mathbb{Z}$. If $\mathcal{G}$ is a group of unitaries in $\mathcal{M}_d$, we call ω $\mathcal{G}$-invariant if $\omega \circ \alpha_U = \omega$ for all $U \in \mathcal{G}$.

We now present the construction and some elementary properties of finitely correlated states. More details can be found in [6]. To construct the so-called C*-finitely correlated (for short finitely correlated states) we need to introduce some auxiliary objects:

(i) an algebra $\mathcal{M}_k$

(ii) a completely positive map $\mathbb{E} : \mathcal{M}_d \otimes \mathcal{M}_k \to \mathcal{M}_k$ that is unity preserving [20, 21]

(iii) a state ρ on $\mathcal{M}_k$, that satisfies $\rho(\mathbb{E}(\mathbf{1} \otimes Y)) = \rho(Y)$ for all $Y \in \mathcal{M}_k$.

There is then a unique translation invariant state ω of $\mathcal{A}_\mathbb{Z}$, such that its local expectation values are given by:

$$\omega(X_m \otimes X_{m+1} \otimes \ldots X_n) = \rho(\mathbb{E}_{X_m} \circ \mathbb{E}_{X_{m+1}} \circ \ldots \mathbb{E}_{X_n}(\mathbf{1}_k)) \qquad (1.1)$$

where $X_i \in \mathcal{M}_d$ is an observable at site i and where for all $X \in \mathcal{M}_d$

$$\mathbb{E}_X : \mathcal{M}_k \to \mathcal{M}_k : Y \mapsto \mathbb{E}_X(Y) = \mathbb{E}(X \otimes Y).$$

Such a state ω will be called the finitely correlated state generated by $(\mathbb{E}, \rho)$. The general behaviour of the correlation functions of ω is determined by the completely positive map $\mathbb{P} = \mathbb{E}_\mathbf{1} : \mathcal{M}_k \to \mathcal{M}_k$. A finitely correlated state ω can be decomposed into ergodic components ω_α generated by $(\mathbb{E}_\alpha, \rho_\alpha)$ such that the eigenvalue 1 of $\mathbb{P}_\alpha$ is non-degenerate. In this paper we will restrict our attention to the ergodic case, *i.e.* we will assume that $\mathbf{1}$ is the unique eigenvector of $\mathbb{P}$ corresponding to the eigenvalue 1. In order to have that ω is clustering one has to require that $\mathbb{P}$ has no other eigenvalue of modulus 1. In this case we will say that $\mathbb{P}$ has a trivial peripheral spectrum; it follows then that ω is exponentially clustering. For an ergodic finitely correlated state ω, it was shown in [6] that the peripheral spectrum is a cyclic group of p-th roots of unity. The state ω can then be written as an average over p p-periodic states of the chain. These periodic components can be considered as translation invariant states of a new chain for which the one site algebra is now obtained by grouping together p consecutive sites of the original chain. Considered as states of the regrouped chain these components are then exponentially clustering. Therefore it will be sufficient for our purposes to consider only the case where $\mathbb{P}$ has a trivial peripheral spectrum.

A finitely correlated state ω is called purely generated if the completely positive unity preserving map $\mathbb{E}$ is pure *i.e.* if there is an isometry $V : \mathbb{C}^k \to \mathbb{C}^d \otimes \mathbb{C}^k$ such that $\mathbb{E}(X) = V^* X V$ for all $X \in \mathcal{M}_d \otimes \mathcal{M}_k$.

It was shown in [6] that purely generated finitely correlated states with trivial peripheral spectrum are pure. Moreover, such a state can be characterized as the unique ground state of an associated translation invariant finite range Hamiltonian. In this situation the ground state energy is separated from the remaining energy spectrum by a non-zero gap [7].

2. ENTROPY ESTIMATES FOR FINITELY CORRELATED STATES

Any state ω of a quantum spin chain $\mathcal{A}_{\mathbb{Z}}$ is completely described in terms of a set of density matrices $\rho_{\{m, \ldots, n\}} \in \bigotimes_m^n \mathcal{M}_d$, such that

$$\omega(A) = \operatorname{Tr}(\rho_{\{m, \ldots, n\}} A) \quad \text{for all } A \in \mathcal{A}_{\{m, \ldots, n\}}.$$

The von Neumann entropy $S_{\{m, \ldots, n\}}$ of the state ω restricted to the volume $\{m, \ldots, n\} \subset \mathbb{Z}$ is then defined by:

$$S_{\{m, \ldots, n\}}(\omega) = -\operatorname{Tr}(\rho_{\{m, \ldots, n\}} \ln \rho_{\{m, \ldots, n\}}).$$

Another measure of the disorder in the state ω was introduced by Rényi [17]. For $q > 1$ the local Rényi entropy $R^q_{\{m, \ldots, n\}}(\omega)$ of order q is defined by:

$$R^q_{\{m, \ldots, n\}}(\omega) = \frac{1}{1-q} \ln \operatorname{Tr}((\rho_{\{m, \ldots, n\}})^q).$$

Remark that the von Neumann entropy $S_{\{m, \ldots, n\}}(\omega)$ is recovered by taking the limit of the Rényi entropies $R^q_{\{m, \ldots, n\}}(\omega)$ for $q \downarrow 1$. These quantities are well known in the context of dynamical systems where one studies the structure of the invariant measure ([8], [9], [11], [12]).

In statistical mechanics one is specially interested in translation invariant (or periodic) states, where one expects the entropies to be extensive quantities. For a general translation invariant state ω of $\mathcal{A}_{\mathbb{Z}}$ it is known that only the von Neumann entropy has sufficiently nice properties to guarantee the existence of its density $s(\omega)$ [5]:

$$s(\omega) = \lim_{n \to \infty} \frac{1}{2n+1} S_{\{-n, \ldots, n\}}(\omega).$$

The Rényi entropy densities $r_q(\omega)$ can be defined as:

$$r_q(\omega) = \limsup_{n \to \infty} \frac{1}{2n+1} R^q_{\{-n, \ldots, n\}}(\omega).$$

For finitely correlated states one can express the density in terms of the defining objects $(\mathbb{E}, \rho)$ of ω. We will mainly use the $r_q(\omega)$ as a technical tool to get lower bounds on the (von Neumann) entropy density of a finitely correlated state. Indeed, one has the following Proposition:

2.1. Proposition. – *Let ω be a translation invariant state of the chain algebra $\mathcal{A}_{\mathbb{Z}}$, then for $1 < q_1 < q_2$:*

$$r_{q_2}(\omega) \leqq r_{q_1}(\omega) \leqq s(\omega).$$

Proof. – Fix $n \in \mathbb{N}$ and let $\rho_{\{-n, \ldots, n\}}$ be the density matrix corresponding to the restriction $\omega_{\{-n, \ldots, n\}}$ of ω to $\mathcal{A}_{\{-n, \ldots, n\}}$. Let $\{r_i\}$ be the set of eigenvalues of $\rho_{\{-n, \ldots, n\}}$ repeated according to multiplicity. Obviously the r_i are non negative, add up to 1 and

$$R^q_{\{-n, \ldots, n\}}(\omega) = \frac{1}{1-q} \ln \sum_i r_i^q.$$

First we show that by Hölder's inequality:

$$R^{q_2}_{\{-n, \ldots, n\}}(\omega) \leqq R^{q_1}_{\{-n, \ldots, n\}}(\omega) \qquad \text{for} \quad 1 < q_1 < q_2. \tag{2.1}$$

Indeed,

$$\begin{aligned} \sum_i r_i^{q_1} &= \sum_i r_i^{q_2 (q_1 - 1)/(q_2 - 1)} r_i^{(q_2 - q_1)/(q_2 - 1)} \\ &\leqq \Big(\sum_i r_i^{q_2}\Big)^{(q_1 - 1)/(q_2 - 1)} \Big(\sum_i r_i\Big)^{(q_2 - q_1)/(q_2 - 1)} \\ &= \Big(\sum_i r_i^{q_2}\Big)^{(q_1 - 1)/(q_2 - 1)} \end{aligned}$$

and so (2.1) follows by taking logarithms. As:

$$S_{\{-n,\ldots,n\}}(\omega)=\lim_{q\downarrow 1} R^{q}_{\{-n,\ldots,n\}}(\omega),$$

we obtain:

$$R^{q_2}_{\{-n,\ldots,n\}}(\omega)\leqq R^{q_1}_{\{-n,\ldots,n\}}(\omega)\leqq S_{\{-n,\ldots,n\}}(\omega).$$

The Proposition follows by dividing this inequality by $2n+1$ and taking the lim sup. ■

Remark that the Proposition immediately extends to a general quasi-local quantum spin algebra. Instead of taking a limit for $n\to\infty$ one should then consider a limit in the sense of van Hove [13].

In the following we will consider the integral order Rényi entropy densities of a finitely correlated state ω generated by $(\mathbb{E},\rho)$. Let $\{A_1,\ldots,A_q\}$ be a set of trace class operators on an Hilbert space $\mathscr{H}$ and let $\{e_i\,|\,i=1,2,\ldots\}$ be an orthonormal basis for $\mathscr{H}$. First observe that for $q=2,3,\ldots$:

$$\begin{aligned}\mathrm{Tr}_{\mathscr{H}}(A_1\ldots A_q)&=\sum_i\langle e_i, A_1\ldots A_q e_i\rangle\\ &=\sum_{i_1,\ldots,i_q}\langle e_{i_1}, A_1 e_{i_2}\rangle\langle e_{i_2}, A_2 e_{i_3}\rangle\ldots\langle e_{i_q}, A_q e_{i_1}\rangle\\ &=\sum_{i_1,\ldots,i_q}\langle e_{i_1}\otimes\ldots e_{i_q}, A_1\otimes\ldots A_q e_{i_2}\otimes\ldots e_{i_q}\otimes e_{i_1}\rangle\\ &=\mathrm{Tr}_{\mathscr{H}\otimes\ldots\mathscr{H}}((A_1\otimes\ldots A_q)\Gamma)\end{aligned}\tag{2.2}$$

where $\Gamma:\varphi_1\otimes\ldots\varphi_q\mapsto\varphi_2\otimes\ldots\varphi_q\otimes\varphi_1$ is the cyclic shift to the left on $\mathscr{H}\otimes\ldots\mathscr{H}$. Applying this to a density matrix ρ corresponding to a state ω one gets:

$$\mathrm{Tr}(\rho^q)=\underbrace{\omega\otimes\ldots\omega}_{q}(\Gamma).\tag{2.3}$$

We will now use this relation to compute the integer Rényi entropies for finitely correlated states. In order to formulate the result we need the following notation: for $q=1,2,\ldots$ define

$$\mathbb{F}^{(q)}:\otimes^q\mathscr{M}_k\to\otimes^q\mathscr{M}_k : X\mapsto\mathbb{F}^{(q)}(X)=\mathbb{E}^{(q)}(\Gamma\otimes X)\tag{2.4}$$

with

$$\begin{gathered}\mathbb{E}^{(q)}:(\otimes^q\mathscr{M}_d)\otimes(\otimes^q\mathscr{M}_k)\to(\otimes^q\mathscr{M}_k):\\ X_1\otimes\ldots X_q\otimes Y_1\otimes\ldots Y_q\mapsto\mathbb{E}(X_1\otimes Y_1)\otimes\ldots\mathbb{E}(X_q\otimes Y_q).\end{gathered}$$

2.2. PROPOSITION. – *Let ω be a finitely correlated state generated by $(\mathbb{E},\rho)$, then for $q=2,3,\ldots$*

$$R^{q}_{\{1,\ldots,n\}}(\omega)=-\frac{1}{q-1}\ln(\otimes^q\rho)((\mathbb{F}^{(q)})^n(\otimes^q\mathbf{1}))$$

in particular

$$r_q(\omega) \geqq -\frac{1}{q-1} \ln \operatorname{spr}(\mathbb{F}^{(q)}), \tag{2.5}$$

where for a linear operator A, spr (A) *denotes the spectral radius of* A.

Proof. — Observe first that for $\Lambda \subset \mathbb{Z}$

$$\underbrace{\omega_\Lambda \otimes \ldots \omega_\Lambda}_{q} = \omega^{(q)} \big|_{\mathscr{A}_\Lambda}$$

where $\omega^{(q)}$ is a finitely correlated state on a product of q copies of the chain: $(\mathscr{M}_d \otimes \ldots \mathscr{M}_d)_\mathbb{Z} \cong \otimes^q \mathscr{A}_\mathbb{Z}$. The state $\omega^{(q)}$ is a product state on $\mathscr{A}_\mathbb{Z} \otimes \ldots \mathscr{A}_\mathbb{Z}$, generated by $(\mathbb{E}^{(q)}, \otimes^q \rho)$. According to (2.3) we have to compute $\omega^{(q)}(\Gamma_{\{1, \ldots, n\}})$ where $\Gamma_{\{1, \ldots, n\}} = \otimes_1^n \Gamma_i$. Here Γ_i is a copy of the cyclic shift on the $\mathbb{C}^d \otimes \ldots \mathbb{C}^d$ at the i-th site of the product chain. So, applying the defining formula (1.1) for finitely correlated states, we calculate the expectation value of $\Gamma_{\{1, \ldots, n\}}$:

$$\begin{aligned} R^q_{\{1, \ldots, n\}}(\omega) &= -\frac{1}{q-1} \ln \omega^{(q)}(\Gamma_{\{1, \ldots, n\}}) \\ &= -\frac{1}{q-1} \ln (\otimes^q \rho)((\mathbb{E}^{(q)}_\Gamma)^n (\otimes^q \mathbf{1})) \\ &= -\frac{1}{q-1} \ln (\otimes^q \rho)((\mathbb{F}^{(q)})^n (\otimes^q \mathbf{1})). \quad \blacksquare \end{aligned}$$

2.3. *Remark.* — *Generically* $\mathbb{F}^{(q)}$ *will only have a single eigenvector belonging to an eigenvalue with modulus equal to* spr$(\mathbb{F}^{(q)})$. *Let us denote by* $\psi_\mathrm{L}^{(q)}$ *and* $\psi_\mathrm{R}^{(q)}$ *the left and right eigenvectors of* $\mathbb{F}^{(q)}$ *corresponding to this eigenvalue.*

If $(\otimes^q \rho)(\psi_\mathrm{R}^{(q)}) \cdot \psi_\mathrm{L}^{(q)}(\otimes^q \mathbf{1}) \neq 0$ *then, as the Rényi entropy density is real, we must have that* spr$(\mathbb{F}^{(q)})$ *is an eigenvalue of* $\mathbb{F}^{(q)}$ *and we actually find that*

$$r_q(\omega) = -\frac{1}{q-1} \ln \operatorname{spr}(\mathbb{F}^{(q)}).$$

In order to prove that the situation described in Remark 2.3 generally holds one would use a result similar to the classical Perron-Frobenius theorem. In our case however, it is not immediately clear that the mappings $\mathbb{F}^{(q)}$ possess the necessary positivity. This lack of manifest positivity can already be traced back to formula (2.3). Since by Proposition 2.1 the Rényi entropy of order 2 gives the best bounds on $s(\omega)$ we shall be especially interested in this case. We show now that the situation described in the above remark indeed holds in this case.

2.4. THEOREM. — *Let* ω *be a finitely correlated state generated by* $(\mathbb{E}, \rho)$ *and suppose that* $\mathbb{F}^{(2)}$ *has only one eigenvalue of maximal modulus, then:*

$$r_2(\omega) = -\ln \operatorname{spr}(\mathbb{F}^{(2)})$$

Proof. — The theorem will follow from Proposition 2.2 if we show that $\operatorname{spr}(\mathbb{F}^{(2)})$ is an eigenvalue of $\mathbb{F}^{(2)}$ and if moreover the right and left eigenvectors of $\mathbb{F}^{(2)}$ have non-zero scalar products with $\rho \otimes \rho$ and $\mathbf{1}_k \otimes \mathbf{1}_k$. The left multiplication $A \in \mathcal{M}_k \otimes \mathcal{M}_k \mapsto FA$ by the flip F on $\mathbb{C}^k \otimes \mathbb{C}^k$ is a unitary transformation on $\mathcal{M}_k \otimes \mathcal{M}_k$ equipped with the tracial scalar product. It will be convenient to introduce the operator

$$T : \mathcal{M}_k \otimes \mathcal{M}_k \to \mathcal{M}_k \otimes \mathcal{M}_k : A \mapsto F\,\mathbb{F}^{(2)}(FA).$$

We can then express the $R^2_{\{1, \dots, n\}}$ as:

$$R^2_{\{1, \dots, n\}} = -\ln(\rho \otimes \rho\, F)\, T^n(F).$$

As $\mathbb{E}$ is a completely positive map there is a (finite) set V_α of linear mappings from $\mathbb{C}^k$ into $\mathbb{C}^d \otimes \mathbb{C}^k$ such that for $X \in \mathcal{M}_d \otimes \mathcal{M}_k$:

$$\mathbb{E}(X) = \sum_\alpha V_\alpha^* X V_\alpha.$$

Denoting as before by Γ the flip on $\mathbb{C}^d \otimes \mathbb{C}^d$ we then compute for $Y \in \mathcal{M}_k \otimes \mathcal{M}_k$:

$$\begin{aligned} T(Y) &= F\,\mathbb{F}^{(2)}(FY) \\ &= F\,\mathbb{E}^{(2)}(\Gamma \otimes FY) \\ &= \sum_{\alpha, \beta} F(V_\alpha^* \otimes V_\beta^*)(\Gamma \otimes F)(\mathbf{1}_d \otimes \mathbf{1}_d \otimes Y)(V_\alpha \otimes V_\beta) \\ &= \sum_{\alpha, \beta} (V_\beta^* \otimes V_\alpha^*)(\mathbf{1}_d \otimes \mathbf{1}_d \otimes Y)(V_\alpha \otimes V_\beta) \end{aligned} \tag{2.6}$$

Consider now in $\mathcal{M}_k \otimes \mathcal{M}_k$ the convex cone $\mathcal{K}$ generated by $\{X^* \otimes X \mid X \in \mathcal{M}_k\}$. By formula (2.6) $\mathcal{K}$ is mapped into itself by T.

Let $\{A_i, i = 1, \dots, k^2\}$ be an orthonormal basis for $\mathcal{M}_k$ equipped with the tracial scalar product $\langle A, B \rangle \equiv \operatorname{Tr}(A^* B)$. We then have that

$$F = \sum_{i=1}^{k^2} A_i \otimes A_i^*.$$

Indeed, if for φ, $\psi \in \mathbb{C}^k$ $|\varphi\rangle\langle\psi|$ denotes the rank 1 operator $\chi \in \mathbb{C}^k \mapsto \langle \psi, \chi \rangle \varphi$, we compute:

$$\begin{aligned} \langle \varphi_1 \otimes \varphi_2, \sum_i A_i^* \otimes A_i \psi_1 \otimes \psi_2 \rangle &= \sum_i \operatorname{Tr}(A_i^* \otimes A_i |\psi_1\rangle\langle\varphi_1| \otimes |\psi_2\rangle\langle\varphi_2|) \\ &= \sum_i \langle A_i, |\psi_1\rangle\langle\varphi_1| \rangle \langle |\varphi_2\rangle\langle\psi_2|, A_i \rangle \\ &= \langle |\varphi_2\rangle\langle\psi_2|, |\psi_1\rangle\langle\varphi_1| \rangle \\ &= \operatorname{Tr}(|\psi_2\rangle\langle\varphi_2, \psi_1\rangle\langle\varphi_1|) \\ &= \langle \varphi_1, \psi_2 \rangle \langle \varphi_2, \psi_1 \rangle \\ &= \langle \varphi_1 \otimes \varphi_2, \psi_2 \otimes \psi_1 \rangle \end{aligned}$$

But this implies that F is an order unit in $\mathcal{K}$.

Applying formula (2.2) we also have that:

$$\mathrm{Tr}((\rho \otimes \rho\, F)(X^* \otimes X)) = \mathrm{Tr}(\rho X^* \rho X).$$

This implies that the functional $Y \in \mathcal{M}_k \otimes \mathcal{M}_k \mapsto \mathrm{Tr}(\rho \otimes \rho\, FY)$ is in the dual of $\mathcal{K}$, and, as ρ was assumed to be faithful, $\mathrm{Tr}(\rho X^* \rho X)$ vanishes iff $X=0$. Therefore $Y \in \mathcal{M}_k \otimes \mathcal{M}_k \mapsto \mathrm{Tr}(\rho \otimes \rho\, FY)$ is also an order unit for the dual cone of $\mathcal{K}$.

From the Theorem of Krein and Rutman ([14], [18]), applied to the case of a finite dimensional space, it now immediately follows that $\mathrm{spr}(\mathbb{F}^{(2)})$ is an eigenvalue of $\mathbb{F}^{(2)}$. Furthermore as F and

$$Y \in \mathcal{M}_k \otimes \mathcal{M}_k \mapsto \mathrm{Tr}(\rho \otimes \rho\, FY)$$

are order units in $\mathcal{K}$ and its dual, it follows that both the right and left eigenvector of T have non-zero scalar products with these order units. ■

3. A QUANTUM SPIN MODEL WITH RESIDUAL ENTROPY

For quantum lattice systems one expects that generically the mean entropy of the equilibrium states converges to zero as the temperature T tends to zero. This is the Third Law of Thermodynamics. It has been known for a long time that there are special interactions that violate this property. The limiting entropy density as T tends to zero is called the residual entropy of the model. A non vanishing residual entropy is closely related to a high degeneracy of the ground states of the model. This was clearly shown in [2]. In classical spin systems the high degeneracy is caused by cancellations in the energy of many configurations due to a special choice of the coupling constants. This is related to the phenomenon of frustation [22]. The residual entropy is then usually determined by counting the ground states configurations ([16], [15], [19]).

Here we will consider a quantum spin chain with SU(2) invariant nearest neighbour interaction. We are not estimating the residual entropy by directly counting the ground state degeneracy. We will show instead that there exists a finitely correlated ground state for this model which has a non-zero mean entropy. This mean entropy is then a lower bound for the residual entropy. In fact we are not able to compute exactly the mean entropy of this finitely correlated state, but, using the results of the preceding section, we will get lower bounds. It is rather easy to obtain upper bounds.

We will heavily use the representation theory of SU(2). It is well known that all the irreducible unitary representations of SU(2) are finite dimensional and that there is exactly one for each dimension. Traditionally they are labelled by a half-integer: the spin $s=0,\ 1/2,\ 1,\ 3/2, \ldots,$ the dimension of the spin-s representation being $2s+1$. We will denote the spin-s irreducible representation by $\mathbf{D}^{(s)}$ *i.e.* for $g \in \mathrm{SU}(2)$, $\mathbf{D}^{(s)}(g)$ is the unitary in $\mathcal{M}_{2s+1}$ representing g. The generators of $\mathbf{D}^{(s)}$ will either be denoted by S^x, S^y, S^z or by the vector $\vec{\mathrm{S}}$. If $\varepsilon_{\alpha\beta\gamma}$ denotes the completely antisymmetric tensor with 3 elements and with $\varepsilon_{xyz}=1$, then the generators satisfy

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

and

$$\vec{\mathrm{S}}.\vec{\mathrm{S}} = \sum_\alpha (\mathrm{S}^\alpha)^2 = s(s+1)\mathbf{1}.$$

For j_1 and j_2 two half-integers the representation $\mathbf{D}^{(j_1)} \otimes \mathbf{D}^{(j_2)}$ is no longer irreducible; its reduction is given by the Clebsch-Gordon series:

$$\mathbf{D}^{(j_1)} \otimes \mathbf{D}^{(j_2)} \cong \mathbf{D}^{(|j_1-j_2|)} \oplus \mathbf{D}^{(|j_1-j_2|+1)} \oplus \ldots \mathbf{D}^{(j_1+j_2)}.$$

From this formula it follows that, up to a phase, there exists for each s such that $s \in \{|j_1-j_2|, |j_1-j_2|+1, \ldots j_1+j_2\}$ a unique intertwining isometry V:

$$\mathbf{D}^{(j_1)}(g) \otimes \mathbf{D}^{(j_2)}(g)\,\mathrm{V} = \mathrm{V}\,\mathbf{D}^{(s)}(g), \qquad g \in \mathrm{SU}(2).$$

The matrix elements of V are precisely the Clebsch-Gordon coefficients. As V is an isometry one has $\mathrm{V}^*\mathrm{V}=\mathbf{1}$ and $\mathrm{VV}^*=\mathrm{P}^{(s)}$ where $\mathrm{P}^{(s)}$ is the orthogonal projection on the subspace of $\mathbb{C}^{2j_1+1} \otimes \mathbb{C}^{2j_2+1}$ that carries the irreducible spin-s subrepresentation of $\mathbf{D}^{(j_1)} \otimes \mathbf{D}^{(j_2)}$. We will now consider a chain of spin-3/2 particles. So the corresponding algebra of observables is the C*-inductive limit of the $\bigotimes_{i \in \Lambda} \mathcal{M}_4$ for $\Lambda \subset \mathbb{Z}$, finite. The local Hamiltonians $\mathrm{H}_{\{m, \ldots, n\}}$, on an interval $\{m, \ldots, n\} \subset \mathbb{Z}$, are given by:

$$\mathrm{H}_{\{m, \ldots, n\}} = \sum_{i=m}^{n-1} \mathrm{P}^{(3)}_{i,i+1}$$

where $\mathrm{P}^{(3)}_{i,i+1}$ is the orthogonal projection onto the spin-3 subspace in $\mathbb{C}^4 \otimes \mathbb{C}^4$, sitting at the nearest neighbour points $i, i+1$. In terms of the generators $\vec{\mathrm{S}}$ this Hamiltonian reads:

$$\mathrm{P}^{(3)}_{i,i+1} = \frac{1}{5{,}760}(495 + 972\,\vec{\mathrm{S}}_i.\vec{\mathrm{S}}_{i+1} + 464\,(\vec{\mathrm{S}}_i.\vec{\mathrm{S}}_{i+1})^2 + 64\,(\vec{\mathrm{S}}_i.\vec{\mathrm{S}}_{i+1})^3).$$

We now first construct a finitely correlated state ω on the spin-3/2 chain by specifying an $\mathbb{E}$ and a ρ that satisfy the compatibility conditions. Consider the uniquely defined intertwining isometry V:

$$\mathbf{D}^{(3/2)} \otimes \mathbf{D}^{(1/2)} \otimes \mathbf{D}^{(1/2)}\,\mathrm{V} = \mathrm{V}\,\mathbf{D}^{(1/2)}$$

define

$$\left.\begin{array}{c}\mathbb{E}:\mathcal{M}_4\otimes\mathcal{M}_2\to\mathcal{M}_2\\ A\otimes B\mapsto\mathbb{E}(A\otimes B)=V^*(A\otimes \mathbf{1}_2\otimes B)V\end{array}\right\}\tag{3.1}$$

and choose for ρ the tracial state on $\mathcal{M}_2$, *i.e.* $\rho(B)=\frac{1}{2}\mathrm{Tr}(B)$. Then $\mathbb{E}(\mathbf{1})=V^*V=\mathbf{1}$ because V is an isometry, and by SU(2) invariance ρ is the unique state on $\mathcal{M}_2$ that satisfies $\rho(B)=\rho(\mathbb{E}_{\mathbf{1}}(B))$.

As the interaction is of finite range we have the well-known result that the local Hamiltonians define a strongly continuous group of automorphisms with generator δ given on local observables by:

$$\delta(X)=\lim_{\Lambda\to\mathbb{Z}}[H_\Lambda, X],\qquad X\in\mathcal{A}_\Lambda,\ \Lambda \text{ finite}.$$

A not necessarily translation invariant state ω of $\mathcal{A}_{\mathbb{Z}}$ is called a ground state of the model if it satisfies:

$$\omega(X^*\delta(X))\geqq 0\quad \text{for all } X\in \mathrm{Dom}(\delta).\tag{3.2}$$

We will show that the finitely correlated state ω determined by the $\mathbb{E}$ and ρ specified above is a ground state of the model in a stronger sense, namely:

$$\omega(P^{(3)}_{i,i+1})=0\quad \text{for all } i\in\mathbb{Z}.\tag{3.3}$$

It is then immediate by the positivity of the interaction that ω is also a ground state of the Hamiltonian in the sense of (3.2). According to the construction of finitely correlated states (1.1) we compute the expectation value of an elementary tensor X_iX_{i+1} of two single site observables living on the nearest neighbour sites $\{i, i+1\}$ as:

$$\omega(X_iX_{i+1})=\frac{1}{2}\mathrm{Tr}_{\mathbb{C}^2}(V^*(\mathbf{1}_4\otimes\mathbf{1}_2\otimes V^*)$$
$$((X_i\otimes\mathbf{1}_2)\otimes(X_{i+1}\otimes\mathbf{1}_2)\otimes\mathbf{1}_2)((\mathbf{1}_4\otimes\mathbf{1}_2\otimes V)V)).\tag{3.4}$$

The range of $(\mathbf{1}_4\otimes\mathbf{1}_2\otimes V)V$ is a two dimensional rotation invariant subspace of $\mathcal{H}=\mathbb{C}^4\otimes\mathbb{C}^2\otimes\mathbb{C}^4\otimes\mathbb{C}^2\otimes\mathbb{C}^2$, that carries a $\mathbf{D}^{(1/2)}$ representation by the intertwining property of V. By the Clebsch-Gordon series the representation $\mathbf{D}^{(3/2)}\otimes\mathbf{D}^{(3/2)}$ on the first and third factors of $\mathcal{H}$ decomposes into a direct sum of irreducible spin 0, 1, 2 and 3 representations. In order to get a non vanishing expectation of $P^{(3)}_{i,i+1}$ the subspace of $\mathcal{H}$ carrying the $\mathbf{D}^{(3)}\otimes\mathbf{D}^{(1/2)}\otimes\mathbf{D}^{(1/2)}\otimes\mathbf{D}^{(1/2)}$ representation should contain a spin-1/2 subspace. This is not the case, which proves (3.3).

Formula (3.1) also shows that ω can be seen as the restriction of a finitely correlated state ω_0 on a double chain. This chain has at each site a spin-3/2 and a spin-1/2 particle, *i.e.* the one site algebra is $\mathcal{M}_4\otimes\mathcal{M}_2$. The finitely correlated state ω_0 on the double chain is generated by $(\mathbb{E}_0, \rho)$

where

$$\mathbb{E}_0(X) = V^* X V \qquad \text{for} \quad X \in \mathcal{M}_4 \otimes \mathcal{M}_2 \otimes \mathcal{M}_2$$

with the same isometry V as in (3.1). We will show in Proposition 3.2 that, if $\mathbb{P}_0$ denotes the completely positive map $X \mapsto \mathbb{E}_0(\mathbf{1}_4 \otimes \mathbf{1}_2 \otimes X)$ from $\mathcal{M}_2$ into itself:

$$\mathbb{P}_0(\mathbf{1}) = \mathbf{1}, \qquad \text{and} \qquad \mathbb{P}_0(\vec{\mathbf{J}}) = -\frac{1}{3}\vec{\mathbf{J}}.$$

where $\vec{\mathbf{J}}$ are the generators of the spin-1/2 representation. From the general results on finitely correlated states it then follows that ω_0 is pure. We have now the following situation: ω_0 is a pure state on a product algebra $\mathcal{A}_1 \otimes \mathcal{A}_2$, where $\mathcal{A}_1 = (\mathcal{M}_4)_{\mathbb{Z}}$ and $\mathcal{A}_2 = (\mathcal{M}_2)_{\mathbb{Z}}$, and we are interested in studying the mean entropy of the restriction of ω_0 to $\mathcal{A}_1$. The following Lemma shows that we can as well study the mean entropy of the restriction of ω_0 to $\mathcal{A}_2$. This will be of interest because the dimension of the local algebras for that subchain is much smaller.

3.1. LEMMA. – *Let for* $i = 1, 2$ $\mathcal{A}_i = (\mathcal{M}_{d_i})_{\mathbb{Z}}$ *and let* ω *be a translation invariant state of* $\mathcal{A}_{12} = \mathcal{A}_1 \otimes \mathcal{A}_2 = (\mathcal{M}_{d_1} \otimes \mathcal{M}_{d_2})_{\mathbb{Z}}$. *Denote by* ω_1*and* ω_2 *the restrictions of* ω *to* $\mathcal{A}_1$ and $\mathcal{A}_2$. *Then*

$$|s(\omega_1) - s(\omega_2)| \leqq s(\omega).$$

In particular, if $s(\omega) = 0$ *then* $s(\omega_1) = s(\omega_2)$.

Proof. – Consider first a finite subset $\Lambda \subset \mathbb{Z}$. It is always possible to find a matrix algebra $\mathcal{B}$ and a pure state σ of $\mathcal{A}_{1,\Lambda} \otimes \mathcal{A}_{2,\Lambda} \otimes \mathcal{B}$ such that the restrictions of σ and ω to $\mathcal{A}_{1,\Lambda} \otimes \mathcal{A}_{2,\Lambda}$ coincide. Here $\mathcal{A}_{1,\Lambda}$ and $\mathcal{A}_{2,\Lambda}$ denote the algebras of observables in the volume Λ of the subchains 1 and 2. By the strong subadditivity property of the entropy [5]:

$$S(\sigma) + S(\sigma|_{\mathcal{A}_{1,\Lambda}}) \leqq S(\sigma|_{\mathcal{A}_{1,\Lambda} \otimes \mathcal{A}_{2,\Lambda}}) + S(\sigma|_{\mathcal{A}_{1,\Lambda} \otimes \mathcal{B}})$$

Now we have also that:

$$S(\sigma) = 0 \text{ because } \sigma \text{ is pure}$$
$$S(\sigma|_{\mathcal{A}_{1,\Lambda}}) = S(\omega_{1,\Lambda})$$
$$S(\sigma|_{\mathcal{A}_{1,\Lambda} \otimes \mathcal{B}}) = S(\sigma|_{\mathcal{A}_{2,\Lambda}}) = S(\omega_{2,\Lambda}) \text{ because } \sigma \text{ is pure.}$$

Indeed, the restrictions of a pure state on a tensor product of two matrix algebras to each of the factors are given by density matrices that have the same eigenvalues taking multiplicities into account, except possibly for the eigenvalue zero. So

$$S(\omega_{1,\Lambda}) - S(\omega_{2,\Lambda}) \leqq S(\omega_\Lambda).$$

Obviously the roles of 1 and 2 are interchangeable. Therefore:

$$|S(\omega_{1,\Lambda}) - S(\omega_{2,\Lambda})| \leqq S(\omega_\Lambda).$$

Dividing by $|\Lambda|$ and taking the limit we obtain the result. ■

Just like Proposition 2.1 this Lemma and its proof immediately generalize to a general quasi-local algebra.

In our situation we have $\mathscr{A}_1=(\mathscr{M}_4)_{\mathbb{Z}}$, $\mathscr{A}_2=(\mathscr{M}_2)_{\mathbb{Z}}$ and the finitely correlated state ω on $\mathscr{A}_1$ which was defined in (3.1) in terms of $(\mathbb{E}, \rho)$ equals $\omega_0|_{\mathscr{A}_1}$ where ω_0 is a pure finitely correlated state. We can therefore apply Lemma 3.1 and we get immediately a dimensional upper bound on $s(\omega)$:

$$s(\omega)=s(\omega_0|_{\mathscr{A}_2})\leqq \ln 2=0.69...$$

In the following Proposition we derive a lower bound for $s(\omega)$, together with a slightly sharper upper bound.

3.2. Proposition:

$$0.654...=-\ln\frac{5+\sqrt{19}}{18}\leqq s(\omega)\leqq \frac{5}{3}\ln 3-\frac{2}{3}\ln 2=0.685...$$

Before entering the proof we state a basic formula for intertwining isometries between representations of SU(2), which will be used repeatedly.

3.3. Lemma. – *Let s, j, j' be (half-) integers with $s+j+j'\in\mathbb{N}$ and $|j-j'|\leqq s\leqq(j+j')$, and let $\mathrm{W}:\mathbb{C}^{2s+1}\to\mathbb{C}^{2j+1}\otimes\mathbb{C}^{2j'+1}$ be the up to a phase unique isometry intertwining $\mathbf{D}^{(s)}$ and $\mathbf{D}^{(j)}\otimes\mathbf{D}^{(j')}$. Let $\vec{\mathbf{S}}$, $\vec{\mathbf{J}}$, $\vec{\mathbf{J}}'$ denote the generators of these representations. Then*

$$(\vec{\mathbf{J}}\otimes\vec{\mathbf{J}}')\mathrm{W}\equiv\sum_{\alpha}(\mathrm{J}^{\alpha}\otimes\mathrm{J}'^{\alpha})\mathrm{W}=\frac{1}{2}\{s(s+1)-j(j+1)-j'(j'+1)\}\mathrm{W}$$

and

$$\mathrm{W}^*(\vec{\mathbf{J}}\otimes\mathbf{1})\mathrm{W}=\lambda\vec{\mathrm{S}}\qquad \textit{with}\quad \lambda=\frac{1}{2}+\frac{1}{2s(s+1)}\{j(j+1)-j'(j'+1)\}.$$

Proof. – By the intertwining property $(\vec{\mathbf{J}}\otimes\mathbf{1}+\mathbf{1}\otimes\vec{\mathbf{J}}')^2\mathrm{W}=\mathrm{W}\vec{\mathbf{S}}^2$. The first relation follows by solving this equation for the mixed term in the expansion of the square on the left hand side. Since $\mathrm{W}^*(\vec{\mathbf{J}}\otimes\mathbf{1})\mathrm{W}$ is a vector operator in $\mathbf{D}^{(s)}$, it must be proportional to $\vec{\mathbf{S}}$. The constant λ is computed from the relation

$$\lambda\vec{\mathbf{S}}^2=\mathrm{W}^*(\vec{\mathbf{J}}\otimes\mathbf{1})\mathrm{W}\vec{\mathbf{S}}=\mathrm{W}^*(\vec{\mathbf{J}}\otimes\mathbf{1})(\vec{\mathbf{J}}\otimes\mathbf{1}+\mathbf{1}\otimes\vec{\mathbf{J}}')\mathrm{W}.\quad ■$$

Proof of 3.2. – In order to obtain the lower and upper bounds we will have to compute some n-point functions of the state. By Lemma 3.1 we can restrict our attention to the spin-1/2 subchain and this will considerably simplify explicit computations.

Consider first the unique isometries:

$$\mathrm{V}_1:\mathbb{C}^2\to\mathbb{C}^4\otimes\mathbb{C}^3\qquad\text{and}\qquad \mathrm{V}_2:\mathbb{C}^3\to\mathbb{C}^2\otimes\mathbb{C}^2$$

intertwining the SU(2) representations $\mathbf{D}^{(1/2)}$ with $\mathbf{D}^{(3/2)} \otimes \mathbf{D}^{(1)}$ and $\mathbf{D}^{(1)}$ with $\mathbf{D}^{(1/2)} \otimes \mathbf{D}^{(1/2)}$, respectively. Then the isometry $V = (\mathbf{1} \otimes V_2) V_1$ intertwines $\mathbf{D}^{(1/2)}$ with $\mathbf{D}^{(3/2)} \otimes \mathbf{D}^{(1/2)} \otimes \mathbf{D}^{(1/2)}$, and must therefore coincide with the operator V of formula (3.1). We will denote by $\vec{\mathbf{J}}$, $\vec{\mathbf{K}}$ and $\vec{\mathbf{S}}$ the generators of the representations $\mathbf{D}^{(1/2)}$, $\mathbf{D}^{(1)}$ and $\mathbf{D}^{(3/2)}$ respectively. We now apply Lemma 3.3, first to V_2 with $(s, j, j') = \left(1, \frac{1}{2}, \frac{1}{2}\right)$, and then to V_1 with $(s, j, j') = \left(\frac{1}{2}, \frac{3}{2}, 1\right)$, to compute

$$\mathbb{E}_0(X) = V_1^* (\mathbf{1}_4 \otimes V_2)^* X (\mathbf{1}_4 \otimes V_2) V_1$$

for some X. We need:

$$\mathbb{E}_0(\mathbf{1}_4 \otimes \mathbf{1}_2 \otimes \vec{\mathbf{J}}) = \mathbb{E}_0(\mathbf{1}_4 \otimes \vec{\mathbf{J}} \otimes \mathbf{1}_2) = -\frac{1}{3}\vec{\mathbf{J}} \tag{3.5}$$

$$\mathbb{E}_0(\mathbf{1}_4 \otimes \vec{\mathbf{J}} \otimes \vec{\mathbf{J}}) = \frac{1}{4}\mathbf{1}_2 \tag{3.6}$$

$$\mathbb{E}_0(\mathbf{1}_4 \otimes J^{\alpha} \otimes J^{\beta}) = \frac{1}{12}\delta_{\alpha,\beta}\mathbf{1}_2. \tag{3.7}$$

Here (3.7) follows from (3.6) and the observation that the range of V_2 is the symmetric subspace of $\mathbb{C}^2 \otimes \mathbb{C}^2$.

The **upper bound** for $s(\omega)$ will be obtained by computing the entropy of the restriction $\rho_{\{1,2\}}$ of the state of the spin-1/2 chain on a pair of neighbouring sites. Indeed, as the mean entropy is given by the infimum of the local mean entropies [5]: $s(\omega) \leqq \frac{1}{2} S(\rho_{\{1,2\}})$. By rotation invariance it is obvious that $\rho_{\{1,2\}}$ is of the form:

$$\rho_{\{1,2\}} = r_0 P^{(0)} + r_1 P^{(1)}$$

where $P^{(0)}$ and $P^{(1)}$ denote the orthogonal projections on the spin-0 and spin-1 subspaces of $\mathbb{C}^2 \otimes \mathbb{C}^2$ respectively. The entropy is then given by:

$$S(\rho_{\{1,2\}}) = -(r_0 \ln r_0 + 3 r_1 \ln r_1).$$

In order to compute r_0 and r_1 we write:

$$\begin{aligned} r_0 = \rho_{\{1,2\}}(P^{(0)}) &= \rho_{\{1,2\}}\left(\frac{1}{4}\mathbf{1} - \vec{\mathbf{J}} \otimes \vec{\mathbf{J}}\right) \\ &= \frac{1}{4} - \rho_{\{1,2\}}(\vec{\mathbf{J}} \otimes \vec{\mathbf{J}}). \end{aligned}$$

Then, by normalization $r_1 = \frac{1}{3}(1-r_0)$. So we need to calculate

$$\begin{aligned}\rho_{\{1,2\}}(\vec{\mathbf{J}}\otimes\vec{\mathbf{J}}) &= \omega_0((\mathbf{1}_4\otimes\vec{\mathbf{J}})\otimes(\mathbf{1}_4\otimes\vec{\mathbf{J}}))\\ &= \frac{1}{2}\operatorname{Tr}(\mathbb{E}_0(\mathbf{1}_4\otimes\vec{\mathbf{J}}\otimes\mathbb{E}_0(\mathbf{1}_4\otimes\vec{\mathbf{J}}\otimes\mathbf{1}_2)))\\ &= \frac{1}{2}\cdot\frac{-1}{3}\operatorname{Tr}(\mathbb{E}_0(\mathbf{1}_4\otimes\vec{\mathbf{J}}\otimes\vec{\mathbf{J}}))\\ &= -\frac{1}{12}.\end{aligned}$$

Hence $r_0 = \frac{1}{3}$ and $r_1 = \frac{2}{9}$. Therefore:

$$S(\rho_{\{1,2\}}) = \frac{5}{3}\ln 3 - \frac{2}{3}\ln 2.$$

To obtain the **lower bound** we compute $r_2(\omega)$ using Theorem 2.4 and then apply Proposition 2.1. In terms of the generators $\vec{\mathbf{J}}$ the flip F on $\mathbb{C}^2\otimes\mathbb{C}^2$ is given by:

$$F = \frac{1}{2}\mathbf{1}_2\otimes\mathbf{1}_2 + 2\vec{\mathbf{J}}\otimes\vec{\mathbf{J}}.$$

The state ω restricted to the spin-1/2 chain is a finitely correlated state given by $(\mathbb{E}_2, \rho)$, where:

$$\mathbb{E}_2 : \mathcal{M}_2\otimes\mathcal{M}_2 \to \mathcal{M}_2 : X\otimes Y \mapsto \mathbb{E}_0(\mathbf{1}_4\otimes X\otimes Y).$$

We have now to compute the spectral radius of

$$\mathbb{F}_2^{(2)} : \mathcal{M}_2\otimes\mathcal{M}_2 \to \mathcal{M}_2\otimes\mathcal{M}_2.$$

Due to rotation invariance we can restrict our attention to the subspace of rotation invariant operators. As a basis in this space we choose $\mathbf{1}_2\otimes\mathbf{1}_2$ and $\vec{\mathbf{J}}\otimes\vec{\mathbf{J}}$.

$$\begin{aligned}\mathbb{F}_2^{(2)}(\mathbf{1}_2\otimes\mathbf{1}_2) &= \mathbb{E}\otimes\mathbb{E}(\mathbf{1}_4\otimes\mathbf{1}_4\otimes F\otimes\mathbf{1}_2\otimes\mathbf{1}_2)\\ &= \mathbb{E}\otimes\mathbb{E}\left(\mathbf{1}_4\otimes\mathbf{1}_4\otimes\left(\frac{1}{2}\mathbf{1}_2\otimes\mathbf{1}_2 + 2\vec{\mathbf{J}}\otimes\vec{\mathbf{J}}\right)\otimes\mathbf{1}_2\otimes\mathbf{1}_2\right)\\ &= \frac{1}{2}\mathbf{1}_2\otimes\mathbf{1}_2 + 2V^*(\mathbf{1}_4\otimes\vec{\mathbf{J}}\otimes\mathbf{1}_2)V\otimes V^*(\mathbf{1}_4\otimes\vec{\mathbf{J}}\otimes\mathbf{1}_2)V\\ &= \frac{1}{2}\mathbf{1}_2\otimes\mathbf{1}_2 + \frac{2}{9}\vec{\mathbf{J}}\otimes\vec{\mathbf{J}}\end{aligned}$$

where we have used (3.5). In a similar way:

$$\begin{aligned}\mathbb{F}_2^{(2)}(\vec{\mathbf{J}}\otimes\vec{\mathbf{J}}) &= \frac{1}{2}V^*(\mathbf{1}_4\otimes\mathbf{1}_2\otimes\vec{\mathbf{J}})V\otimes V^*(\mathbf{1}_4\otimes\mathbf{1}_2\otimes\vec{\mathbf{J}})V\\ &= 2\sum_{\alpha,\beta}V^*(\mathbf{1}_4\otimes J^\alpha\otimes J^\beta)V\otimes V^*(\mathbf{1}_4\otimes J^\alpha\otimes J^\beta)V\\ &= \frac{1}{18}\vec{\mathbf{J}}\otimes\vec{\mathbf{J}}+\frac{1}{24}\mathbf{1}_2\otimes\mathbf{1}_2.\end{aligned}$$

Therefore the spectral radius of $\mathbb{F}_2^{(2)}$ is the largest eigenvalue of:

$$\begin{pmatrix}1/2 & 2/9\\ 1/24 & 1/18\end{pmatrix}$$

which is $\dfrac{5+\sqrt{19}}{18}$. ■

Finally, we show how a small perturbation of the Hamiltonian destroys the ground state degeneracy. Let H^s denote the "staggered" perturbation operator

$$H^s_{\{m,\ldots,n\}}=\sum_{i=m;\, i\text{ even}}^{n-1}P^{(2)}_{i,i+1}.$$

This interaction is not translation invariant but only periodic with period 2, but it is fully SU(2)-invariant. Then we claim that for all positive ε the interaction $H^\varepsilon=H+\varepsilon H^s$ has a unique ground state ω^s with a spectral gap, and that the gap with go to zero as $\varepsilon\to 0$. It will be clear from the construction that ω^s is also a ground state for the original Hamiltonian H.

We shall construct ω^s as a finitely correlated state with period 2. For this we need two completely positive unit preserving maps

$$\mathbb{E}^+:\mathcal{A}\otimes\mathcal{M}_2\to\mathcal{M}_3\qquad\text{and}\qquad\mathbb{E}^-:\mathcal{A}\otimes\mathcal{M}_3\to\mathcal{M}_2.$$

We also need a state ρ^+ on $\mathcal{M}_2$ and a state ρ^- on $\mathcal{M}_3$ such that $\rho^\pm\,\mathbb{E}^\pm(\mathbf{1}\otimes X)=\rho^\mp(X)$. As usual we shall write $\mathbb{E}^\sigma_X(Y)=\mathbb{E}^\sigma(X\otimes Y)$. The formula for the state analogous to (1.1) is then

$$\omega(X_m\otimes X_{m+1}\otimes\ldots X_n)=\rho^{\sigma(m)}(\mathbb{E}^{\sigma(m)}_{X_m}\circ\mathbb{E}^{\sigma(m+1)}_{X_{m+1}}\circ\ldots\mathbb{E}^{\sigma(n)}_{X_n}(\mathbf{1})),\quad(3.8)$$

where $\sigma(i)=(-1)^i$. We shall take $\mathbb{E}^\pm(X)=V^*_\pm XV_\pm$, where $V_\pm$ are intertwining isometries between the respective representations of SU(2), and let $\rho^\pm$ be the unique rotation invariant states, *i.e.* the normalized traces in $\mathcal{M}_2$ and $\mathcal{M}_3$. When i is even we have

$$\omega(X_i\otimes X_{i+1})=\rho^+(V^*_+(\mathbf{1}_4\otimes V^*_-)(X_i\otimes X_{i+1}\otimes\mathbf{1}_2)(\mathbf{1}_4\otimes V_-)V_+).$$

As before we conclude that $(P^{(2)}\otimes\mathbf{1}_2\otimes\mathbf{1}_2)(\mathbf{1}_4\otimes V_-)V_+$ must vanish, since otherwise this operator would be a non-zero intertwiner between $\mathbf{D}^{(1/2)}$ and $\mathbf{D}^{(2)}\otimes\mathbf{D}^{(1/2)}$. It follows that ω^s is a ground state of $H+\varepsilon H^s$ in the same strong sense as ω is a ground state for H. The uniqueness of this ground state, and the fact that it has a gap follow from the general theory in [6]. To apply this theory one merely has to note that the two-step transition operator $\mathbb{E}^{+-}: X_1 \otimes X_2 \otimes Y \mapsto \mathbb{E}^+ (X_1 \otimes \mathbb{E}^- (X_2 \otimes Y))$ is generated by the isometry $(\mathbf{1}_4 \otimes V_-) V_+$ so that the state ω^s is "purely generated". One also has to check that the eigenvalue 1 of $\mathbb{E}_{\mathbf{1}}^{+-} = \mathbb{P}^{+-}$ is the only one of modulus 1. We do this by computing the decay constant of the correlation functions of ω^s. These are determined by the powers of $\mathbb{P}^{+-}$, which can be computed in the basis $\{\mathbf{1}, \vec{\mathbf{J}}\}$ of $\mathcal{M}_2$. By rotation invariance it suffices to compute the constant μ such that $\mathbb{P}^{+-}(\vec{\mathbf{J}}) = \mu \vec{\mathbf{J}}$, and to show that $|\mu| < 1$. From Lemma 3.3 we immediately get $\mu = \frac{1}{6}$. Recall that the decay constant of ω was $-\frac{1}{3}$, meaning $\frac{1}{9}$ for two step transitions. Hence the correlations in the pure ground state ω^s go to zero slightly less rapidly than in the highly degenerate ground state ω.

As the ground state ω^s of H^s is non-degenerate we can obtain the spectral gap $\gamma_0(\varepsilon)$ as the least $\gamma \geqq 0$ such that for all local observables X:

$$\omega^s (X^* [H^\varepsilon, X]) \leqq \gamma (\omega^s (X^* X) - |\omega^s (X)|^2)$$

By making an explicit choice for the X we will obtain an upper bound for $\gamma_0(\varepsilon)$. More specifically we will estimate $\gamma_0(\varepsilon)$ by studying the spin-wave spectrum of H^ε, *i.e.* we choose

$$X_N(q) = \frac{1}{\sqrt{N}} \sum_{j=-N}^{N} e^{iqj} S_j^z.$$

As $\omega^s(\vec{S}) = 0$ and $\omega^s(X H^\varepsilon_{\{m, \ldots, n\}}) = 0$ for all observables X we obtain the estimate:

$$\gamma_0(\varepsilon) \leqq \inf_q \lim_{N \to \infty} \frac{\omega^s (X_N^*(q) H^\varepsilon X_N(q))}{\omega^s (X_N^*(q) X_N(q))}$$

We now compute the limits of the numerator and denominator:

$$\begin{aligned}\lim_{N \to \infty} \omega^s (X_N^*(q) X_N(q)) &= \omega^s ((S_0^z)^2) + \omega^s ((S_1^z)^2) \\ &\quad + \sum_{j=1}^{\infty} e^{2ijq} (\omega^s (S_0^z S_{2j}^z) + \omega^s (S_1^z S_{2j+1}^z)) + \text{h.c.} \\ &\quad + \sum_{j=1}^{\infty} e^{i(2j-1)q} (\omega^s (S_0^z S_{2j-1}^z) + \omega^s (S_1^z S_{2j}^z)) + \text{h.c.}\end{aligned}$$

The sums can be evaluated using the following results for the two-point correlation function, which can be obtained by applying Lemma 3.3: for

$j>0$

$$\omega^s(S_0^\alpha S_0^\beta)=\omega^s(S_1^\alpha S_1^\beta)=\frac{5}{4}\delta_{\alpha,\beta}$$

$$\omega^s(S_0^\alpha S_{2j-1}^\beta)=-\frac{25}{216}\left(\frac{1}{6}\right)^j$$

$$\omega^s(S_0^\alpha S_{2j}^\beta)=\frac{25}{32}\left(\frac{1}{6}\right)^j$$

$$\omega^s(S_1^\alpha S_{2j}^\beta)=-\frac{25}{144}\left(\frac{1}{6}\right)^j$$

$$\omega^s(S_1^\alpha S_{2j+1}^\beta)=\frac{50}{9}\left(\frac{1}{6}\right)^j$$

The denominator then becomes

$$\frac{34\,485+19\,890\cos 2q-1\,250\cos q}{432\,(37-12\cos 2q)}$$

For the numerator one gets

$$\lim_{N\to\infty}\omega^s(X_N^*(q)\,H^\varepsilon X_N(q))=\frac{7}{24}(1-\cos q)+\varepsilon\left(\frac{35}{72}-\frac{5}{72}\cos q\right)$$

Taking $q=0$ we obtain

$$\gamma_0(\varepsilon)\leqq\frac{36}{425}\varepsilon$$

which shows that the gap disappears when $\varepsilon\downarrow 0$.

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REFERENCES

[1] L. Accardi and A. Frigerio, Markovian Cocycles, *Proc. R. Ir. Acad.*, Vol. **83A**, (2), 1983, pp. 251-263.

[2] M. AIZENMAN and E. H. LIEB, The third law of thermodynamics and the degeneracy of the ground state for lattice systems, *J. Stat. Phys.*, Vol. **24**, 1981, pp. 279-297.
[3] I. AFFLECK and E. H. LIEB, A proof of part of Haldane's conjecture on quantum spin chains, *Lett. Math. Phys.*, Vol. **12**, 1986, pp. 57-69.
[4] I. AFFLECK, T. KENNEDY, E. H. LIEB and H. TASAKI, Valence bond ground states in isotropic quantum antiferromagnets, *Commun. Math. Phys.*, Vol. **115**, 1988, pp. 477-528.
[5] O. BRATTELI and D. W. ROBINSON, *Operator algebras and quantum statistical mechanics*, 2 volumes, Springer Verlag, Berlin, Heidelberg, New York 1979 and 1981.
[6] M. FANNES, B. NACHTERGAELE and R. F. WERNER, Finitely correlated states of quantum spin chains, *Commun. Math. Phys.*, Vol. **144**, 1992, pp. 443-490.
[7] M. FANNES, B. NACHTERGAELE and R. F. WERNER, Valence bond states on quantum spin chains as ground states with spectral gap, *J. Phys. A*, Vol. **24**, 1991, pp. L185-L190.
[8] P. GRASSBERGER and I. PROCACCIA, Measuring the strangeness of strange attractors, *Physica*, Vol. **9D**, 1983, pp. 189-205.
[9] P. GRASSBERGER and I. PROCACCIA, Dimensions and entropies of strange attractors from a fluctuating dynamics point of view, *Physica*, Vol. **13D**, 1984, pp. 34-54.
[10] F. D. M. HALDANE, Continuum dynamics of the 1-D Heisenberg antiferromagnet: identification with the O(3) nonlinear sigma model, *Phys. Lett.*, Vol. **93A**, 1983, pp. 464-468.
[11] T. C. HALSEY, M. H. JENSEN, L. P. KADANOFF, I. PROCACCIA and B. I. SHRAIMAN, Fractal measures and their singularities: the characterization of strange sets, *Phys. Rev.*, Vol. **33A**, 1986, pp. 1141-1151.
[12] H. G. E. HENTSCHEL and I. PROCACCIA, The infinite number of generalized dimensions of fractals and strange attractors, *Physica*, Vol. **8D**, 1983, pp. 435-444.
[13] L. VAN HOVE, Quelques propriétés générales de l'intégrale de configuration d'un système de particules avec interaction, *Physica*, Vol. **15**, 1949, pp. 951-961.
[14] M. G. KREĬN and M. A. RUTMAN, Linear operators leaving invariant a cone in a Banach space, *Transl. Am. Math. Soc. Series* 1, Vol. **10**, 1966, pp. 199-325.
[15] B. NACHTERGAELE and L. SLEGERS, The ground state and its entropy for a class of one dimensional classical lattice systems, *Physica*, Vol. **149A**, 1988, pp. 432-446.
[16] S. REDNER, One-dimensional Ising chain with competing interactions: exact results and connection with other statistical models, *J. Stat. Phys.*, Vol. **25**, 1981, pp. 15-23.
[17] A. RÉNYI, On measures of entropy and information, *Proc. 4th Berkeley Symp. Math. Statist. Prob.*, 1960, University of California Press Berkeley, 1961.
[18] H. H. SCHAEFER, *Topological vector spaces*, Springer-Verlag, New York, Heidelberg, Berlin, 1971.
[19] L. SLEGERS, The residual entropy for a class of one-dimensional lattice models, *J. Phys.*, Vol. **21A**, 1988, pp. 3489-3500.
[20] W. F. STINESPRING, Positive functions on C*-algebras, *Proc. Amer. Math. Soc.*, Vol. **6**, 1955, pp. 211-216.
[21] E. STØRMER, Positive maps of C*-algebras, in A. HARTKÄMPER, and H. NEUMANN Eds., *Foundations of quantum mechanics and ordered linear spaces*, Lecture Notes in Physics 29, Springer Verlag, Berlin, Heidelberg, New York, 1974.
[22] G. TOULOUSE, Theory of the frustration effect in spin glasses: I, *Commun. Phys.*, Vol. **2**, 1977, pp. 115-119.

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