DIAS-STP-89-22

Exact Antiferromagnetic Ground States of Quantum Spin Chains

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Abstract: We recall a simple class of translation invariant states for an infinite quantum spin chain, which was introduced by L.Accardi. Those states have exponential decay of correlation functions, and a subclass contains the ground states of a certain class of finite range interactions. We consider, in particular, a family of states for integer spin chains, containing as its simplest member the ground state of a spin 1 Heisenberg antiferromagnet recently studied by I.Affleck, T.Kennedy, E.H.Lieb, and H.Tasaki. For this family we compute explicitly the correlation functions and other properties.

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We consider an infinite chain of quantum mechanical systems of spin J. This is to say that the systems are labelled by sites n= ...,−1,0,1,... , and the observables of the system at each site are given by the algebra $\mathcal{M}_{2J+1}$ of (2J+1)x(2J+1) matrices. A state of the chain assigns an expectation value $\langle X_n\otimes\ldots\otimes X_{n+m}\rangle$ to the observables $X_n,\ldots,X_{n+m}$, where X_i is an observable at site i. This assignment has to satisfy the positivity condition $\langle A^*A\rangle\geq 0$, the consistency condition

$$\langle X_n\otimes\ldots\otimes X_{n+m}\rangle = \langle 1_{n-1}\otimes X_n\otimes\ldots\otimes X_{n+m}\rangle = \langle X_n\otimes\ldots\otimes X_{n+m}\otimes 1_{n+m+1}\rangle .$$

and the normalization condition $\langle 1\rangle=1$. The aim of this letter is to call attention to "finitely correlated states", which have been introduced by Accardi [1] under the name of "Quantum Markov Chains". These states are invariant under translations along the chain and are characterized by the additional property that there are only finitely many linearly independent functionals of the form

$$(X_1,\ldots X_n) \longmapsto \langle Y_{-m}\otimes\ldots\otimes Y_0\otimes X_1\otimes\ldots\otimes X_n\rangle .$$

In the cases we consider here, the space of these functionals can be parametrized by an auxiliary matrix algebra $\mathcal{M}_k$, and the states are explicitly constructed as follows:

We start from a map $\mathbb{E}:\mathcal{M}_{2J+1}\otimes\mathcal{M}_k\longrightarrow\mathcal{M}_k$ and a density matrix $\rho\in\mathcal{M}_k$ such that $\mathbb{E}(1\otimes 1)=1$, and $\mathrm{tr}[\rho\mathbb{E}(1\otimes A)]=\mathrm{tr}[\rho A]$ for all $A\in\mathcal{M}_k$. It will be convenient to introduce for each $X\in\mathcal{M}_{2J+1}$ the map $\tilde{\mathbb{E}}[X]:\mathcal{M}_k\longrightarrow\mathcal{M}_k$, given by $\tilde{\mathbb{E}}[X](A)=\mathbb{E}(X\otimes A)$. An important operator in this theory is $\tilde{\mathbb{E}}[1]$, which we shall abbreviate by $\hat{\mathbb{E}}$. In terms of $\hat{\mathbb{E}}$ the above conditions on $\mathbb{E}$ and ρ become $\hat{\mathbb{E}}(1)=1$ and $\mathrm{tr}[\rho\,\hat{\mathbb{E}}(A)]=\mathrm{tr}[\rho A]$. The state $\langle\ldots\rangle$ is now given explicitly by

$$\langle X_n\otimes\ldots\otimes X_{n+m}\rangle = \mathrm{tr}\Big[\rho\ \tilde{\mathbb{E}}[X_n]\circ\tilde{\mathbb{E}}[X_{n+1}]\circ\ldots\circ\tilde{\mathbb{E}}[X_{n+m}](1)\Big], \qquad (1)$$

where "∘" means composition of maps. The consistency conditions for the state then follow from the properties of $\hat{\mathbb{E}}$ and ρ. Translation invariance follows because we have chosen $\mathbb{E}$ to be independent of the site. It remains to establish conditions on $\mathbb{E}$ that will ensure the positivity of the functional $\langle\ldots\rangle$. For this it suffices to take $\mathbb{E}$ to be completely positive [2], which is in turn guaranteed if we take $\mathbb{E}$ of the form

$$\mathbb{E}(X\otimes A)= V^{*}(X\otimes A)V \tag{2}$$

for an isometry $V:\mathbb{C}^{k}\longrightarrow \mathbb{C}^{2J+1}\otimes\mathbb{C}^{k}$.

A nice feature of finitely correlated states is that their correlation functions can be computed in a very simple way: for two single site observables $X,Y\in\mathcal{M}_{2J+1}$ at distance n from each other the correlation function is

$$\langle X\otimes\underbrace{1\otimes\ldots\otimes 1}_{n-1\ \text{factors}}\otimes Y\rangle = \mathrm{tr}\left[\rho\ \tilde{\mathbb{E}}[X]\circ\hat{\mathbb{E}}^{n-1}\circ\tilde{\mathbb{E}}[Y](1)\right]. \tag{3}$$

Thus the computation of all correlation functions is reduced to the diagonalization of the single linear operator $\hat{\mathbb{E}}:\mathcal{M}_{k}\longrightarrow\mathcal{M}_{k}$, i.e. a $k^2 x k^2$-matrix. Generically, the eigenvalue 1 (with eigenvector $1\in\mathcal{M}_{k}$) is non-degenerate, and the other eigenvalues are less than one in absolute value. Therefore the state exhibits pure exponential clustering and only a finite number of decay rates can appear. Negative eigenvalues of $\hat{\mathbb{E}}$ correspond to alternating signs in correlation functions, which are typical of antiferromagnetic behaviour. The simplicity of computations with finitely correlated states makes them an interesting set of trial states in variational computations. Minimizing, for example, the mean energy for the usual spin 1/2 Heisenberg antiferromagnet over the finitely correalated states with the smallest possible value k=2 leads to an estimated energy density, which is about 25% off the exact value. This is a considerable improvement over the mean-field approximation (corresponding in our setting to the trivial choice k=1), which does not describe antiferromagnetism at all [3].

We illustrate these general properties of finitely correlated states by explicitly constructing a family of such states (labelled by a half-integer $j\geq J/2$) for spin chains with integer spin J. We shall compute their correlation functions by diagonalizing $\hat{\mathbb{E}}$, and discuss some of their properties, which follow easily from the above construction. The simplest case of our construction (J=1, j=1/2) gives a state recently studied by I.Affleck, T.Kennedy, E.H.Lieb, an H.Tasaki [4] and also by J.Chayes, L.Chayes, and S.Kivelson [5] in terms of the "resonating valence bonds" introduced by P.Anderson [6]. They are also the exact ground states of a type of models discovered by Klein [7] (see also [8]). Thus our construction offers a simple alternative to the computation of the correlation functions of these models, replacing the diagrammatic technique used in [4].

We start from the representations $D^{(J)}$ and $D^{(j)}$ of SU_2, and denote their generators by $\vec{S}=(S_1,S_2,S_3)$ and $\vec{L}=(L_1,L_2,L_3)$, respectively. Then if J is integer and $2j\geq J$, there is an up to a phase unique isometry

$$V:\mathbb{C}^{2j+1}\longrightarrow \mathbb{C}^{2J+1}\otimes\mathbb{C}^{2j+1}$$

intertwining $D^{(j)}$ and $D^{(J)}\otimes D^{(j)}$. Then eq.2 defines the required map $\mathbb{E}:\mathcal{M}_{2J+1}\otimes\mathcal{M}_k\longrightarrow \mathcal{M}_k$ with $k=2j+1$. Since V is an isometry the property $\hat{\mathbb{E}}(1)=\mathbb{E}(1\otimes 1)=1$ is obvious. Moreover, $A\longmapsto tr[\hat{\mathbb{E}}(A)]$ defines a rotation invariant functional on $\mathcal{M}_{2j+1}$. Since $D^{(j)}$ is irreducible, this must be proportional to the trace itself. Hence we can (and must) take $\rho=(2j+1)^{-1}\cdot 1$.

It is clear from the intertwining property of V that the operator $\hat{\mathbb{E}}$ commutes with the action $\beta_g(A)=D_g^{(j)}AD_g^{(j)*}$ of SU_2 on $\mathcal{M}_k$. The representation β on the $(2j+1)^2$-dimensional space $\mathcal{M}_k$ can be decomposed into irreducible representations $\beta\cong\oplus_{\chi=0}^{2j}D^{(\chi)}$. The irreducible subspaces of this decomposition $\hat{\mathbb{E}}$ are eigenspaces for $\hat{\mathbb{E}}$ and we only have to compute the corresponding eigenvalues $\lambda(\chi,J,j)$. These are invariants constructed from the representations $D^{(J)}$, $D^{(j)}$, and $D^{(\chi)}$, which suggests that they can be expressed by a 6j-symbol. In fact, a straightforward computation observing the conventions of [9] yields

$$\lambda(\chi,J,j)=(-1)^{\chi}\ (2j+1)\begin{Bmatrix} j & j & J\\ j & j & \chi\end{Bmatrix}. \tag{4}$$

The case of principal interest is $\chi=1$, because the generators L_1, L_2, and L_3 transform according to $D^{(1)}$. We give a simple direct calculation of $\lambda=\lambda(1,J,j)$ and the spin-spin correlation function to show that the 6j-machinery is not essential for many cases. From the intertwining property of V we get $(1\otimes\vec{L}+\vec{S}\otimes 1)V=V\vec{L}$. Using $\vec{L}^2=j(j+1)$ and $\vec{S}^2=J(J+1)$ the relation $(1\otimes\vec{L}+\vec{S}\otimes 1)^2V=V\vec{L}^2$ becomes $2\vec{L}\cdot\vec{S}\ V=-J(J+1)\ V$. Hence with $\hat{\mathbb{E}}\ \vec{L}==\mathbb{E}(1\otimes\vec{L})=\lambda\vec{L}$ we find $\mathbb{E}(1\otimes\vec{L})\cdot\vec{L}=V^*1\otimes\vec{L}\cdot(1\otimes\vec{L}+\vec{S}\otimes 1)V=j(j+1)-\frac{1}{2}J(J+1)=\lambda\vec{L}^2=\lambda\ j(j+1)$. This determines

λ, and $\tilde{\mathbb{E}}[\vec{S}]$ satisfies $\tilde{\mathbb{E}}[\vec{S}](1)= \vec{L} - \hat{\mathbb{E}}\,\vec{L}= (1-\lambda)\vec{L}$, and $\tilde{\mathbb{E}}[\vec{S}]\cdot\vec{L}= V^*(\vec{S}\otimes 1)V\cdot\vec{L}= V^*\vec{S}\otimes 1\cdot(1\otimes\vec{L}+\vec{S}\otimes 1)V= J(J+1)-\frac{1}{2}J(J+1)= \frac{1}{2}J(J+1)$. The spin-spin correlation at distance n is defined as $C_{ik}(n)= \langle S_i\otimes 1\ldots\otimes 1\otimes S_k\rangle$, where n-1 factors 1 appear on the right. Since the 3x3-matrix C(n) is rotation invariant it is a multiple of the Kronecker symbol δ_{ik}, and it suffices to compute its trace. Inserting the above formulas into eq.3, we get

$$C_{ik}(n)= \delta_{ik}\ \frac{1}{2}\ J^2(J+1)^2\ \left(1-\frac{J(J+1)}{2j(j+1)}\right)^{n-1} . \tag{5}$$

The representation of SU_2 associated with n neighbouring sites is $D^{(J)}\otimes\ldots\otimes D^{(J)}$. A characteristic property of the family of states under consideration is that they vanish on most of the irreducible subspaces appearing in the decomposition of this tensor product representation. The relation

$$\tilde{\mathbb{E}}[D_g^{(J)}]^n(A)= D_g^{(j)}\ \hat{\mathbb{E}}^n\left(D_g^{(j)*}\cdot A\right)$$

follows directly from the intertwinig property of V for n=1, and generalizes to all n by induction. Inserting this into eq.1 we find

$$\underbrace{\langle D_g^{(J)}\otimes\ldots\otimes D_g^{(J)}\rangle}_{n\ \text{factors}} = \mathrm{tr}\left[\rho\ D_g^{(j)}\cdot\ \hat{\mathbb{E}}^n\left(D_g^{(j)*}\right)\right]. \tag{6}$$

Now the right hand side, considered as a function of $g\in SU_2$, can be expressed as a sum of matrix elements of the representation $D^{(j)}\otimes D^{(j)}$. Hence the support of the state $\langle\ldots\rangle$ is contained in the subspace of $\left(\mathbb{C}^{2J+1}\right)^{\otimes n}$ carrying representations $D^{(\varkappa)}$ with $\varkappa\le 2j$. In short, the sum of any row of consecutive spins (of arbitrary length n) is bounded under $\langle\ldots\rangle$ by 2j.

These considerations have an immediate bearing on nearest neighbour Hamiltonians of the form $H= \sum_{i\in\mathbb{Z}} h^{(i)}$, where $h^{(j)}$ denotes a copy of a fixed operator $h\in \mathcal{M}_{2J+1}\otimes\mathcal{M}_{2J+1}$ in the i^{th} and $(i+1)^{th}$ factor of the chain. Suppose that h is positive and vanishes on the subspaces with $\varkappa>2j$. For J=1 and j=1/2 this fixes h up to trivial scalings to be the Hamiltonian

$$h= \frac{1}{3} + \frac{1}{2}\ \vec{S}_1\cdot\vec{S}_2 \ + \frac{1}{6}\ (\vec{S}_1\cdot\vec{S}_2)^2,$$

studied in [4]. Then by the previous paragraph $\langle\ldots\rangle$ is a ground state for H, in the sense [4] that $\langle h^{(i)}\rangle$ attains its minimal value 0 for all i. In fact, it was shown in [4] that $\langle\ldots\rangle$ is the only state with that property.

This ground state property can be established in our framework without taking into account any special symmetry (e.g. rotation invariance), using only the special form eq.2 of $\mathbb{E}$, together with the assumptions that $\hat{\mathbb{E}}^n(A)\xrightarrow[n\to\infty]{} \mathrm{tr}[\rho A]\cdot 1$, and ρ is non-singular. We state the main results, leaving a discussion of this assumption and detailed proofs to a later publication.

It will be convenient to choose some basis ψ_μ, $\mu=1,..,2J+1$ in $\mathbb{C}^{2J+1}$. Then V can be expressed in terms of matrices $v(\mu)\in\mathcal{M}_k$ as $V\chi = \sum_\mu \psi_\mu\otimes(v(\mu)\chi)$. For each $n\in\mathbb{N}$ we define a map $\Omega_n : \mathcal{M}_k \longrightarrow \left(\mathbb{C}^{2J+1}\right)^{\otimes n}$ by

$$\Omega_n(A) = \sum_{\mu_1,\ldots\mu_n} \psi_{\mu_1}\otimes\ldots\otimes\psi_{\mu_n} \ \mathrm{tr}\Big[A\cdot v(\mu_1)\cdot\ldots\cdot v(\mu_n)\Big]. \tag{7}$$

On n consecutive sites the state $\langle\ldots\rangle$ is given by a density matrix in $\left(\mathbb{C}^{2J+1}\right)^{\otimes n}$. The support of this density matrix is contained the range of Ω_n, which we shall denote by $\mathcal{R}_n$. Clearly, $\dim \mathcal{R}_n \le \dim \mathcal{M}_k = k^2$. Equality holds for some n if the $(2J+1)^n$ operators $v(\mu_1)\cdot\ldots\cdot v(\mu_n)$ span the vector space $\mathcal{M}_k$. Under the above assumptions this is true for all $n\ge N-1$, for some N. Now let h be a positive semi-definite matrix in $\left(\mathbb{C}^{2J+1}\right)^{\otimes N}$ whose null-eigenspace coincides with $\mathcal{R}_N$. Let $h^{(i)}$ denote a copy of h, acting in the algebra of the sites i+1, i+2,..., i+N. Then $H=\sum_{i\in\mathbb{Z}} h^{(i)}$ is an interaction of range N for the spin chain. We can then show that $\langle\ldots\rangle$ is the unique ground state for H in the sense of [4]. This implies, in particular, that the state $\langle\ldots\rangle$ is a pure state on the quasi-local algebra of the chain.

The conditions for this conclusion are generically true for any choice of V, and $(2J+1)^{N-1} \ge k^2$. They are easily verified for the above family of rotation invariant states. For example, $j\le J\le 2j$ implies $\dim \mathcal{R}_2 = (2j+1)^2$, so the corresponding states are ground states for suitable interactions of nearest and next-nearest neighbours. The smallest admissable value of j, namely j=J/2, gives a state, which is the unique ground state of any nearest neighbour interaction vanishing on the spin $\leq J$ subspace of $\left(\mathbb{C}^{2J+1}\right)^{\otimes 2}$.

The technique we presented can be generalized without major changes to models on Cayley-trees, and the basic construction of finitely correlated states can be generalized to higher dimensional lattices and general graphs.

Acknowledgement: Part of this work was done while one of us (M.F.) was visiting the University College of Dublin on an Erasmus project of the EEC. He would also like to thank DIAS for the warm hospitality which was extended to him. R.F.W would like to thank Zhong-Qi Ma for helpful discussions and an independent verification of eq.4. He also gratefully acknowledges the financial support of the Alexander-von Humboldt Foundation.

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