Factorized ground state in dimerized spin chains

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Abstract. The possibility of observing factorized ground states in dimerized spin systems is studied. A set of sufficient conditions is derived which allows one to establish whether or not it is possible to have factorization both in nearest-neighbor and long-range Hamiltonians. These conditions can be derived by forcing factorization for each of the pairwise terms of the total Hamiltonian. Due to the peculiar structure of a dimerized chain, an antiferromagnetic factorized ground state of the kind $|\nearrow\rangle, |\nearrow\rangle, |\nwarrow\rangle, |\nwarrow\rangle$ (forbidden in regular chains) is possible.

1. Introduction

Entanglement properties of many-body quantum critical systems are an attractive research field [1, 2, 3, 4]. During last years, an increasing number of papers have been concerned with the problem of the existence of fully factorizable ground states. The phenomenon of ground-state factorization (GSF) in spin chains, first discovered by Kurmann *et al.* [5], then observed in two-dimensional lattices through quantum Monte Carlo methods [6, 7], has been analyzed by Giampaolo *et al.* in [8], where the factorizing field has been determined for a quite general class of translationally-invariant models through an appropriate measure of entanglement, the so-called extremal single-qubit unitary operation (E-SQUO), which vanishes at the factorizing point. As shown in [9], the critical point turns out to separate two regions with qualitatively different bipartite entanglement. It has been shown in [10] that, in the vicinity of the factorizing field, the range of concurrence diverges, and that such divergence corresponds the appearance of a characteristic length scale in the system. Factorization in generalized inhomogeneous ferrimagnets is discussed in [11].

The extension to dimerized chains has been done in [12]. It has been shown that, in the case of the XY chain, the factorizing point represents an accidental degeneracy point of the Hamiltonian. For every number of spins, at the factorizing field, the Hamiltonian symmetry is broken. This consideration can be used in the opposite direction. That is, there is factorization only if there is degeneracy, apart from special cases, like the isotropic XX chain, are considered. In this paper, I will show that sufficient conditions for the existence of GSF can be derived, without introducing the E-SQUO, just exploiting the pairwise structure of the Hamiltonians, for a large class of dimerized systems. In section 2, I will introduce the method to calculate the factorizing field, and the sufficient conditions to get it. I will specialize the calculation to nearest-neighbor Hamiltonians in section 3, and the results will be extended to long-range systems in section 4. Conclusions are given in section 5.

2. Sufficient condition for GSF

To start the discussion, let us introduce the following Hamiltonian

$$H = \sum_{\alpha=x,y,z} \sum_{l=1}^{N/2} \sum_{i=1}^{2} J_i^\alpha \sigma_{2l-2+i}^\alpha \sigma_{2l-1+i}^\alpha - h \sum_{l=1}^{N} \sigma_l^z, \tag{1}$$

It describes a chain of spins 1/2 with nearest-neighbor interaction in the presence of a transverse field (throughtout the paper only positive fields will be considered). This chain is dimerized in the sense that the coupling coefficients between spins assume alternate values. Boundary conditions are taken assuming $\sigma_{N+1}^\alpha = \sigma_1^\alpha$. The pairwise structure of H allows us to decompose the Hamiltonian as a sum of two-body operators $H = \sum_{l=1}^{N/2} (H_l^{(1)} + H_l^{(2)})$, with

$$H_l^{(i)} = \sum_{\alpha=x,y,z} J_i^\alpha \sigma_{2l-2+i}^\alpha \sigma_{2l-1+i}^\alpha - h_i \left(\sigma_{2l-2+i}^z + \sigma_{2l-1+i}^z\right) \tag{2}$$

with h_1 and h_2 such that $h = h_1 + h_2$. The decomposition of the transverse term is arbitrary, but the form assumed in 2 is suggested by the overall symmetry of the model. Note that the value of h_1 and h_2 is not specified.

Now, let us assume that one eigenstate of H is factorized ($|\Psi\rangle = \otimes_{l=1}^{N} |\psi_l\rangle$). The corresponding eigenvalue should be $E_\Psi = \sum_{l=1}^{N/2} \sum_{i=1}^{2} E_\Psi^{l,i}$, with

$$E_\Psi^{l,i} = \langle\psi_{2l-2+i}|\langle\psi_{2l-1+i}|H_l^{(i)}|\psi_{2l-2+i}\rangle|\psi_{2l-1+i}\rangle \tag{3}$$

It is easy to show that if $E_\Psi^{l,i}$ is the minimun eigenvalue of $H_l^{(i)}$, E_Ψ is the ground state energy of H. In fact, given a whatever state $|\Phi\rangle$, $\langle\Phi|H_l^{(i)}|\Phi\rangle \geq E_\Psi^{l,i}$. As a consequence, $\langle\Phi|H|\Phi\rangle \geq E_\Psi$, and this ends the proof.

3. Short-range Hamiltonians

Coming back to the search for a factorized ground state of 1, we can divide our problem in two steps. The first step will consist in the determination of the conditions under which each $H_l^{(i)}$ admits GSF, while in the second step we will check that the state we find in this way is also eigenstate of the total Hamiltonian. Given the sufficient criterion derived before, this is enough to ensure that this state is the ground state of H.

3.1. Step 1

The central feature of $H_l^{(i)}$ is the invariance under rotations of π around the z axis. This is formalized by the vanishing of the commutator $[H_l^{(i)}, P_l^{(i)}] = 0$, where $P_l^{(i)} = \sigma_{2l-2+i}^z \sigma_{2l-1+i}^z$ is the parity operator, since its eigenvalues are $+1$ or -1, according to the number of down spins in the z direction being even or odd. The above commutation relation then requires also the eigenstates of $H_l^{(i)}$ to have definite parity. Now, since $H_l^{(i)}$ is not diagonal in the σ^z basis ($|\uparrow,\uparrow\rangle$, $|\downarrow,\downarrow\rangle$, $|\uparrow,\downarrow\rangle$, and $|\downarrow,\uparrow\rangle$ are not eigenstates of $H_l^{(i)}$), $|\psi_{2l-2+i}\rangle|\psi_{2l-1+i}\rangle$ can be its ground state only if it can be written as $(\cos\theta_{2l-2+i}|\uparrow\rangle + \sin\theta_{2l-2+i}|\downarrow\rangle) \otimes (\cos\theta_{2l-1+i}|\uparrow\rangle + \sin\theta_{2l-1+i}|\downarrow\rangle)$. In other words, the system cannot support a ground state which is at the same time both symmetric and separable. Then, to try to observe GSF we must force symmetry breaking, by imposing the degeneracy between the lower eigenstates of the two symmetry sectors:

$$E^{(ev)} = E^{(odd)}, \tag{4}$$

($E^{(ev)}$ and $E^{(odd)}$ are, respectively, the lowest energies of the even and the odd sector of $H_l^{(i)}$). Because of these symmetry properties, the matrix representation of $H_l^{(i)}$ in the basis $|\uparrow\uparrow\rangle, |\downarrow\downarrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle$ is block diagonal, each block being a 2×2 matrix. The action of $H_l^{(i)}$ on the even parity basis vectors is given by

$$H_l^{(i)}\,|\uparrow,\uparrow\rangle = (J_i^x - J_i^y)\,|\downarrow,\downarrow\rangle + (J_i^z - 2h_i)\,|\uparrow,\uparrow\rangle \tag{5}$$

$$H_l^{(i)}\,|\downarrow,\downarrow\rangle = (J_i^x - J_i^y)\,|\uparrow,\uparrow\rangle + (J_i^z + 2h_i)\,|\downarrow,\downarrow\rangle \tag{6}$$

yielding the energy eigenvalues

$$E^{(ev)} = J_i^z \pm \sqrt{4h_i^2 + (J_i^x - J_i^y)^2}. \tag{7}$$

Obviously, the ground state will correspond to the sign $-$, while the sign $+$ will determine the excited state.

The analogous computation in the odd parity sector gives

$$H_l^{(i)}\,|\uparrow,\downarrow\rangle = (J_i^x + J_i^y)\,|\downarrow,\uparrow\rangle - J_i^z\,|\uparrow,\downarrow\rangle \tag{8}$$

$$H_l^{(i)}\,|\downarrow,\uparrow\rangle = (J_i^x + J_i^y)\,|\uparrow,\downarrow\rangle - J_i^z\,|\downarrow,\uparrow\rangle \tag{9}$$

and the corresponding eigenvalues are

$$E^{(odd)} = -J_i^z \pm (J_i^x + J_i^y) \tag{10}$$

In this case, the identification of the ground state cannot be done without fixing the value of the coupling parameters. If $(J_i^x + J_i^y) > (<)0$, the ground state corresponds to the sign $-(+)$, and it is characterized by an antiferromagnetic (ferromagnetic) order. Since $H_l^{(1)}$ is different from $H_l^{(2)}$, we could have, for instance, a situation where $(J_1^x + J_1^y) > 0$ and $(J_2^x + J_2^y) < 0$. As seen in [12], this opens up the possibility of observing an antiferromagnetic Neél-type ground state, whose unitary cell is represented by a pair of spins.

Ferromagnetic case As said, it corresponds to $(J_i^x + J_i^y) < 0$ both for $i = 1$ and $i = 2$. The condition 4 implies for the two-spin factorizing field

$$h_i^{(F)} = \sqrt{(J_i^z - J_i^y)(J_i^z - J_i^x)}. \tag{11}$$

The parameteres defining the ground state are

$$\tan\theta_{2l-2+i} = \pm\sqrt{\frac{J_i^x + J_i^y - 2J_i^z + 2\sqrt{(J_i^z - J_i^y)(J_i^z - J_i^x)}}{J_i^x - J_i^y}} \tag{12}$$

and $\theta_{2l-2+i} = \theta_{2l-1+i}$.

Antiferromagnetic case In this case, $(J_i^x + J_i^y) > 0$ both for $i = 1$ and $i = 2$. Under this constraint, 4 is satisfied if

$$h_i^{(F)} = \sqrt{(J_i^z + J_i^y)(J_i^z + J_i^x)}, \tag{13}$$

while the eigenvectors are such that

$$\tan\theta_{2l-2+i} = \pm\sqrt{\frac{J_i^x + J_i^y + 2J_i^z - 2\sqrt{(J_i^z + J_i^y)(J_i^z + J_i^x)}}{J_i^x - J_i^y}} \tag{14}$$

and $\theta_{2l-2+i} = -\theta_{2l-1+i}$. It is equivalent to choose $\theta_{2l} = -\theta_{2l+1}$.

Mixed case Let us assume, for instance, $(J_1^x + J_1^y) > 0$ and $(J_2^x + J_2^y) < 0$. This choice would allow to have different eigenstates and factorizing field depending on the dimer we select. In fact, we find

$$h_1^{(F)} = \sqrt{(J_1^z + J_1^y)(J_1^z + J_1^x)} \tag{15}$$

$$h_2^{(F)} = \sqrt{(J_2^z - J_2^y)(J_2^z - J_2^x)} \tag{16}$$

with

$$\tan\theta_{2l-1} = \pm\sqrt{\frac{J_1^x + J_1^y + 2J_1^z - 2\sqrt{(J_1^z + J_1^y)(J_1^z + J_1^x)}}{J_1^x - J_1^y}} \tag{17}$$

$$\tan\theta_{2l} = \pm\sqrt{\frac{J_2^x + J_2^y - 2J_2^z + 2\sqrt{(J_2^z - J_2^y)(J_2^z - J_2^x)}}{J_2^x - J_2^y}} \tag{18}$$

and $\theta_{2l-1} = -\theta_{2l}$ while $\theta_{2l} = +\theta_{2l+1}$.

3.2. Step 2

So far, we listed the conditions under which every single two-spin Hamiltonian can get factorized, and we calculated the relevant quantities. To go further, we need to merge all dimers in the whole chain. Since each single spin belongs to two different dimers, the angle θ corresponding to a given site should be independent on which of the two dimers are taken into account.

Ferromagnetic case In the ferromagnetic case this condition this happens if the parameter satisfy the conditions $J_2^x = \kappa J_1^x$, $J_2^y = \kappa J_1^y$, and $J_2^z = \kappa J_1^z$. As a result of this assumption, all angles equal to each other. Because of the $\pm$ before the external square root in 12, two solutions are possible which have the form $|\Psi^{\pm}\rangle = \otimes_{l=1}^{N} |\psi_l^{\pm}\rangle$, with $|\psi_l^{\pm}\rangle = \cos\theta|\uparrow\rangle \pm \sin\theta|\downarrow\rangle$. The factorizing field is given as

$$h^{(F)} = (1+\kappa)\sqrt{(J_1^z - J_1^y)(J_1^z - J_1^x)}. \tag{19}$$

Antiferromagnetic case The constraint $\theta_{2l} = -\theta_{2l+1}$ leads to two possible factorized states whit the usual antiferromagnetic structure $|\Psi^{\pm}\rangle = \otimes_{l=1}^{N/2} |\psi_{2l-1}^{\pm}\rangle|\psi_{2l}^{\mp}\rangle$. The consistency conditions are the same given in the presence of ferromagnetic coupling ($J_1^x = \kappa J_2^x$, $J_1^y = \kappa J_2^y$, and $J_1^z = \kappa J_2^z$) while factorization takes place if

$$h^{(F)} = (1+\kappa)\sqrt{(J_1^z + J_1^y)(J_1^z + J_1^x)}. \tag{20}$$

Mixed case With the assumptions $(J_1^x + J_1^y) > 0$ and $(J_2^x + J_2^y) < 0$, satisfying 17 and 18 under the constraints $\theta_{2l-1} = -\theta_{2l}$ and $\theta_{2l} = \theta_{2l+1}$ is possible only if we choose $J_1^x = -\kappa J_2^x$, $J_1^y = -\kappa J_2^y$, and $J_1^z = \kappa J_2^z$. The factorizing field has the same value of 20. Even in this case two different factorized ground states can be buildt which are $|\Psi^{\pm}\rangle = \otimes_{l=1}^{N/4} |\psi_{4l-3}^{\pm}\rangle|\psi_{4l-2}^{\pm}\rangle|\psi_{4l-1}^{\mp}\rangle|\psi_{4l}^{\mp}\rangle$. Obviously, this structure can be coherently assumed in a finite-size system only if $N/4$ is integer.

4. Long-range Hamiltonians

The problem of searching a factorized ground state in dimerized spin chains can be extended to systems exhibiting longe-range correlations. They can be described through

$$H = \sum_r H_r - h \sum_{l=1}^{N} \sigma_l^z, \tag{21}$$

with

$$H_r = \sum_{\alpha=x,y,z} \sum_{l=1}^{N/2} \left(J_{r,1}^{\alpha} \sigma_{2l-1}^{\alpha} \sigma_{2l-1+r}^{\alpha} + J_{r,2}^{\alpha} \sigma_{2l}^{\alpha} \sigma_{2l+r}^{\alpha} \right), \tag{22}$$

where $J_{r,i}^{\alpha}$ are the dimerized coupling constants between spin pairs at odd distance r. The existence of alternate coupling on even distances cannot be univocally introduced, and it will be dropped. For the sake of clarity, we will consider one-dimensional chains, since the extension to multi-dimensional chains does not imply the emergence of qualitatively new results. To avoid the appearance of frustation for finite chains, N/r should be integer for any value of r appearing in H. As in the nearest-neighbor case, we can split the Hamiltonian as a sum of two-body operators: $H = \sum_{l,r,i} H_{l,r}^{(i)}$, where

$$H_{l,r}^{(i)} = \sum_{\alpha} J_{r,i}^{\alpha} \sigma_{2l-2+i}^{\alpha} \sigma_{2l-2+i+r}^{\alpha} - h_{r,i} \left(\sigma_{2l-2+i}^z + \sigma_{2l-2+i+r}^z \right), \tag{23}$$

and $h_{r,1}$, $h_{r,2}$ such that $h = \sum_r (h_{r,1} + h_{r,2})$.

Now, each single spin belongs to many different two-body terms, depending on the range of interaction. To find the existence of the factorized ground state, we shall repeat the two steps made in the previous section. While the diagonalization of the two-spin Hamiltonian gives obviously the same results, the presence of long-range coupling causes the appearence of new constraints on the Hamiltonian parameters.

4.1. Step 1

For reasons that will appear clear in the following, we make the following classification: We say that the coupling is ferromagnetic if $\left(J^x_{1,i} + J^y_{1,i}\right) < 0$ both for $i = 1$ and $i = 2$. When $\left(J^x_{1,i} + J^y_{1,i}\right) > 0$ for $i = 1, 2$, we are in the presence of antiferromagnetism. The mixed case we will use is defined through $\left(J^x_{1,1} + J^y_{1,1}\right) > 0$ and $\left(J^x_{1,2} + J^y_{1,2}\right) < 0$.

All the parameters being dependent on r, the field factorizing the two-body Hamiltonian $H^{(i)}_{l,r}$ is, in the ferromagnetic case

$$h^{(F)}_{r,i} = \sqrt{(J^z_{r,i} - J^y_{r,i})(J^z_{r,i} - J^x_{r,i})}, \tag{24}$$

while the angles defining the ground state are (in analogy with 12)

$$\tan\theta_{r,2l+i} = \pm\sqrt{\frac{J^x_{r,i} + J^y_{r,i} - 2J^z_{r,i} + 2\sqrt{(J^z_{r,i} - J^y_{r,i})(J^z_{r,i} - J^x_{r,i})}}{J^x_{r,i} - J^y_{r,i}}} \tag{25}$$

with $\theta_{r,2l+i} = \theta_{r,2l+i+r}$.

In the purely antiferromagnetic case, we have to generalize 13, 14, and get

$$h^{(F)}_{r,i} = \sqrt{(J^z_{r,i} + J^y_{r,i})(J^z_{r,i} + J^x_{r,i})} \tag{26}$$

and

$$\tan\theta_{r,2l+i} = \pm\sqrt{\frac{J^x_{r,i} + J^y_{r,i} + 2J^z_{r,i} - 2\sqrt{(J^z_{r,i} + J^y_{r,i})(J^z_{r,i} + J^x_{r,i})}}{J^x_{r,i} - J^y_{r,i}}} \tag{27}$$

with $\theta_{r,2l+i} = -\theta_{r,2l+i+r}$.

Last generalization (in the mixed case) amounts to write

$$h^{(F)}_{r,1} = \sqrt{(J^z_{r,1} + J^y_{r,1})(J^z_{r,1} + J^x_{r,1})} \tag{28}$$

$$h^{(F)}_{r,2} = \sqrt{(J^z_{r,2} - J^y_{r,2})(J^z_{r,2} - J^x_{r,2})} \tag{29}$$

with

$$\tan\theta_{r,2l-1} = \pm\sqrt{\frac{J^x_{r,1} + J^y_{r,1} + 2J^z_{r,1} - 2\sqrt{(J^z_{r,1} + J^y_{r,1})(J^z_{r,1} + J^x_{r,1})}}{J^x_{r,1} - J^y_{r,1}}} \tag{30}$$

$$\tan\theta_{r,2l} = \pm\sqrt{\frac{J^x_{r,2} + J^y_{r,2} - 2J^z_{r,2} + 2\sqrt{(J^z_{r,2} - J^y_{r,2})(J^z_{r,2} - J^x_{r,2})}}{J^x_{r,2} - J^y_{r,2}}} \tag{31}$$

and $\theta_{r,2l-1} = -\theta_{r,2l-1+r}$ while $\theta_{r,2l} = +\theta_{r,2l+r}$.

4.2. Step 2

As said, each single spin belongs to more than two dimers. To have a factorized ground state, we should find the same value of θ for each of the dimers of a given site. It should be independent both on r and i.

Ferromagnetic case The independence of θ is achieved if the parameters are such that $J^{\alpha}_{r,i} = \gamma_r J^{\alpha}_{1,i}$ and $J^{\alpha}_{r,2} = \kappa J^{\alpha}_{r,1}$. The value of the factorizing field is then $h^{(F)} = (1+\kappa)\sqrt{(\mathcal{J}^z_1 - \mathcal{J}^x_1)(\mathcal{J}^z_1 - \mathcal{J}^y_1)}$, where the $\mathcal{J}^\alpha$ are the global interactions along different axes: $\mathcal{J}^\alpha_i = \sum_r J^\alpha_{r,i}$. The structure of the state is the same obtained with short-range interaction: the solutions are $|\Psi^\pm\rangle = \otimes^N_{l=1}|\psi^\pm_l\rangle$.

Antiferromagnetic case The scaling conditions that ensure factorization are $J^{\alpha}_{r,2} = \kappa J^{\alpha}_{r,1}$, $J^{x,y}_{r,i} = (-1)^r \gamma_r J^{x,y}_{1,i}$, and $J^z_{r,i} = \gamma_r J^z_{1,i}$. As said before, dimerization on even distances is not comprised in our model. On the other hand, we could introduce coupling putting $J_{2r,1} = J_{2r,2}$. In this situation, the constraint on $J^{x,y}_{r,i}$ is nesessary to guarantee ferromagnetism on even distances, since the states we obtain are $|\Psi^\pm\rangle = \otimes^{N/2}_{l=1}|\psi^\pm_{2l-1}\rangle|\psi^\mp_{2l}\rangle$. The factorized point amounts to $h^{(F)} = (1+\kappa)\sqrt{(\mathcal{J}^z_1 - \mathcal{J}^x_1)(\mathcal{J}^z_1 - \mathcal{J}^y_1)}$, with $\mathcal{J}^z_1 = \sum_r J^z_{r,1}$ and $\mathcal{J}^{x,y}_1 = \sum_r (-1)^r J^{x,y}_{r,1}$.

Mixed case In this last case, the possibility of having the eigensolutions $|\Psi\rangle = \otimes^{(N/4)-1}_{l=0}|\psi^\pm_{4l+1}\rangle|\psi^\pm_{4l+2}\rangle|\psi^\mp_{4l+3}\rangle|\psi^\mp_{4l+4}\rangle$ is related to the conditions $J^{x,y}_{r,2} = -\kappa J^{x,y}_{r,1}$, $J^z_{r,2} = \kappa J^z_{r,1}$, $J^z_{r,i} = \gamma_r J^z_{1,i}$, and $J^{x,y}_{r,i} = (-1)^{(r-1)/2}\gamma_r J^{x,y}_{1,i}$. The value of the factorizing field is, as in the other cases, $h^{(F)} = (1+\kappa)\sqrt{(\mathcal{J}^z_1 - \mathcal{J}^x_1)(\mathcal{J}^z_1 - \mathcal{J}^y_1)}$, with $\mathcal{J}^z_1 = \sum_r J^z_{r,1}$ and $\mathcal{J}^{x,y}_1 = \sum_r (-1)^{(r-1)/2} J^{x,y}_{r,1}$.

5. Conclusions

In summary, we discussed the existence of a fully unentangled ground state in a class of dimerized spin chains. It has been shown that a sufficient condition for factorization can be derived by exploiting the pairwise character of the Hamiltonian. We applied this method both to nearest-neighbor and long-range Hamiltonians, calculating the condition that should be satisfied by the parameters of the system to observe factorization. Together with the usual ferromagnetic and antiferromagnetic regimes, we studied a third case, with no analogous in translationally-invariant systems, consisting of an antiferromagnetic Neél-type ground state where pairs of adjacent spins represent the unitary cell.

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