Antiferromagnetic ordering of energy levels for $SU(N)$ Hubbard chain

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The talk

The Lieb-Mattis theorem on the antiferromagnetic ordering of energy levels of bipartite $SU(2)$ Heisenberg spin lattice systems is generalized to $SU(N)$ extended Hubbard model with Heisenberg exchange and pair-hopping terms.

It is proved that

- The minimum energy levels among the states from equivalent representations are nondegenerate
- They are ordered according to the partial dominance order of corresponding Young diagrams.
- The ground states form a unique antisymmetric multiplet.

We shall

- Shortly review the Lieb-Mattis theorem on antiferromagnetic ordering of energy levels for usual spin systems.
- Describe $SU(N)$ generalization of extended Hubbard chain.
- Formulate $SU(N)$ analogue generalization of the antiferromagnetic ordering of energy levels for this system.
- Describe the proof based on Perron-Frobenius theorem and representation theory of unitary group.

Motivation

- The structure of the ground state (GS) (degeneracy, quantum numbers) is very important
- Bethe ansatz can be applied to the restricted class of integrable models *only*
- SU(N) symmetric point exists in spin ladders, spin-orbital model, spin-1 chain with a biquadratic exbhange, etc.

The conditions (bipartness, usual $SU(2)$ spins) of the original ordering therem [Lieb, Mattis, 1962] can be weakened or extended. In particular, it is extended

- To extended $t-J$ and Hubbard chains [Xiang, d'Ambrumenil, 1992];
- To frustrated (non-bipartite) quasi-1d spin ladder systems, including diagonal and four-spin interactions [Hakobyan, 2007,2008].

Antiferromagnetic ordering of levels on bipartite Heisenberg systems

Exact results on the Heisenberg spin lattice systems

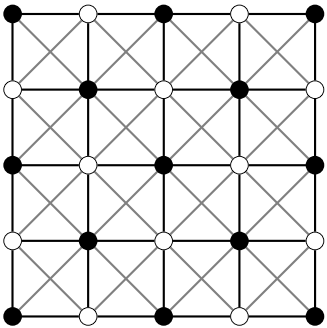
$$H_{\text{Heis}} = \sum_{\langle x,y \rangle} J_{xy} \vec{S}_x \cdot \vec{S}_y :$$

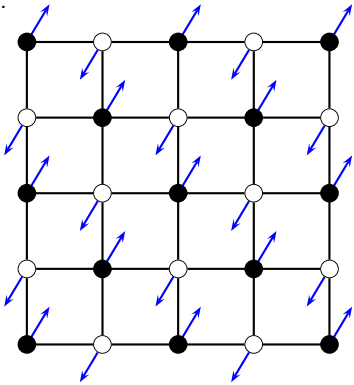
- Exact solution of spin-1/2 ring [Bethe, 1931].
- Spin-1/2 ring has unique ground state (GS), [Marshall, 1955].
- On general *bipartite* lattice [Lieb, Mattis, 1962]:
  - $S_{\text{GS}} = |S_A - S_B|$, where S_A (S_B) is the *highest* possible spin on sublattice A (B);
  - Energy level ordering, i. e. $\mathcal{E}(S_1) > \mathcal{E}(S_2)$ if $S_1 > S_2 \geq S_{\text{GS}}$, where $\mathcal{E}(S)$ is the *lowest* energy value in spin-S sector;
  - The levels $\mathcal{E}(S)$ and, hence, GS are nondegenerated.

The bipartite lattices L are splitted into two sublattices A and B such that the spin exchange between sites of different lattices are antiferromagnetic: $J_{AB} \geq 0$, while the exchanges within the same lattice are ferromagnetic: $J_{AA}, J_{BB} \leq 0$.

The bipartite and frustrated systems

The frustrated (nonbipartite) spin system on the left and bipartite system on the right. All spin exchange couplings are positive.





- The classical ground state on bipartite systems is the rotationally degenerate Neel state with $|S_{\mathrm{GS}}| = |S_A - S_B|$.
- The quantum ground state is a unique multiplet with the same spin.

$SU(N)$ Hubbard and Sutherland chains

Extended Hubbard model: fermions $c^{\pm}_{x,\alpha}$ are given by flavor $\alpha = 1, \ldots, N$ and position x.

$$H_{\text{Hub}} = \sum_{x,\alpha} -t_x (c^{+}_{x+1,\alpha} c_{x,\alpha} + c^{+}_{x,\alpha} c_{x+1,\alpha}) + V(n_1, \ldots, n_L) + H_{\text{Suth}}$$
$$- \sum_{x,\alpha>\beta} K_x (c^{+}_{x+1,\alpha} c^{+}_{x+1,\beta} c_{x,\beta} c_{x,\alpha} + c^{+}_{x,\alpha} c^{+}_{x,\beta} c_{x+1,\beta} c_{x+1,\alpha}),$$
$$H_{\text{Suth}} = \sum_{x,a} J_x T^a_x T^a_{x+1}$$

$J_x = J$ exactly solvable by Bethe ansatz [Sutherland, 1975]

$$T^a_x = \sum_{\alpha,\beta} c^{+}_{x,\alpha} \mathcal{T}^a_{\alpha\beta} c_{x,\beta}, \quad a = 1, \ldots, N^2 - 1 = \dim SU(N),$$

The $SU(2)$ case for fermionic chain was studied by [Xiang, d'Ambrumenil, 1992].

The symmetries of H_{Hub} and H_{Suth}

The symmetry group of H_{Suth} is $SU(N)$, while the symmetry group of H_{Hub} is $U(N) = SU(N) \times U(1)$.
The $U(1)$ charge M is the number of particles

$$M = \sum_{x,\alpha} c^{+}_{x,\alpha} c_{x,\alpha}.$$

The $SU(N)$ conserved charges are

$$T^{a} = \sum_{x,\alpha,\beta} c^{+}_{x,\alpha} \mathcal{T}^{a}_{\alpha\beta} c_{x,\beta},$$

where $\mathcal{T}^{a}_{\alpha\beta}$ are the generators in N-dimensional defining representation.
Each site x has 2^N states with fermion number $0 \leq k \leq N$. The states

$$c^{+}_{\alpha_1} \dots c^{+}_{\alpha_k} |0\rangle$$

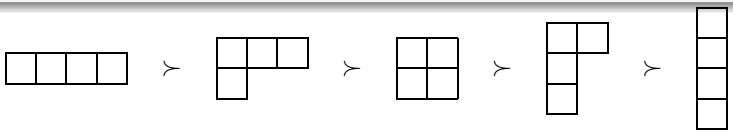
form the $d = \binom{N}{k}$ antisymmetric $SU(N)$ multiplet.

The main result: Ordering of energy levels

The $U(N)$ multiplets are described by Young tableaux $\mathbb{Y}$ with M boxes and no more than N rows.

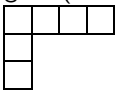
- Due to $U(N)$ symmetry, the Hamiltonian of the extended Hubbard chain remains invariant on the individual sectors $\mathbb{Y}$ combining the equivalent representations.
- The number of boxes in $\mathbb{Y}$ is the $U(1)$ charge corresponding to the number of particles M.
- The dominance order among Young diagrams [book: Macdonald, Symmetric functions and Hall polynomials]:

$\mathbb{Y}' \succ \mathbb{Y}$ if $\mathbb{Y}$ may be obtained from $\mathbb{Y}'$ by the displacement of some of its boxes from the upper rows to the lower ones, for example:



Properties of the dominace order:

- It is a partial order: there are Young diagrams, which are not related by this order for higher ($N > 2$) algebras and higher ($M > 5$) box numbers.

  Examples:  and  .

- The Young diagrams with different number of boxes are not related to each other also.

The main result:

For the extended $SU(N)$ Hubbard model

- The minimum energy levels $E(\mathbb{Y})$ in the sectors characterized by different Young diagrams are satisfy the dominance ordering:

$$E(\mathbb{Y}_2) > E(\mathbb{Y}_1) \quad \text{if} \quad \mathbb{Y}_2 \succ \mathbb{Y}_1.$$

- The levels $E(\mathbb{Y})$ are nondegenerate, up to the trivial $SU(N)$ degeneracy.

Ground state

- There is a lowest diagram $\mathbb{Y}_{\rm gs}$ among all diagrams containing the same amount M of boxes:
$$\mathbb{Y} \succ \mathbb{Y}_{\rm gs}$$
- All columns in $\mathbb{Y}_{\rm gs}$ have the maximal length N besides the last one having
$$m = M \mod N$$
Thus, it corresponds to the m-th order antisymmetric representation.

According to the ordering rule,

- The ground states of the extended Hubbard chain with M particles form a unique $\binom{N}{m}$-dimensional antisymmetric $SU(N)$ multiplet.
- In particular, if the number of particles is the multiplicity of N, the ground state is a unique singlet.

Ground state: examples

- $SU(2)$ case: the ground state is a spin singlet for even number of particles M, while for odd M it is a spin doublet in agreements with the results [Xiang, d'Ambrumenil, 1992].
- $SU(3)$ case: depending on the value of the remainder m, the ground state is a singlet, a three-dimensional defining representation $\mathbf{3}$, or its complex conjugate one $\bar{\mathbf{3}}$. Here they are for $M = 6, 7, 8$:

$$\mathbb{Y}^{\mathbf{0}}_{\mathrm{gs}} = \begin{array}{|c|c|}\hline \ & \ \\ \hline \ & \ \\ \hline \ & \ \\ \hline \end{array}\,, \qquad \mathbb{Y}^{\mathbf{3}}_{\mathrm{gs}} = \begin{array}{|c|c|c|}\hline \ & \ & \ \\ \hline \ & \ \\ \cline{1-2} \ & \ \\ \cline{1-2} \end{array}\,, \qquad \mathbb{Y}^{\bar{\mathbf{3}}}_{\mathrm{gs}} = \begin{array}{|c|c|c|}\hline \ & \ & \ \\ \hline \ & \ & \ \\ \hline \ & \ \\ \cline{1-2} \end{array}\,.$$

Note that using the described method we can not compare the ground states having different amount of particles.

Steps of the proof

The proof based on Perron-Frobenius theorem: For the connected matrix A with nonpositive off-diagonal elements, i.e. $A_{ij} \leq 0$ for $i \neq j$,

- The lowest eigenvalue is nondegenerate,
- All coefficients of corresponding eigenvector can be choosen to be positive, i.e. $\psi_i > 0$ for all i.

The connectness of A means that for any two indexes i, j there is a sequence of indexes $i_1, i_2, \ldots, i_n$ such that $A_{ii_1} A_{i_1 i_2} \ldots A_{i_n j} \neq 0$.

- On each subspace of states with fixed $S^z = M$ choose the basis, where the matrix of Hamiltonian obeys the conditions of the Perron-Frobenius theorem.
- This proves the uniqueness of so-called relative ground state Ω_M on $S^z = M$ subspace.
- Choose some simple trial state Ψ_M with certain value of the total spin $S = s$, which overlaps with Ω_M. Due to the uniqueness, Ω_M will have the same spin value. In most cases, $s = |M|$.
- Since each spin-S multiplet have representative in any M-subspace with $|M| \leq S$, $E(S_1) > E(S_2)$ for $S_1 > S_2$.

Nonpositive basis

Then nonzero off-diagonal elements of H_{Hub} are negative in the basis

$$\{x^\alpha\} = \{x_1^\alpha, \ldots, x_{M_\alpha}^\alpha | x_1^\alpha < \cdots < x_{M_\alpha}^\alpha\},$$

where the particles of the same flavor are grouped together, while withing each flavor are ordered according to their positions:

$$|\{x^1\}, \ldots, \{x^N\}\rangle = \prod_{\alpha=1}^{N} (c^+_{x_1^\alpha,\alpha} c^+_{x_2^\alpha,\alpha} \ldots c^+_{x_{M_\alpha}^\alpha,\alpha})|0\rangle.$$

The hopping term $c^+_{x\pm1,\alpha} c_{x,\alpha}$ acts nontrivially on the states having one α-fermion per two adjacent states. It just replaces $c^+_{x,\alpha}$ by $c^+_{x\pm1,\alpha}$, so the off-diagonal matrix elements are non-positive.

This basis was first described and used for the $SU(N)$ Heisenberg chains [Affeck, Lieb, 1986]. Its $SU(2)$ analogue was applied for the extended $t-J$ and Hubbard models [Xiang, d'Ambrumenil, 1992]. It was applied for $t-J$ model with $SU(N_b) \times SU(N_f)$ symmetry [Angelucci, Sorella, 1996] and for $SU(4)$ Hubbard model [Li, Tian, Ma, Lin, 2004].

Nonpositive basis for H_{Suth}

The Sutherland interaction H_{Suth} preserves the number of particles on each site. In particular, its restriction on the sector with one fermion per site, gives the Sutherland spin chain:

$$\sum_a T_x^a T_{x+1}^a = 2P_{x,x+1} - 2/n,$$

where $P_{x,y}$ is the permutation of two sites.

The usual Ising (Potts) basis is

$$|\alpha_1, \ldots, \alpha_L\rangle = c^+_{1,\alpha_1} c^+_{2,\alpha_2} \ldots c^+_{L,\alpha_L} |0\rangle = (-1)^{p_{\alpha_1 \ldots \alpha_L}} |x^1, \ldots, x^N\rangle,$$

Here $p_{\alpha_1 \ldots \alpha_L}$ is the number of inversions in the sequence.

The this basis was used in the study of spin chains with higher symmetries [Hakobyan 2004; Li, 2001].

Relative ground states

The Hamiltonian is invariant on any subspace with fixed number M_α of fermions of each type α. It is a weight subspace under the $U(N)$ action. The weight is given by the set $\{M_\alpha\}_{\alpha=1}^{N}$.
It is easy to see that any two basic states from the same subspace are connected by the kinetic terms of the Hamiltonian. Then, according to the Perron-Frobenius theorem,

The relative ground state of the Hamiltonian in any M_α-subspace is unique, and its all coefficients in the nonnegative basis are straightly positive:

$$\Omega_{M_1\dots M_N} = \sum_{\substack{\{x^1\},\dots,\{x^N\} \\ \#\{x^\alpha\}=M_\alpha}} \omega_{\{x^1\}\dots\{x^N\}} |\{x^1\},\dots,\{x^N\}\rangle, \quad \omega_{\{x^1\}\dots\{x^N\}} > 0.$$

Multiplet of the relative ground state:

$\Omega_{M_1\dots M_N}$ belongs to a single irreducible $U(N)$ representation characterized by the Young diagram $\mathbb{Y}_{M_\alpha}$ with row lengths given by the nonzero numbers from the set $M_1,\dots,M_N$.

- The irreducible representations of $U(N)$ are labeled by the Young diagrams $\mathbb{Y}$ with at most N rows. Every box of $\mathbb{Y}$ is associated with a single particle.
- Symmetrize the flavors over the rows, then antisymmetrize over the columns. The spatial coordinates are kept fixed during this process.
- The states constructed in this way form an irreducible representation of $U(N)$.
- The states, where flavors do not decrease along the rows from left to right and increase along the columns from top to bottom, form the standard basis of the multiplet.
- Among them there is the highest weight state, in which the i-th rows is filled by the particles with the flavor $\alpha = i$.

$$(c^+_{x,\alpha}c^+_{y,\beta} + c^+_{x,\beta}c^+_{y,\alpha})|0\rangle = \boxed{{}^x\alpha}\boxed{{}^y\beta}, \qquad (c^+_{x,\alpha}c^+_{y,\beta} - c^+_{x,\beta}c^+_{y,\alpha})|0\rangle = \begin{array}{|c|}\hline {}^x\alpha \\ \hline {}^y\beta \\ \hline \end{array}.$$

$$(c^+_{x,\alpha}c^+_{y,\beta}c^+_{z,\gamma})(c^+_{x,\mu}c^+_{z,\nu})c^+_{x,\delta}|0\rangle \quad \longrightarrow \quad \begin{array}{|c|c|c|}\hline {}^x\alpha & {}^y\beta & {}^z\gamma \\ \hline {}^x\mu & {}^z\nu \\ \cline{1-2} {}^x\delta \\ \cline{1-1} \end{array}.$$

The construction of the trial state $\Psi_{M_1 \dots M_N}$

- The row lengths of $\mathbb{Y}$ are given by $\{M_\alpha\}$, the j-th column containing particles on j-th site.
- Fill the first row by α_1-type fermions, where M_{α_1} is the largest number from the set, then the second row by α_2-type fermions, where M_{α_2} is the next largest number, and so on.
- The symmetrization-antisymmetrization procedure is trivial.
- The state $\Psi_{M_1 \dots M_N}$ is a basic state.

The examples for $SU(3)$ chain:

$$\Psi_{3,2,1} = \begin{array}{|c|c|c|} \hline {}^{1}1 & {}^{2}1 & {}^{3}1 \\ \hline {}^{1}2 & {}^{2}2 \\ \cline{1-2} {}^{1}3 \\ \cline{1-1} \end{array} \qquad \Psi_{2,3,1} = \begin{array}{|c|c|c|} \hline {}^{1}2 & {}^{2}2 & {}^{3}2 \\ \hline {}^{1}1 & {}^{2}1 \\ \cline{1-2} {}^{1}3 \\ \cline{1-1} \end{array} \qquad \Psi_{2,0,4} = \begin{array}{|c|c|c|c|} \hline {}^{1}3 & {}^{2}3 & {}^{3}3 & {}^{4}3 \\ \hline {}^{1}1 & {}^{2}1 \\ \cline{1-2} \end{array}$$

Since the constructed state participates in the decomposition of the relative ground state, it overlaps: $\langle \Psi_{M_1 \dots M_N} | \Omega_{M_1 \dots M_N} \rangle = \omega_{M_1, \dots, M_N} > 0$. Due to the uniqueness of $\Omega_{M_1 \dots M_N}$, both states are the members of equivalent multiplets.

Extention of the oscillation theorem to many particles

Consider the quantum mechanical system of $1d$ identical fermions

$$H_{\mathrm{QM}} = -\frac{1}{2m}\sum_{i=1}^{M}\frac{\partial^2}{\partial x_i^2} + V(x_1, \ldots, x_M).$$

- For $M = 1$ particle, well-kown oscillation theorem: the wavefunction of nth level contains n zeroes.
- H_{QM} is invariant with respect to the symmetric group $\mathcal{S}_M^{\mathrm{space}}$ of coordinate permutations.
- The irreducible representations of S_M are classified by Young diagrams $\mathbb{Y}$ with M boxes.
- The lowest energy levels $E(\mathbb{Y}')$ among the states belonging to the $\mathbb{Y}'$ symmetry classes are nondegenerate and obey the inverse dominance order [Lieb, Mattis, Phys. Rev. 1962; book: Mattis, The Theory of Magnetism, 2004]:

$$E(\mathbb{Y}'_1) > E(\mathbb{Y}'_2) \text{ if } \mathbb{Y}'_1 \prec \mathbb{Y}'_2.$$

Simple explanation

In particular, the highest energy level corresponds to the fermionic, while the lowest level – to bosonic wavefunctions.

Analogy with one-particle case:

- $\mathbb{Y}'_1 \prec \mathbb{Y}'_2 \quad \Rightarrow \quad$ the wavefunction $\Psi_{\mathbb{Y}'_1}$ is "more antisymmetric" than $\Psi_{\mathbb{Y}'_2}$ $\Rightarrow$ it has more zeroes $\Rightarrow$ its energy level is higher: $E(\mathbb{Y}'_1) > E(\mathbb{Y}'_2)$.

The two-particle case:

- $\Psi_{\begin{smallmatrix}\square\\\square\end{smallmatrix}}(x_1, x_2) = -\Psi_{\begin{smallmatrix}\square\\\square\end{smallmatrix}}(x_2, x_1)$ and $x_1 = x_2$ is a zero line
- $\Psi_{\square\square}(x_1, x_2) = \Psi_{\square\square}(x_1, x_2)$ and can avoid zeroes.

Ordering for the QM system with interacting $SU(N)$ fermions

Suppose now that we have identical quantum mechanical fermions with additional $SU(N)$ flavors. Since H_{QM} does not depend on $SU(N)$ spin degrees of freedom, its symmetry group consists of three independent parts:

$$\mathcal{S}_M^{\mathrm{space}} \times \mathcal{S}_M^{\mathrm{spin}} \times SU(N)$$

According to the Schur-Weyl duality, the joint action of $\mathcal{S}_M^{\mathrm{spin}} \times SU(N)$ decomposes into a direct sum of tensor products of irreducible modules:

$$\sum_{\mathbb{Y}} \pi_{\mathbb{Y}} \otimes \rho_{\mathbb{Y}}.$$

$\pi_{\mathbb{Y}}$ and $\rho_{\mathbb{Y}}$ are the irreducible representations of $\mathcal{S}_M^{\mathrm{spin}}$ and $SU(N)$.

$$\sum_{\mathbb{Y}',\mathbb{Y}} \pi_{\mathbb{Y}'} \otimes \pi_{\mathbb{Y}} \otimes \rho_{\mathbb{Y}}.$$