Extension of the Lieb-Schultz-Mattis and Kolb theorem

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Abstract

The theorem of Lieb, Schultz and Mattis (LSM) [1], which states that the S=1/2 XXZ spin chain has gapless or degenerate ground states, can be applied to broader models. Independently, Kolb [7] considered the relation between the wave number $q$ and the twisting boundary condition, and he obtained a similar result as LSM. However, in frustrating cases it is known that there exist several exceptions for the assumption of the unique lowest state for the finite size, which is important in the traditional LSM theorem. In our previous paper, without the assumption of the uniqueness, we have extended the LSMK theorem for frustrating and non-symmetric cases. However, there remains a complexity in the proof of continuity. In this paper, we will simplify the proof than the previous work.

Keywords: Lieb-Schultz-Mattis, rigorous theorem, frustration, one-dimension, Dzyalosinskii-Moriya

1 Introduction

In statistical physics, rigorous theorems play important role; the Mermin-Wagner theorem, the Marshall-Lieb-Mattis theorem [2,3], the Lieb-Schultz-Mattis theorem [1] etc, which do not give quantitative but qualitative results, and can be applied to broad models. And one can use them to check the consistency of approximations, experiments, or numerical data.
Lieb, Schultz and Mattis (LSM) studied the S=1/2 XXZ spin chain. In appendix B of [1], they stated two theorems. For the finite \( L \) size, the uniqueness of the ground state was proved in the first theorem. In the second theorem, they proved that there exists a low-energy \( O(1/L) \) excited state; in the infinite limit, this means that either there are degenerate ground states or a vanishing gap. The first theorem was nothing more than an extension of Marshall’s theorem [2], later generalized [3], therefore it is appropriate to call the first theorem the “Marshal-Lieb-Mattis (MLM) theorem”. However the MLM theorem is limited in non-frustrated cases. The second LSM theorem was extended for general spin \( S \) and was applied for various models [4, 5].

For rational magnetizations, by using the LSM discussion, Oshikawa et al. [6] pointed out that there are multiple degenerate energy states with a gap in the infinite limit (relating to the spontaneous translation symmetry breaking) or gapless. In addition, they emphasized the discrete symmetry (the space inversion or the spin reversal or the time reversal symmetry), besides the U(1) and the translation symmetry. Although the discrete symmetry simplifies the proof of the LSM theorem, it excludes non-symmetric cases.

Independently of the LSM discussions [1, 4], Kolb [7] studied the energy spectra of the XXZ spin chain with the twist boundary condition. He pointed out the shift of the (pseudo) wave number \( q \) when varying the twist boundary condition. For the \( S \) half-odd-integer case, he showed the nontrivial periodicity \( (q \to q + \pi) \) of the energy spectra in the Brillouin zone, which means the two-fold pseudo degenerate ground states. In section II of [8], Fáth and Sólyom combined the Kolb’s idea and LSM theorem, and they argued the continuity of the energy spectra for \( S^z_T = \pm 1, \pm 2, \cdots \).

One limitation of the traditional LSM theorem is the assumption of the unique ground state for the finite size (or the unique lowest energy state in the fixed magnetization subspace). However, when including frustrations, there exist counterexamples for this assumption; one is the double-fold ground states in the Majumdar-Ghosh model [9] (\( \alpha = 1/2 \) in [1])

\[
\hat{H} = \sum_j \hat{S}_j \cdot \hat{S}_{j+1} + \alpha \hat{S}_j \cdot \hat{S}_{j+2}
\]  

(1)

(more generally multi-fold lowest states in matrix product models), another is the double-well energy spectrum observed in one spin flip from the fully aligned state in the incommensurate region (\( \alpha > 1/4 \) in [1]).

In our previous paper [10], we separated the LSM theorem from the MLM one, without the assumption of the uniqueness of the ground state, using a
squeeze theorem type method, and combing the LSM theorem with Kolb’s discussion (hereafter we call the LSM theorem with Kolb’s one as LSMK theorem). Also we tried not to use the discrete symmetry in the proof process. Therefore we can extend the LSMK theorem for frustrating or non-symmetric models. However, in our previous work, the proof of the continuity of energy spectra was not straightforward. In this paper, we will polish it.

The layout of the paper as follows. In section 2, we introduce the definition of symmetry operations. Section 3 is the main part of this work: we prove the continuity and the nontrivial periodicity of the lowest energy spectra as a function of wave number \( q \), assuming the U(1) and the translational symmetries plus the short-range interaction. Section 4 is the conclusion.

2 Model, symmetries, eigenstates

In this section we consider the symmetries of the spin chain. As a typical model, we treat the following generalized XXZ spin chain:

\[
\hat{H} = \sum_{j=1}^{L} \sum_{r=1}^{HL} \left( J(r) (\hat{S}_j^x \hat{S}_{j+r}^x + \hat{S}_j^y \hat{S}_{j+r}^y) + \Delta(r) \hat{S}_j^z \hat{S}_{j+r}^z \right) + \hbar \sum_{j=1}^{L} \hat{S}_j^z \]

where \((\hat{S}_j)^2 = S(S + 1)\) \((S = 1/2, 1, \cdots)\), \(L\) denotes the system size, \(HL = [L/2] - 1\), and the periodic boundary condition (PBC). We can also include multibody and nonsymmetric interactions, as will be shown later.

2.1 Symmetries

Next we enumerate the symmetry operations. Hereafter we denote

\[
\hat{S}_T^x \equiv \sum_{j=1}^{L} \hat{S}_j^x, \quad \hat{S}_T^y \equiv \sum_{j=1}^{L} \hat{S}_j^y, \quad \hat{S}_T^z \equiv \sum_{j=1}^{L} \hat{S}_j^z. \]

1. Rotation operator around the z-axis: \(\hat{U}_\theta \equiv \exp(-i\theta \hat{S}_T^z)\).

The rotation operator satisfies:

\[
(\hat{U}_\theta)^\dagger \hat{S}_j^z \hat{U}_\theta = \hat{S}_j^z \exp(\pm i\theta), \quad (\hat{U}_\theta)^\dagger \hat{S}_j^\pm \hat{U}_\theta = \hat{S}_j^\pm. \]
2. Translation operator by one-site: $\hat{U}_{\text{trl}}$.

$$\hat{U}_{\text{trl}}^\dagger \hat{S}_{j}^{x,y,z} \hat{U}_{\text{trl}} = \hat{S}_{j+1}^{x,y,z}. \quad (5)$$

3. The operators $\hat{S}_{j}^{x,y,z}$ are invariant under the translation.

2.2 Eigenstates

We write the eigenstate for the total spin $\hat{S}_{T}^{z}$ and the translation:

$$\hat{S}_{T}^{z}|S_{T}^{z};q\rangle = S_{T}^{z}|S_{T}^{z};q\rangle, \quad \hat{U}_{\text{trl}}|S_{T}^{z};q\rangle = \exp(iq)|S_{T}^{z};q\rangle, \quad (6)$$

where the total spin eigenvalue is related with the magnetization as $M \equiv S_{T}^{z}/L$, and $q$ is the wave number.

Since the Hamiltonian is $\text{U}(1)$ and translational invariant, one can choose

$$\hat{H}|S_{T}^{z};q\rangle = E(S_{T}^{z};q)|S_{T}^{z};q\rangle. \quad (7)$$

Energy spectra are $2\pi$ periodic with the wave number $q$:

$$E(S_{T}^{z};q+2\pi) = E(S_{T}^{z};q). \quad (8)$$

3 Extension of the LSMK theorem

In this section, we will extend the LSMK theorem without the assumption of the uniqueness of the lowest energy, by using squeeze theorem type methods. And we will use only the $\text{U}(1)$ and the translational symmetry. We do not assume the discrete symmetry such as the space inversion or the spin reversal or the time reversal. Hereafter we express $|S_{T}^{z};q\rangle$ as one of the lowest energy eigenstates in the subspace of $S_{T}^{z}$ and $q$ for the Hamiltonian $\hat{H}$ with PBC.

In the subsection 3.1, we define the twisted boundary condition (TBC) and the twisting operator; although in this paper we will only use PBC, for the purpose of the Taylor expansion [18] later, we mention TBC. In the subsection 3.2, we review the LSMK theorem according to [10, 11, 12], since the formalism in [6, 8] was somewhat cumbersome because of the wave-function treatment, and higher order calculations become simpler than [4] when multi-body interactions are included. Using the squeezing method, we discuss the periodicity for the rational magnetization in 3.3, and the continuity for the irrational magnetization in 3.4.
3.1 Twisted boundary condition and twisting operator

We introduce the twisted boundary condition (TBC):

\[
\hat{S}^\pm_{L+j} = \hat{S}^\pm_j \exp(\pm i\Phi), \quad \hat{S}^z_{L+j} = \hat{S}^z_j, \tag{9}
\]

and we shall denote the Hamiltonian (2) with TBC as \( \hat{H}_\Phi \).

Next we define the twisting unitary operator [10, 11] :

\[
\hat{U}_{\text{tw}} \equiv \exp\left(-i\frac{\Phi}{L} \sum_{j=1}^{L} j(\hat{S}^z_j - S)\right), \tag{10}
\]

then we obtain

\[
(\hat{U}_{\text{tw}}^\dagger \hat{S}^\pm_j \hat{U}_{\text{tw}}) = \hat{S}^\pm_j \exp(\pm i\Phi j/L), \quad (\hat{U}_{\text{tw}}^\dagger \hat{S}^z_j \hat{U}_{\text{tw}}) = \hat{S}^z_j, \tag{11}
\]

and \([\hat{U}_{\text{tw}}, \hat{U}_{\text{tr}}^\dagger] = 0\).

Applying the twisting operator (10) for \( \hat{H}_\Phi \), we obtain

\[
(\hat{U}_{\text{tw}}^\dagger \hat{H}_\Phi \hat{U}_{\text{tw}} - \hat{H}_\Phi) = \sum_{j=1}^{L} \sum_{r=1}^{HL} \frac{J(r)}{2} (\hat{S}^+_{j} \hat{S}^z_{j+r} \exp(-i\frac{\Phi r}{L}) - 1) + \text{h. c.}. \tag{12}
\]

Note that we will only use this expression in the Taylor expansion (18) around \( \Phi = 0 \) to \( \Phi = 2\pi l (l: \text{integer}) \) (PBC).

3.2 LSM theorem and translation operator

Lemma 1. (Translation operator and twisting operator)

\[
\hat{U}_{\text{tw}}^\dagger \hat{U}_{\text{tr}} \equiv \hat{U}_{\text{tr}} \hat{U}_{\text{tw}} \tag{13}
\]

Proof.

\[
\hat{U}_{\text{tr}} \hat{U}_{\text{tw}} \hat{U}_{\text{tr}} = \exp\left(-i\frac{\Phi}{L} \sum_{j=1}^{L} j(\hat{S}^z_{j+1} - S)\right)
= \exp\left(-i\frac{\Phi}{L} \left(\sum_{j=2}^{L} (j-1)(\hat{S}^z_j - S) + L(\hat{S}^z_{L+1} - S)\right)\right)
= \hat{U}_{\text{tw}} \exp\left(i\frac{\Phi}{L} (\hat{S}^z_T - SL)\right) \exp(-i\Phi(\hat{S}^z_1 - S)), \tag{14}
\]
where we used \( \hat{S}_{L+1}^z = \hat{S}_1^z \). By setting \( \Phi = 2\pi l \) and using the fact that the eigenvalue of \( \hat{S}_1^z - S \) is an integer, we obtain \(^{13}\).

**Theorem 1.** In the subspace with a quantum number \( S_T^z \), on the lowest energies of the two wave numbers \( q \) and \( q - 2\pi l S_T^z / L + 2\pi l S \) (\( l \) is an integer \( |l| \ll L \)), the next inequality holds:

\[
E(S_T^z; q - 2\pi l S_T^z / L + 2\pi l S) - E(S_T^z; q) \leq O(l^2 / L).
\]

(15)

**Proof.** The following combination

\[
(\hat{U}_{2\pi l}^\dagger \hat{H} \hat{U}_{2\pi l} - \hat{H}),
\]

(16)
is translational invariant from the Lemma 1. Also from the Lemma 1, we obtain

\[
\hat{U}_{1l}(\hat{U}_{2\pi l}^\dagger S_T^z; q) = \exp(i(q - 2\pi l S_T^z / L + 2\pi l S))(\hat{U}_{2\pi l}^\dagger S_T^z; q)).
\]

(17)

Next we consider the Taylor expansion:

\[
(\hat{U}_\Phi^\dagger \hat{H} \Phi \hat{U}_\Phi) = \hat{H}_{\Phi=0} + \Phi \left[ \frac{d}{d\Phi} \left( (\hat{U}_\Phi^\dagger \hat{H} \Phi \hat{U}_\Phi) \right) \right]_{\Phi=0} + O(\Phi^2).
\]

(18)

By the way, using the next relation

\[
\left[ \frac{d}{d\Phi} \left( (\hat{U}_\Phi^\dagger \hat{H} \Phi \hat{U}_\Phi) \right) \right]_{\Phi=0} = - \left[ \hat{H}, \frac{i}{L} \sum_{j=1}^L j(\hat{S}_j^z - S) \right],
\]

(19)

and the fact

\[
\langle S_T^z; q | [\hat{H}, \sum_{j=1}^L j(\hat{S}_j^z - S)] | S_T^z; q \rangle = 0,
\]

(20)

we obtain

\[
\langle S_T^z; q | \left[ \frac{d}{d\Phi} \left( (\hat{U}_\Phi^\dagger \hat{H} \Phi \hat{U}_\Phi) \right) \right]_{\Phi=0} | S_T^z; q \rangle = 0.
\]

(21)
Using equations (16), (17), (18) and (21) for models (2), we can prove the following inequality:

\[
E(S^z_T; q - 2\pi l S^z_T/L + 2\pi l S) - E(S^z_T; q)
\leq \langle S^z_T; q | (\hat{U}^{tw}_{2\pi l})^\dagger \hat{H} U^{tw}_{2\pi l} - \hat{H}) | S^z_T; q \rangle
\]

\[
= \sum_{j=1}^{L} \sum_{r=1}^{HL} J(r) \kappa \left( \frac{r l}{L} \right) \langle S^z_T; q | \hat{S}_j^+ \hat{S}_{j+r}^- | S^z_T; q \rangle + \text{h. c.}
\]

\[
\leq 2 \sum_{j=1}^{L} \sum_{r=1}^{HL} |J(r)| \left| \kappa \left( \frac{r l}{L} \right) \right| \langle S^z_T; q | \hat{S}_j^+ \hat{S}_{j+r}^- | S^z_T; q \rangle \leq O(L^2/L),
\]

(22)

where \( \kappa(\phi) \equiv \frac{1}{2}(\exp(-2\pi i \phi) - (1 - 2\pi i \phi)) \approx O(\phi^2) \)

In the course of proof, we have used the variational principle, the translational invariance, the boundedness of spin operators \( |\langle S^z_T; q | \hat{S}_j^+ \hat{S}_{j+r}^- | S^z_T; q \rangle| \leq 4S^2 \), and that the transverse interaction is short-range (for details, see appendix).

**Remarks**

1. Although the form of (22) seems specific for the model (2), one can prove it for general U(1) symmetric models; the multibody interactions: \( \langle \hat{S}_j \cdot \hat{S}_{j+r_1} \rangle \langle \hat{S}_{j+r_2} \cdot \hat{S}_{j+r_3} \rangle \) and the Dzyaloshinskii-Moriya type interaction: \( \langle \hat{S}_j \times \hat{S}_{j+1} \rangle \) etc. They are expressed as a sum of terms

\[
\hat{S}_j^+ \hat{S}_{j+r_1}^- \hat{S}_{j+r_2}^+ \hat{S}_{j+r_3}^- \ldots,
\]

where the number of the raising operators must be equal to the number of the lowering operators from the U(1) symmetry. Then it is easy to show the inequality (22).

2. The longitudinal interaction \( \Delta(r) \) and the magnetic field \( h \) give no restriction on Theorem 1.

3. One can prove a similar result as the Lemma 1 for the fermion \([15, 16]\) and the boson \([17]\). However, in the proof process of the Theorem 1, we have used the boundedness of operators. Thus, it is safe to apply the LSM theorem for interacting fermions systems on a lattice \([15, 16]\), whereas for the boson operator which is not bounded, one cannot prove the LSM theorem.
3.3 Nontrivial periodicity of energy spectra for rational magnetizations

**Theorem 2.** The lowest energy spectrum in the subspace of \( S^z_T = (S - m/n)L \) \((m, n \text{ are coprime integers, independent of } L)\) is non-trivially periodic as \( q \to q + 2\pi/n \) in the infinite limit:

\[
\lim_{L \to \infty} |E(S^z_T; q) - E(S^z_T; q + 2\pi/n)| = 0. \tag{24}
\]

**Proof.** From the Theorem 1, we obtain

\[
E(S^z_T; q + 2\pi ml/n) - E(S^z_T; q) \leq O(l^2/L), \tag{25}
\]

Secondly, applying the Theorem 1 to the lowest energy state with \( q + 2\pi ml/n \), we obtain

\[
E(S^z_T; q) - E(S^z_T; q + 2\pi ml/n) \leq O(l^2/L), \tag{26}
\]

therefore

\[
|E(S^z_T; q) - E(S^z_T; q + 2\pi ml/n)| \leq O(l^2/L). \tag{27}
\]

Finally, since \( m, n \) are coprime, one can choose integers \( l, k \):

\[
ml + nk = 1, \tag{28}
\]

and remembering \((\clubsuit)\), we obtain

\[
|E(S^z_T; q) - E(S^z_T; q + 2\pi/n)| \leq O(l^2/L). \tag{29}
\]

[Remarks]

1. Naively, the number of minima of the lowest energy spectrum in the Brillouin zone \((-\pi \leq q < \pi)\) should be \( n \) from the Theorem 2. However, there exist the cases where the number of minima is \( 2n, 3n, \cdots \).

2. The nontrivial periodicity of the Theorem 2 is valid only for the lowest energy spectrum.
3.4 Continuity of energy spectra for irrational magnetizations

**Theorem 3.** The lowest energy spectrum in the subspace of \( S^z_T = (S - m/n)L + \Delta S^z_T \) \((m, n\) are coprime integers, independent of \( L\); \( \Delta S^z_T\) is an integer with \( |\Delta S^z_T| \ll L\) is continuous as a function of the wavenumber \( q\) in the infinite limit, except \( \Delta S^z_T = 0\).

*Proof.* By taking the twist operator as \( \hat{U}^{tw}_{2\pi n} \), and using the Theorem 1 with (8), we obtain
\[
E(q + 2\pi n \Delta S^z_T/L) - E(q) \leq O(n^2/L). \tag{30}
\]
Conversely we can show
\[
E(q) - E(q + 2\pi n \Delta S^z_T/L) \leq O(n^2/L). \tag{31}
\]
Therefore we obtain
\[
|E(q) - E(q + 2\pi n \Delta S^z_T/L)| \leq O(n^2/L), \tag{32}
\]
that is, the lowest energy spectrum is continuous in the infinite limit. \(\square\)

[Remarks]

1. One cannot prove the continuity of the lowest energy spectrum in the \( S^z_T = (S - m/n)L \) subspace.
2. Although the lowest energy spectrum of \( \Delta S^z_T = \pm 1, \pm 2, \cdots \) is continuous, the derivative of the spectrum may be discontinuous.

4 Conclusion

We have extended the LSMK theorem including the frustrated case, because we have not used the uniqueness condition of the lowest state in each \( S^z_T \) subspace. We have also extended the LSMK theorem for the non-symmetric case, for example, the Dzyaloshinskii-Moriya interaction.

Although there are many researches on the traditional LSM theorem, almost all of them have assumed the *uniqueness of the lowest energy state for the finite system* or more restrictively the MLM (Perron-Frobenius) theorem.
Fáth and Sólyom did not mention explicitly the assumption of the uniqueness of the lowest energy state in the fixed magnetization, however, they did not discuss carefully to avoid the uniqueness assumption. Although in the original statement of LSM, the unique lowest state assumption is harmless, for further applications of the LSM theorem, for example, the magnetic plateaux where a multi-fold degeneracy may occur, or the continuity of the energy spectra, this assumption may become an obstacle. Interestingly, Affleck et al. touched that the assumption of a unique ground state can fail for some cases, but did not discuss profoundly.

Another assumption, the discrete symmetry such as the space inversion or the spin reversal or the time reversal, was introduced in and has been widely used. Although these discrete symmetries simplify the proof of the LSMK theorem (especially for multibody interactions), they exclude the non-symmetric interactions. However, reexamining the proof process, these discrete symmetries are not needed in the LSMK theorem (the first one who noticed this point was).

Another by-product of the separation of the MLM theorem and the discrete symmetry from the LSMK theorem is that the requirement of the evenness of system size \( L \) can be omitted.

When the magnetization is irrational, i.e., \( S^z = (S-m/n)L+\Delta S^z \), \( \Delta S^z = \pm 1, \pm 2, \cdots \), the lowest energy spectrum is continuous for the wave number \( q \) in the infinite limit. For the rational magnetization \( S^z = (S-m/n)L \), the lowest energy spectrum has the periodicity \( q \rightarrow q + 2\pi/n \) in the wave number space, and the energy spectrum is gapless or gapped with \( n \) (maybe \( 2n, 3n, \cdots \))-fold degeneracy (indeed there are \( 2n \)-fold degeneracy cases: Néel state in \( S=1 \) XXZ chain etc.). Note that for the gapless case, there are \( n \) (maybe \( 2n, 3n, \cdots \)) soft modes for the rational magnetization, from the periodicity \( q \rightarrow q + 2\pi/n \).

Finally, the original LSM theorem has been applied for the spin ladder model, the fermion system on the lattice, and the quantum Hall effect. It will be interesting to consider our methods for fermion models with frustrations. For the interacting boson, although the LSM-like results were expected, one can not prove the LSM theorem because the boson operator is not bounded; it would be needed some conditions, for example the hard core (repulsive) interaction, to prove the LSM-like results for the interacting boson, or boson systems might be intrinsically different from the bounded operator cases (spin or fermion).
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A Condition on the interaction range

Here we discuss the condition of the interaction range. From the latter part of (22), we obtain

\[ \sum_{r=1}^{H,L} |J(r)| |\kappa (rl/L)| = \frac{l^2}{L^2} \sum_{r=1}^{H,L} r^2 |J(r)| \left| \frac{\kappa (rl/L)}{(rl/L)^2} \right| \leq C \frac{l^2}{L^2} \sum_{r=1}^{H,L} r^2 |J(r)|, \]  

(33)

where we have used the boundedness \(|\kappa (\phi)|/\phi^2 \leq C, (C > 0)\) in the interval \(0 \leq \phi \leq l\), since \(|\kappa (\phi)|/\phi^2\) is a continuous function. Therefore, when

\[ \lim_{L \to \infty} \sum_{r=1}^{H,L} r^2 |J(r)| = \text{Constant}, \]  

(34)

we obtain the result of Theorem 1. Moreover, with the weaker condition

\[ \lim_{L \to \infty} \frac{1}{L} \sum_{r=1}^{H,L} r^2 |J(r)| = 0, \]  

(35)

we can obtain similar results as Theorems 1,2,3 with slight modifications (the condition (35) is somewhat different from [12]). Note that (35) gives only the sufficient condition for Theorem 1,2,3. Other model may be gapless or may have degenerate ground states. The S=1/2 Heisenberg chain with long-range interactions \(J(r) = 1/r^2\) [19,20] is such an example.

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