The A-Cycle Problem In XY model with Ring Frustration

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Traditionally, the transverse spin-1/2 XY model is mapped to a fermionic "c-cycle" problem, where the prior periodic boundary condition is applied to the fermionic chain and the additional boundary term has been neglected. However, the "a-cycle" problem (the original problem without any approximation) has not been treated seriously up to now. In this paper, we consider the XY model with ring frustration and diagonalize it without any approximation with the help of parity constraint. Then two peculiar gapless phases have been found.

Keywords: XY Model; ring frustration; phase diagram.

1. Introduction
The spin-1/2 XY model in a transverse magnetic filed

\[ H = \sum_{j=1}^{N} \left( \frac{1 + \gamma}{2} \sigma_j^x \sigma_{j+1}^x + \frac{1 - \gamma}{2} \sigma_j^y \sigma_{j+1}^y \right) - h \sum_{j=1}^{N} \sigma_j^z, \]  

(1)

with Pauli matrices \( \sigma^\alpha \) (\( \alpha=x, y, z \)) and ring structure \( \sigma_{N+1}^z=\sigma_1^z \) is one of the most fundamental systems endowed with interesting phenomenon, which plays a central role in the study of many-body quantum systems \[123\]. It can be mapped to a model of spinless fermions using the Jordan-Wigner transformation \( \sigma_j^x=(\sigma_j^x+i\sigma_j^y)/2=c_j^\dagger \exp \left( i \pi \sum_{l<j} c_l^\dagger c_l \right) \), which map an ↑ spin or a ↓ spin at any site to the presence or absence of a spinless fermion at that site \[4\]. Following the Jordan-Wigner transformation, Eq. (1) takes the form

\[ H = Nh - 2h \sum_{j=1}^{N} c_j^\dagger c_j + \sum_{j=1}^{N-1} \left( \gamma c_j^\dagger c_{j+1}^\dagger + c_j^\dagger c_{j+1} + h.c. \right) \]
\[- \exp(i \pi M) \left( \gamma c_N^\dagger c_1^\dagger + c_N^\dagger c_1 + h.c. \right), \]

(2)
where $M = \sum_{j=1}^{N} c_j^\dagger c_j$ is the total number of fermions. Traditionally, one can get a standard quadratic Hamiltonian which can be diagonalized easily after applying periodic boundary condition (PBC) to the fermionic chain and neglecting the additional term $[\exp(i\pi M) + 1] \left( \gamma c_N^\dagger c_1^\dagger + c_N^\dagger c_1 + h.c. \right)$ in the thermodynamic limit. This is the "c-cycle" problem for the XY model.

Recently, we have shown that for the odd-numbered antiferromagnetic Ising Model ($\gamma = 1$), i.e. the Ising Model which suffers a ring frustration, the "c-cycle" problem is not equivalent to the original periodic Ising chain even in the thermodynamic limit so we must consider the "a-cycle" problem, i.e. the original problem without any approximation. In fact, we impose PBC on the original spin model rather than on the fermionic chain and we have no reason to neglect the additional term. In this sense, the "a-cycle" problem is more appropriate. In this paper, we will focus on the "a-cycle" problem of an periodic antiferromagnetic XY chain.

The paper is organized as follows: In Section 2, we diagonalize the XY model with ring frustration for the "a-cycle" problem. In Section 3, we analyse the phase diagram. Finally, we draw our conclusion in Section 4.

2. Diagonalization

We only consider a periodic chain with an odd number of lattice sites because it suffers a ring frustration. In the limit $\hbar \to 0$, the fully anti-aligned Néel state cannot complete periodically, as it requires an even total number of spins.

Eq. (2) is not a standard quadratic Hamiltonian due to the presence of the factor $\exp(i\pi M)$. To diagonalize this Hamiltonian without any approximation, we should deal with it carefully. First, we note that though the total number of fermions $M$ does not conserve, its evenness or oddness is invariant, so that the parity of the system $P = \exp(i\pi M)$ is invariant. When $M$ is even, $P = 1$, we will refer to as even channel, we can define anti-PBC condition $c_1^\dagger = -c_{N+1}^\dagger$. When $M$ is odd, $P = -1$, we will refer to as odd channel, and we can define PBC condition $c_1^\dagger = c_{N+1}^\dagger$. In both cases, Eq. (2) can be rewritten as

$$H = N\hbar - 2\hbar \sum_{j=1}^{N} c_j^\dagger c_j + \sum_{j=1}^{N} \left( \gamma c_j^\dagger c_{j+1}^\dagger + c_j^\dagger c_{j+1} + h.c. \right)$$ (3)

The Hamiltonian Eq. (3) is quadratic form in fermion creation and annihilation operators and can be diagonalized by introducing Fourier transformation $c_q = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} c_j \exp(iqj)$ and Bogoliubov transformation $\eta_q = u_q c_q - i v_q c_q^\dagger$, where the lattice spacing $a$ is set to be unit and the momentum $q$ lies in the first Brillouin zone $(-\pi, \pi]$ and is quantized in units of $2\pi/N$. The even channel implies the momentum $q$ must take a value in the set

$$q^e = \left\{ -\frac{N-2}{N}\pi, \ldots, \frac{1}{N}\pi, \frac{1}{N}\pi, \ldots, \frac{N-2}{N}\pi, \pi \right\}.$$ (4)

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while the odd channel means the momentum \( q \) must take a value in the following set
\[
q^o = \{-\frac{N-1}{N}\pi, \ldots, -\frac{2}{N}\pi, 0, \frac{2}{N}\pi, \ldots, \frac{N-1}{N}\pi\},
\]
where the superscript \( e \) denotes even channel and \( o \) denotes odd channel\(^7\).

We can arrive at the diagonalized Hamiltonian given by
\[
H^e = 2 \sum_{q \in q^e, q \neq \pi} \omega(q) \eta_q^c \eta_q + \Lambda_e + 2(h + 1) - 2(h + 1) c^c_x c_x.
\]
\[
H^o = 2 \sum_{q \in q^o, q \neq 0} \omega(q) \eta_q^o \eta_q + \Lambda_o + |h - 1| + (h - 1) - 2(h - 1) c^o_0 c_0.
\]
with
\[
\omega(q) = \sqrt{(\cos q - h)^2 + (\gamma \sin q)^2}, \quad 2u_q v_q = \frac{\gamma \sin q}{\omega(q)}
\]
\[
u_q^2 = \frac{\omega(q) + \cos q - h}{2\omega(q)}, \quad v_q^2 = \frac{\omega(q) - \cos q + h}{2\omega(q)}
\]
\[
\Lambda_e = -\sum_q \omega(q), \quad \Lambda_o = -\sum_q \omega(q)
\]

We must notice that there is no need of Bogoliubov transformation for \( q = \pi \) and \( q = 0 \). The Hamiltonian \( H^e \) means only even number fermionic occupation states are valid states for the original spin model due to the even parity constraint, such as \(|\phi^e\rangle, \eta^1 \eta^c_c |\phi^e\rangle, \eta^1 \eta^c_c |\phi^e\rangle\), where the vacuum state \(|\phi^e\rangle\) is defined as \( c_x |\phi^e\rangle = 0\), \( \eta_q |\phi^e\rangle = 0 \) for all \( q \in q^e \neq \pi \). While the Hamiltonian \( H^o \) implies that only odd number fermionic occupation states are correct states, such as \( c^0_0 |\phi^o\rangle, \eta^1 \eta^c_c |\phi^o\rangle\), \( \eta^1 \eta^c_c |\phi^o\rangle \). Similarly, the vacuum state \(|\phi^o\rangle\) satisfies \( c^0_0 |\phi^o\rangle = 0\), \( \eta_q |\phi^o\rangle = 0 \) for all \( q \in q^o \neq 0 \). Due to the parity constraint\(^12\), the valid states for the both channels are \( 2^{N-1} \), thus we can get \( 2^N \) states totally which is in accordance with the original spin model. The core of the "a-cycle" problem lies in this parity constraint which helps us to obliterate the redundant degree of freedom in each channel exactly and reconstruct the correct states of the original spin problem. On the contrary, the parity factor \( \exp(i\pi M) \) in the "c-cycle" problem is not treated seriously\(^1\).

3. The Phase diagram

In this section we discuss the phase diagram of the transverse XY ring for the "a-cycle" problem. As shown in Fig.4\(^1\) there are two special gapless phase which is not exist in the "c-cycle" problem. As a function of \( q \), the dispersion relation \( \omega(q) \) has a minimum at the point 0 in the gapped phase and the gapless phase I. While in the gapless phase II, the point is \( k_0 \) which is given by \( k_0 = \arccos \left( \frac{h}{1-\gamma^2} \right) \). In Ref.\(^7\), the special gapless phase for the Ising case \( (\gamma = 1, h < 1) \) has been discussed.
Fig. 1. The phase diagram of the transverse XY model with ring frustration for the "a-cycle" problem. The horizontal line $h = 1$ denotes the phase transition between the gapped phase and the gapless phase I. The vertical line $\gamma = 0$, $0 < h < 1$ stands for the phase transition in the gapless phase II. The dotted line given by the equation $\gamma^2 + h - 1 = 0$, denotes the boundary between the gapless phase I and II. The ground state in the gapless phase I and gapped phase is $c^\dagger_0 |\phi_o\rangle$, the 2-fold degenerate ground states in the gapless phase II are given by $\eta^\dagger_\pi c^\dagger_\pi |\phi_e\rangle$, $\eta^\dagger_\pi -c^\dagger_\pi |\phi_e\rangle$ or $\eta^\dagger_\pi k^\dagger_\pi |\phi_o\rangle$, $\eta^\dagger_\pi -k^\dagger_\pi |\phi_o\rangle$, depending on the lattice number $N$ and parameter $h$, $\gamma$.

in detail by the aid of band structure analysis method. In the Ising case, when $h = 0$, the fully anti-aligned Neél state cannot complete periodically due to the ring frustration. Thus there has to be at least one defect, which are sometimes called kink or domain wall. The ground state is $2N$ fold degenerate because the position of the up-up or down-down kink is arbitrary. When a small transverse field is applied, as a source of quantum tunnelling, the high level of degenerate ground state would split into a gapless band. Similarly, a transverse XY ring with an odd number of lattice sites would also possess the special gapless phase. Next, we will discuss the phase diagram in detail.

In the gapped phase ($h > 1$), the lowest energy states in even channel are $\eta^\dagger_\pi c^\dagger_\pi |\phi_e\rangle$ and $\eta^\dagger_\pi -c^\dagger_\pi |\phi_e\rangle$ rather than the vacuum state $|\phi_e\rangle$ due to the presence of the minus sign in the term $-2(h+1)c^\dagger_\pi c_\pi$ in Eq. (6). The corresponding lowest energy is given by $2\omega(\pi_N) + \Lambda_e$. Likewise, the lowest energy state in odd channel is $c^\dagger_0 |\phi_o\rangle$, and its energy reads $\Lambda_o$. In the thermodynamic limit, we have $\Lambda_e = \Lambda_o = -N \int_{-\pi}^{\pi} \frac{dq}{2\pi} \omega(q)$. Compare the expression $2\omega(\pi_N) + \Lambda_e$ with $\Lambda_o$, we found that the true ground state comes from odd channel, i.e. $|GS\rangle = c^\dagger_0 |\phi_o\rangle$. And the first excited state comes from even channel. Thus the energy gap in this region is given by $2(h - 1)$ when $N \rightarrow \infty$.

In the gapless phase I ($0 < h < 1$, $\gamma^2 + h - 1 > 0$), using the same method, we can found that the ground state is also given by $c^\dagger_0 |\phi_o\rangle$. But the corresponding energy is $\Lambda_o + 2(1-h)$ rather than $\Lambda_o$, because the absolute value of the term $|h-1|$ in Eq. (7) takes different value in different regions. We can rewrite the ground state energy as $2\omega(0) + \Lambda_o$. Together with the excited energy $2\omega(\pi_N) + \Lambda_o$, $2\omega(\pi_N) + \Lambda_e$, etc. in odd channel and the excited energy $2\omega(\pi_N) + \Lambda_e$, $2\omega(\pi_N) + \Lambda_e$, etc. in even channel, they form a continuous gapless energy band in the thermodynamic limit $N(\text{odd}) \rightarrow \infty$. A quantum phase transition occurs at a value of transverse
Similarly, in odd channel, they are given by $k$ and $\omega$ limit, the ground state energy per site is given by $2\frac{\omega(k^c) + \Lambda_e}{N}$ in even channel form a continuous gapless energy band in the thermodynamic limit (m and n are integer). The energy value of the corresponding state is readily read out from the diagonalized Hamiltonian, Eq. (6) or Eq. (7).

| States | Even channel | States | Energy | States | Energy |
|--------|--------------|--------|--------|--------|--------|
| $|c^\dagger_1|\phi^c\rangle$ | $2\omega(k^c) + \Lambda_e$ | $|c^\dagger_1|\phi^c\rangle$ | $2\omega(k^c) + \Lambda_e$ |
| $|c^\dagger_1|\phi^c\rangle$ | $2\omega(k^c + \frac{\pi n}{N}) + \Lambda_e$ | $|c^\dagger_1|\phi^c\rangle$ | $2\omega(k^c + \frac{\pi n}{N}) + \Lambda_e$ |
| $|c^\dagger_1|\phi^c\rangle$ | $2\omega(k^c + \frac{\pi m}{N}) + \Lambda_e$ | $|c^\dagger_1|\phi^c\rangle$ | $2\omega(k^c + \frac{\pi m}{N}) + \Lambda_e$ |
| $\cdots$ | $\cdots$ | $\cdots$ | $\cdots$ |

Table 1. The states $\eta^\dagger_{k^{c} \pm \frac{2\pi n}{N}}|\phi^c\rangle$ (k$^c$ $\pm$ $\frac{2\pi m}{N}$ $\in$ q$^c$) in odd channel and the states $\eta^\dagger_{k^{c} \pm \frac{2\pi n}{N}}c^\dagger_1|\phi^c\rangle$ (k$^e$ $\pm$ $\frac{2\pi n}{N}$ $\in$ q$^e$) in even channel form a continuous gapless energy band in the thermodynamic limit (m and n are integer). The energy value of the corresponding state is readily read out from the diagonalized Hamiltonian, Eq. (6) or Eq. (7).

field given by $h = 1$, because the second derivative of the ground state energy per site $\int_{-\pi}^{\pi} \frac{dq}{q} \omega(q)$ has a divergent peak in this line.

In the gapless phase II ($0 < h < 1, \gamma^2 + h - 1 < 0$), as mentioned before, $\omega(q)$ has a minimum at the point $k_0$ which is given by $k_0 = \text{arccos} \left( \frac{h}{1-\gamma^2} \right)$. Thus the ground state in this phase is no longer given by $c^\dagger_0|\phi^c\rangle$. To obtain the properties in the thermodynamic limit, we can keep $N$ as a variable, and then let $N \to \infty$. The special point $k_0$ which depends on the transverse filed $h$ and the anisotropy parameter $\gamma$ may neither belong to $q^e$ nor belong to $q^o$ for an finite chain because $q^e$ and $q^o$ are quantized in units of $2\pi/N$. So the problem became even more complicated in this phase. But for an arbitrary finite chain, we can always find some special values $k^c \in q^c$ in even channel and $k^o \in q^o$ in odd channel that minimize the dispersion relation respectively. Then the 2-fold degenerate lowest energy states and the corresponding energy in even channel are $\eta^\dagger_{k^c}c^\dagger_1|\phi^c\rangle$, $\eta^\dagger_{-k^c}c^\dagger_1|\phi^c\rangle$ and $2\omega(k^c) + \Lambda_e$.

Similarly, in odd channel, they are given by $\eta^\dagger_{k^o}|\phi^o\rangle$, $\eta^\dagger_{-k^o}|\phi^o\rangle$ and $2\omega(k^o) + \Lambda_o$, respectively. The ground states can come from even channel or odd channel, depending on the lattice number $N$ and parameter $h, \gamma$. One can check that $k^c \to k_0$ and $k^o \to k_0$ as the number of lattice sites $N \to \infty$. Thus in the thermodynamic limit, the ground state energy per site is given by $2\omega(k_0)/N - \int_{-\pi}^{\pi} \frac{dq}{q} \omega(q)$. Its second derivative has a divergent peak in the line $\gamma = 0, 0 < h < 1$. The system undergoes a quantum phase transition in this line. Furthermore, to understand the formation of the gapless energy band, we also list some excited states in Table 1.

### 4. Conclusion

In this paper we have provided an extensive discussion of the "a-cycle" problem of an odd-numbered periodic antiferromagnetic XY chain, i.e. the transverse XY model with ring frustration. The presented material covers several aspects. First, we pay a special attention to the parity of the system $P = \text{exp}(i\pi M)$ which plays an important role in the "a-cycle" problem. We can diagonalize the original Hamiltonian in two
channels, depending on the parity of the system. Secondly, with the help of the parity constraint, the true ground states in different phases are obtained. When the applied transverse field is weak $h < 1$, two peculiar gapless phases are founded due to the ring frustration.

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