Bloch oscillations of multi-magnon excitations in a Heisenberg XXZ chain

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The studies of multi-magnon excitations will extend our understandings of quantum magnetism and strongly correlated matters. Here, by using the time-evolving block decimation algorithm, we investigate the Bloch oscillations of two-magnon excitations under a gradient magnetic field. Through analyzing the symmetry of the Hamiltonian, we derive a rigorous and universal relation between ferromagnetic and anti-ferromagnetic systems. Under strong interactions, in addition to free-magnon Bloch oscillations, there appear fractional bounded-magnon Bloch oscillations which can be understood by an effective single-particle model. To extract the frequencies of Bloch oscillations and determine the gradient of magnetic field, we respectively calculate the fidelity in the time domain and the sub-standard deviation in the frequency domain. Our study not only explore the interaction-induced Bloch oscillations of multi-magnon excitations, but also provides an alternative approach to determine the gradient of magnetic field via ultracold atoms in optical lattices.

I. INTRODUCTION

Heisenberg spin chain, a paradigmatic model in many-body physics, is benefit to study collective excitations and low-energy properties of quantum magnets. Particularly, the elementary aspects of quantum magnetism can be well described by spin excitations. The spin-wave theory provides a fundamental insight that magnons are the quasi-particle excitations over the ferromagnetic ground states [1, 2]. The Bethe ansatz has predicted the existence of bound states (BSs) of magnons in Heisenberg chains [3]. It renders an attractive research subjects to identify the signatures of magnons [4–7]. The quench dynamics is considered as an effective way to probe magnon BSs [8, 9]. It has demonstrated that ultracold atomic ensembles offer an ideal platform to simulate spin excitations [10, 11]. In particular, single-magnon excitations and multi-magnon BSs have been observed in cold atom experiments [12, 13].

On the other hand, if a constant force is applied, a quantum particle in a periodic potential will undergo Bloch oscillations (BOs) [14, 15]. The BOs have been directly observed with ultracold atoms [16–18]. In multi-particle systems, inter-particle interaction will have an huge influence on the BOs. For strongly interacting few-body system, novel fractional BOs can arise at a double (or multiple) Bloch frequency that of single-particle BOs [19]. Fractional BOs have been studied in various systems, such as photonic systems [20, 21], cold atom systems [22–24], electronic systems [25], etc. Similar to the BOs of an electron in a static electric field, single-magnon dynamics in spin chains subjected to a gradient magnetic field is examined [26–28]. However, the BOs of multi-magnon excitations are still unclear. In particular, how to characterize and extract the novel effects induced by the inter-magnon interactions?

This paper aims to explore two-magnon dynamics in the Heisenberg spin chain under a gradient magnetic field. We provide a dynamical symmetry analysis to explore the relation between ferromagnetic and anti-ferromagnetic systems. By analyzing the spin-spin correlations, we track the dynamical difference for different interactions via using the time-evolving block decimation (TEBD) algorithm [29, 30]. From the time-evolution of spin distributions and instantaneous spin-spin correlations, we find the dynamical signature of free-magnon BOs to bounded-magnon BOs. We also calculate the sub-standard deviation to extract the multi-frequency BOs and determine the gradient of magnetic field. This paper is organized as follows. In Sec. II, we describe the spin-1/2 Heisenberg XXZ chain within a gradient magnetic field and analyze its symmetry. In Sec. III, we simulate the BOs of two-magnon excitations via the TEBD algorithm. In Sec. IV, we calculate the sub-standard deviation in the frequency domain to extract the effects induced by the interactions and determine the magnetic field gradient. In Sec. V, we give a brief summary and discussions.

II. MAGNON EXCITATIONS AND THEIR DYNAMICAL SYMMETRY

We consider a spin-1/2 Heisenberg XXZ chain in the presence of a gradient magnetic field,

$$\hat{H} = \sum_l \left( J \hat{S}_l^+ \hat{S}_{l+1}^- + h.c. + \Delta \hat{S}_l^z \hat{S}_{l+1}^z + lB \hat{S}_l^x \right).$$

(1)
Here, $\hat{S}_l^z (i = x, y, z)$ are spin-1/2 operators for the $l$-th site, $\hat{S}_l^\pm = \hat{S}_l^x \pm i \hat{S}_l^y$ are spin raising and lowering operators for the $l$-th site, $J$ is the spin exchange energy which is set as unit (i.e. $J = \hbar = 1$), $\Delta$ is the interaction between nearest-neighbor spins, and $B$ is the magnetic field gradient.

When $B = 0$, there are three types of ground states: the critical phase in $-1 < \Delta < 1$, the ferromagnetic phase in $\Delta < -1$, and the anti-ferromagnetic phase in $\Delta > 1$. In ferromagnetic phase regime $\Delta < -1$, the excitation of a magnon is equal to the flipping of one spin $1/2$. For a sufficiently large ferromagnetic interaction $\Delta \ll 0$, the ground state is a completely ferromagnetic state $|0\rangle$ with all spin downward $\downarrow\downarrow\downarrow\downarrow\downarrow$ or upward $\uparrow\uparrow\uparrow\uparrow\uparrow$. Our initial state is chosen as the two-magnon excitations, which is prepared by flipping two neighboring spins in the completely ferromagnetic state $\downarrow\downarrow\downarrow\downarrow\downarrow$.

The Hamiltonian (1) exhibits a $U(1)$ symmetry under global spin rotations around the $z$-axis and the number of its total magnetization $\hat{S}^z = \sum_l \hat{S}_l^z$ is conserved (i.e. $[\hat{H}, \hat{S}^z] = 0$). This means that the subspaces with different numbers of spin excitations are decoupled. Using the mapping: $|l\rangle \leftrightarrow |0\rangle$, $|l\rangle \leftrightarrow |1\rangle$, $\hat{S}_l^+ \leftrightarrow \hat{a}_l^+ \hat{S}_l^z \leftrightarrow \hat{a}_l^+ - \hat{n}_l - \frac{1}{2}$, the Hamiltonian (1) can be mapped onto $\hat{H} = \sum_l \left( \frac{1}{2} \hat{a}_l^+ \hat{a}_{l+1} + h.c. + \Delta \hat{n}_l \hat{n}_{l+1} + B \hat{n}_l \right)$, with $\hat{n}_l = \hat{a}_l^+ \hat{a}_l$. Here, $\hat{a}_l^+$ is particle creation (annihilation) operator at the $l$-th site and they satisfy the commutation relations for hard-core bosons. Thus one can understand the two-magnon excitations in the picture of two hard-core bosons.

Inter-magnon interaction is a key ingredient in the formation of BSS and also has an influence on the dynamics. Intuitively, ferromagnetic interactions ($\Delta < 0$) and anti-ferromagnetic ones ($\Delta > 0$) may affect the dynamics in different ways. Nevertheless, a symmetry protected dynamical symmetry (SPDS) theorem [31] indicates that different interactions are related and the certain symmetry of the static Hamiltonian can guarantee the interaction-induced dynamical symmetry. Different from the single-point operators in [31], we extend its conclusions to two-point operators. According to the SPDS theorem, we divide the Hamiltonian (1) into two parts $\hat{H} = \hat{H}' + \hat{H}''$ with

$$\hat{H}' = \sum_l \frac{1}{2} \left( \hat{S}_l^+ \hat{S}_{l+1}^- + \hat{S}_l^- \hat{S}_{l+1}^+ \right),$$

and

$$\hat{H}'' = \Delta \sum_l \hat{S}_l^x \hat{S}_l^z + \sum_l lB \hat{S}_l^z.$$  

For the system with only nearest-neighbor spin exchange, one can decompose it as odd-lattices $\mathcal{A}$ and even-lattices $\mathcal{B}$, thus we can define an operator $\hat{W}$ related to the bipartite lattice symmetry,

$$\hat{W}^{-1} \hat{S}_l^- \hat{W} = \begin{cases} \hat{S}_l^-, & \text{if } l \in \mathcal{A}, \\ -\hat{S}_l^- & \text{if } l \in \mathcal{B}. \end{cases}$$

Combining with the time-reversal operator $\hat{R}$, we find an operator $\hat{Q} = \hat{R} \hat{W}$ ensuring that $\hat{Q}$ anti-commutes with $\hat{H}'$ and commutes with $\hat{H}''$,

$$\{\hat{Q}, \hat{H}'\} = 0, \quad [\hat{Q}, \hat{H}''] = 0.$$  

In order to reveal the spin correlation, we concentrate on initial states which are two-magnon excitations at the adjacent sites, $|\psi(0)\rangle = \hat{S}_{l_0}^z \hat{S}_{l_1}^z |0\rangle$, where $|0\rangle = \downarrow\downarrow\downarrow\downarrow\downarrow$. The initial states are naturally invariant under the transformation $\hat{Q}$, just adding a global phase,

$$\hat{Q}^{-1} |\psi(0)\rangle = - |\psi(0)\rangle,$$

and the spin correlation between $l'$ and $l''$ sites at time $t$ is defined as

$$C_{l',l''}(t) = \langle \psi(t) | \hat{S}_{l'}^z \hat{S}_{l''}^z | \psi(t) \rangle.$$  

Obviously, the two-spin operator $\hat{S}_{l'} \hat{S}_{l''}$ satisfies

$$\hat{Q}^{-1} \hat{S}_{l'} \hat{S}_{l''} \hat{Q} = \hat{S}_{l'''} \hat{S}_{l''},$$

Combining Eqs. (5),(6),(8) with the identity $\hat{Q}^{-1} e^{-iHt} \hat{Q} = e^{-iHt} \hat{Q}$, we obtain,

$$C_{l',l''}(t) \Delta_{l',l''} = \langle \psi(0) | e^{i(H'+H'')t} \hat{S}_{l'}^z \hat{S}_{l''}^z e^{-i(H'+H'')t} | \psi(0) \rangle = \langle \psi(0) | \hat{Q} e^{i(H'+H'')t} \hat{S}_{l'}^z \hat{S}_{l''}^z \hat{Q}^{-1} e^{-i(H'+H'')t} | \psi(0) \rangle = \langle \psi(0) | e^{i(H'-H'')t} \hat{S}_{l'}^z \hat{S}_{l''}^z e^{-i(H'-H'')t} | \psi(0) \rangle = C_{l',l''}(t) \Delta_{l',l''}.$$  

This means that the time-dependent spin correlation is the same when we simultaneously change the signs of interaction $\Delta$ and magnetic field gradient $B$. We can find a direct connection between the spin correlations with $(\Delta,B)$ and $(-\Delta,-B)$. When the sign of gradient magnetic field is flipped, the system is invariant if we reverse the lattice around the center position of the initial state $l_c^0 = 1/2$, this is, the lattice index is changed from $l$ to $2l_c - l$. The relation (9) is further given as

$$C_{l',l''}(t) \Delta_{l',l''} = C_{2l_c - l' - l''} \Delta_{l',l''}.$$  

Thus we can conclude

$$C_{l',l''}(t) \Delta_{l',l''} = C_{2l_c - l' - l''} \Delta_{l',l''}.$$  

which indicates that, when the sign of interaction $\Delta$ is changed, the time-evolution of spin correlation is symmetrical about the center position of the initial state $l_c^0$.

In Fig. 1, we compare the spin correlation $C_{-10,-9}(t)$ with anti-ferromagnetic interaction $(-\Delta)$ and the spin correlation $C_{10,11}(t)$ with ferromagnetic interaction $(\Delta)$. The parameters are chosen as $\Delta = -1.5$, $B = 0.05$ and the total chain length $L_t = 101$. The numerical results completely follow the relation (11). This is to say, once we know the spin correlation under ferromagnetic interaction, we can deduce the results under antiferromagnetic interaction. Therefore, below we only consider the system with ferromagnetic interactions $\Delta < 0$. 

FIG. 1. (Color online) Dynamical symmetry of spin correlations under the parameters ($\Delta, B$) and ($-\Delta, B$). The time-evolution of two-spin correlations in 10th and 11th with ferromagnetic interaction (left half) and the ones in -10th and -9th with anti-ferromagnetic interaction (right half).

III. SIGNATURE OF BLOCH OSCILLATIONS IN SPIN CORRELATIONS

In this section, we consider how the interactions affect the dynamics of spin excitations under a gradient magnetic field. The initial state is chosen as $|\downarrow...\downarrow\uparrow\uparrow\downarrow...\downarrow\rangle$, which is a two-spin excitation at the adjacent central sites. In the time-evolution, the spin excitations will undergo BOs. To show the interaction effects on BOs, we calculate the spin distributions $S^z_l(t) = \langle \psi(t) | \hat{S}^z_l | \psi(t) \rangle$ (12) as a function of time, and the instantaneous correlations $C_{l',l''}(t) = C_{l',l''}/C_{l',l''}^{\text{max}}$ at the different times marked as A-E in (a). The parameters are chosen as $\Delta = 0, B = 0.05$, and the total chain length $L_t = 101$.

Since there is no interaction, each magnon behaves as a free particle and the time-evolution recovers the breathing mode in the single-particle BOs.

In Fig. 2 (b)-(f), we show the spin-spin correlations $C_{l',l''} = \langle \hat{S}^z_{l'} \hat{S}^z_{l''} \rangle$ at different times: A($t = 0$), B($t = T_B/4$), C($t = T_B/2$), D($t = 3T_B/4$) and E($t = T_B$). In one period, the spin-spin correlation behaves like a cross for each instantaneous state. As the spin excitations expand and shrink, the region of cross becomes larger at B($t = T_B/4$), reaches the maximum at C($t = T_B/2$), gradually decreases at D($t = 3T_B/4$) and finally recovers the initial state at E($t = T_B$). The wide of the crosses in Fig. 2 (b)-(f) are in excellent agreement with the wide of spin distributions in (A)-(E) in Fig. 2 (a), respectively.

A. Dynamics of free magnons

We first consider the BOs of magnons in a noninteracting system. The eigen-values form a Wannier-Zeeman ladder with equidistant level spacing $\Delta E = B$ [32], which directly gives the Bloch frequency. We numerically compute the time-evolution of the spin-spin correlations via the TEBD algorithm. The parameters are chosen as $\Delta = 0, B = 0.05$, and the total chain length $L_t = 101$. The noninteracting magnons independently undergo BOs with period $T_B = \frac{2\pi}{\Delta B}$, see Fig. 2 (a). The spin excitations periodically widen and shrink in an interval $|l| < \frac{2}{B} \sin Bt$ (13).

B. Dynamics of strongly interacting magnons

Under strong interactions, through implementing the many-body degenerate perturbation analysis, we derive an effective single-particle Hamiltonian and explore the interaction-induced fractional BOs [34-37].

Under the condition of $|\Delta| \gg (1/2, |B|)$, one can treat
the hopping term and the gradient magnetic field term
\[ \hat{H}_1 = \frac{1}{2} \sum_l (\hat{S}_l^z \hat{S}_{l+1}^- + \hat{S}_l^z \hat{S}_{l+1}^+) + \sum_l i B \hat{S}_l^z, \] (14)
as a perturbation to the interaction term
\[ \hat{H}_0 = \Delta \sum_l \hat{S}_l^+ \hat{S}_{l+1}^-. \] (15)
The effective single-particle Hamiltonian can be written as
\[ \hat{H}_{\text{eff}} = \frac{1}{4\Delta} \sum_m (\hat{C}_m^+ \hat{C}_{m+1}^+ + \hat{C}_m^+ \hat{C}_m^-) + \sum_m 2Bm \hat{C}_m^+ \hat{C}_m^-, \] (16)
whose detailed derivation can be found in Appendix (A). Here, the operator \( \hat{C}_m^+ = \hat{S}_m^+ \hat{S}_{m+1}^+ \) means simultaneously flipping two adjacent spins at \( m \)-th and \((m + 1)\)-th sites, and \( \hat{C}_m^- = (\hat{C}_m^+)^\dagger \). The two-magnon excitations behave like a single particle in the tilted lattices with doubled frequency \( \omega_B^f/2 = 2B \). The two magnons tend to travel together and undergo fractional BOs, see Fig. 3(a). The initial state and parameters are the same as those in Fig. 2, except for \( \Delta = -5 \). The spin distribution width is given as
\[ \langle |l| \rangle < \frac{1}{2\Delta B} \sin(Bt). \] (17)
Compared with Fig. 2(a), the distribution width is reduced by a factor of \( 1/(4\Delta) \) while the oscillation frequency becomes double. The numerical results are well consistent with the analytical ones (17).

The spin-spin correlations \( C_{\nu,\nu'} = \langle \hat{S}_\nu^z \hat{S}_{\nu'}^z \rangle \) reveal the effective single-particle dynamics. Similarly, in one period, the spin-spin correlations behave like a cross for each instantaneous state, see Fig. 3(b)-(f). As the spin distributions expand and shrink, the region of cross reaches the maximum at B(t = \( T_B/4 \), recovers the initial state at C(t = \( T_B/2 \), increases to the maximum again at D(t = \( 3T_B/4 \) and finally recovers the initial state again at E(t = \( T_B \). It clearly manifests that the two strongly interacting magnons undergo a breathing motion with the half-period of the free-magnon breathing motion. The width of the crosses in Fig. 3(b)-(f) are in excellent agreement with the width of spin distributions in (A)-(E) in Fig. 3(a), respectively.

C. Dynamics of moderately interacting magnons

At last, we study the dynamics of two-magnon excitations in the moderate-interaction case. The initial state and the parameters are the same as those in Fig. 2 except for \( \Delta = -1.5 \). The spin distributions exhibit the coexistence of two breathing modes, see Fig. 4(a). The outer and inner breathing modes correspond to the oscillations of free magnons and bounded magnons, respectively. This is because that the initial state is prepared as the superposition of scattering and bound states (see Appendix (B) for more details). Nevertheless, the outer breathing mode is slightly asymmetric about the initial position \( t_0 \), different from the breathing mode of free magnons. The asymmetry may come from the interaction-induced scattering of free magnons.

Similar to the spin distributions, the instantaneous spin-spin correlations also show the coexistence of inner and outer pattern, see Fig. 4(c)-(f) for different times: B(t = \( T_B/4 \), C(t = \( T_B/2 \), D(t = \( 3T_B/4 \) and E(t = \( T_B \). The correlations partially recover the initial correlations at C(t = \( T_B/2 \). This is because that the bound-state component returns to the initial ones while the scattering-state component is not yet. At E(t = \( T_B \), both two components return to the initial state, see Fig. 4(f).

So far, we examine the role of spin-spin interaction on the dynamics of magnon excitations among the spin chain. By increasing the interaction strength, one may observe clear enhancement of the correlated tunneling of two magnons. Moreover, the spin-spin correlations can be utilized to characterize the multi-magnon BOs.
FIG. 4. (Color online) The Bloch dynamics of two moderately interacting magnons. (a) The spin distributions $S^z(t)$ versus the rescaled time $t/T_B$. (b)-(f) The rescaled instantaneous correlations $C_{\ell',\ell''} = C_{\ell',\ell''}/C_{\ell',\ell''}^{\max}$ at the different time marked as A-E in (a). The parameters are the same as those in Fig. 2 except for $\Delta = -1.5$.

IV. EXTRACTING MAGNETIC FIELD GRADIENT FROM MULTI-MAGNON BLOCH OSCILLATIONS

In this section, we discuss how to determine the magnetic field gradient from the multi-magnon BOs. When two-magnon excitations are launched on the adjacent central sites of the spin chain under a gradient magnetic field, it may exhibit a dynamical localization in a period. The time-dependent spin distributions and spin-spin correlations both show the coexistence of two components when the interaction strength is moderate. However, we cannot accurately determine the magnetic field gradient (which determines the Bloch frequency) via the spin distributions or spin-spin correlations. Below, we analyze the fidelity in the time domain and the sub-standard deviation in the frequency domain to extract the gradient of magnetic field and the Bloch frequency.

A. Fidelity in time domain

In this subsection, we present how to use the time-dependent fidelity to extract the multi-frequencies of BOs, especially when the bound-state component and scattering-state component coexist. By simulating the time-evolution with the TEBD algorithm, we calculate the time-dependent fidelity

$$F(t) = |\langle \Psi(0)|\Psi(t) \rangle|^2.$$  \hspace{1cm} (18)

It characterizes the probability of the time-evolved state returning to the initial state.

FIG. 5. (Color online) Fidelity versus the rescaled time $t/T_B$ for different values of $\Delta$: (a) 0, (b) $-1$, (c) $-1.5$ and (d) $-5$. The other parameters are chosen as $B = 0.05$ and the total chain length $L_t = 101$.

A slight change of the interaction may have a huge influence on the dynamics. We discuss the fidelity versus the rescaled time $t/T_B$ for different interaction strengths $\Delta$: (a) 0, (b) $-1$, (c) $-1.5$ and (d) $-5$, see Fig. 5. The gradient of magnetic field is chosen as $B = 0.05$, and the total length of spin chain is $L_t = 101$. For clear visibility, the evolution time is set to be $t = 4T_B$. Without interaction, the sharp peaks perfectly emerge at the integer multiple of period $T_B$, see Fig. 5(a). When the interaction increases, in addition to the peaks at the integer multiple of period $T_B$, there also appear peaks at the integer multiple of half-period $T_B/2$, see Fig. 5(b)-(d). For the moderate-interaction strength $\Delta = -1.5$, we find the coexistence of peaks at both the integer multiple of periods $T_B/2$ and $T_B$, see Fig. 5(c). The period $T_B$ and half-period $T_B/2$ correspond the the free-magnon Bloch frequency $B$ and the bounded-magnon Bloch frequency $2B$. For stronger interaction strength $\Delta = -5$, the dynamics transfers from the independent BOs to the effective single-magnon BOs, and the half-period oscillation of fidelity is dominant, see Fig. 5(d). To explain how the interaction affects the fidelity, we project the initial state onto the scattering and the bound states. We find that the occupation on BSs becomes larger as the interaction increases (see Appendix (B) for more details). Thus the peaks at the half-period $T_B/2$ become higher as the interaction increases.

There are two typical schemes to measure the force based on the delocalization-enhanced BOs and driving resonance tunneling effects [38]. Here we find that, once
we determine the position of the peak of fidelity, the magnetic field gradient can be accurately given. However, when the free-magnon component dominates in the weak interaction case, it is difficult to distinguish the bound-state component from the scattering-magnon component by directly observing the time-evolution of the fidelity. Under such a moderate interaction, the periodicity of fidelity is destroyed due to the appearance of irregular behaviors (such as quantum chaos), see Fig. 5(b). In the next subsection, we will consider another observable to distinguish different BOs as well as precisely extract the gradient of magnetic field.

B. Sub-standard deviation in frequency domain

In above, it has been found that two-magnon BSs undergo fractional BOs with frequency doubling. The frequency doubling appears in the power spectrum is an excellent indicator for judging the appearance of two-magnon BSs. Here, we will analyze the frequency spectrum of the time-dependent generalized deviation,

$$D^x(t) = \sum_l \langle \hat{S}_l^z \rangle + 1/2 \langle l(t) - l_c(t) \rangle^x,$$  \hspace{1cm} (19)

which can characterize the fluctuation of spin excitations in spatial distribution. Here $\langle \hat{S}_l^z \rangle$ represents the spin magnetization at site $l$ and $l_c$ is the centroid of the time evolved state. When $x = 2$, the generalized deviation becomes traditional standard derivation. Instead of traditional standard deviation, we define the super-standard deviation for $x > 2$ and sub-standard deviation for $x < 2$ to highlight the bounded and free magnons, respectively. After a series of trials, we find that one may choose sub-standard deviation with $x = 1/2$ to extract the multiple Bloch frequencies.

The time-dependent sub-standard deviations show that the spatial region of spin excitations decreases as the interaction strength increases, see the insets in Fig. 6. Making a fast Fourier transform of the sub-standard derivations to obtain $f(\omega)$, one can observe sharp peaks center at the multiple of $\omega_B$ in the frequency domain. The maximum peak centers at $\omega_B$ for noninteracting systems, see Fig. 6(a). As the interaction increases, the peak at $\omega_B$ becomes lower while the peak at $2\omega_B$ becomes higher, and the peak at $2\omega_B$ becomes dominant under strong interactions, see Fig. 6(b)-(d). Since the peaks at $\omega_B$ and $2\omega_B$ are mainly induced by BOs of scattering and bounded magnons, respectively, the dominant of peak at $2\omega_B$ is a clear signature of two-magnon BSs. Numerical results reveal that, when the interaction strength increases, the individual magnon BOs gradually vanish while the bounded-magnon fractional BOs become dominant.

The Fourier transform $f(\omega)$ can not only efficiently reflect the oscillation mode with different frequencies, but also provide a method to precisely determine the magnetic field gradient $B$. The sharp peak at $\omega_B$ enables us to extract the accurate value of $B$. Compared with measuring the fidelity, measuring $f(\omega)$ gives more accurate value of the magnetic field gradient, even in the weak interaction regime.

V. SUMMARY AND DISCUSSIONS

In this work, through considering a Heisenberg XXZ chain under a gradient magnetic field, we study how the interaction affects the BOs of two-magnon excitations and give a quantitative methods to extract the magnetic field gradient from the multi-frequency BOs. We extend the theory of dynamical symmetry of single-point operators to the one of two-point operators, and find that the dynamics in anti-ferromagnetic systems can be directly derived from the corresponding ferromagnetic ones. As the interaction increases, we find that the spin distribution or spin-spin correlation dynamics gradually transfers from BOs of free magnons to the fractional BOs of bounded magnons. The interaction-induced fractional BOs provide a new perspective to observe the BSs. Moreover, we use the fidelity in the time domain and the sub-standard deviation in the frequency domain to probe the multi-frequency BOs and determine the magnetic field gradient. The sub-standard deviation is an excellent candidate to probe the magnon BSs and accurately determine the magnetic field gradient.

Based on the current techniques in engineering ultracold atoms, it is possible to simulate our Heisenberg spin chain. By loading two-state $^{87}$Rb atoms into a one-dimensional optical lattice in the Mott regime with one particle per lattice site, the two hyperfine states with different magnetic dipole moments can be labeled as spin-up and spin-down, respectively. Applying a gradient magnetic field along the lattice, our spin-dependent lattices

![FIG. 6. (Color online) The Fourier transform of the sub-standard deviation for different values of $\Delta$: (a) 0, (b) $-1$, (c) $-1.5$ and (d) $-5$. The insets are the sub-standard deviation versus the rescaled time $t/T_B$. The other parameters are chosen as $B = 0.05$ and the total chain length $L_t = 101$.](image-url)
can be realized. The dynamics of spin density distribution and spin-spin correlation can be tracked via the techniques of atomic microscope [12, 13]. The interaction between magnons can be tuned via Feshbach resonance techniques [39, 40]. With the observed spin density distributions and spin-spin correlations, the fidelity and the sub-standard deviation can be given.

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Appendix A: Effective single-particle Hamiltonian for strongly interacting magnons

Under strong ferromagnetic interactions, the magnons prefer to travel together instead of the individual propagation. In order to explain this phenomena, we analytically construct an effective single-particle Hamiltonian by using the many-body degenerate perturbation theory.

When $|\Delta| \gg (1/2, |B|)$, we can divide the Hamiltonian into the $\hat{H}_0$ as a dominant term and $\hat{H}_1$ as a perturbation term. In the two-magnon basis $\{|l_1' l_2' \rangle = \hat{S}_l^{+} \hat{S}_l^{+} |0\rangle : -L \leq l_1' < l_2' \leq L\}$, the $\hat{H}_0$ consists of two subspaces $\mathcal{U}$ and $\mathcal{V}$. The total chain length $L_t = 2L + 1$. The degenerate eigen-states $\{|G_m\rangle = |m, m+1\rangle : -L \leq m \leq L\}$ form the subspace $\mathcal{U}$ with eigen-values $E_0 = \Delta$. Correspondingly, the degenerate eigen-states $\{|E_{l_1 l_2}\rangle = |l_1, l_2\rangle : l_1 \neq l_2 \pm 1, -L \leq l_1 < l_2 \leq L\}$ form the subspace $\mathcal{V}$ with eigen-values $E_1 = 0$. The projection operators define as $\hat{P}_U = \sum_m \langle G_m | \langle G_m \rangle$ onto $\mathcal{U}$ and $\hat{P}_V = \sum_{l \neq l_1, \pm 1} \frac{E_0 - E_l}{E_0 - E_{l_1}} |E_{l_1 l_2}\rangle \langle E_{l_1 l_2}|$ onto $\mathcal{V}$. The second-order effective Hamiltonian is written as

$$\hat{H}_{eff} = \hat{h}_0 + \hat{h}_1 + \hat{h}_2$$

$$= E_0 \hat{P}_U + \hat{P}_U \hat{H}_1 \hat{P}_U + \hat{P}_U \hat{H}_1 \hat{P}_U \hat{H}_1 \hat{P}_U. \quad (A1)$$

The first-order perturbation reads as

$$\hat{h}_1 = \hat{P}_U \hat{H}_1 \hat{P}_U$$

$$= \sum_{l, m, m'} \langle G_m | \langle G_m | (lB \hat{S}_l^{+}) | G_{m'} \rangle \langle G_{m'} |. \quad (A2)$$

Since

$$\sum_l \langle G_m | (lB \hat{S}_l^{+}) | G_{m'} \rangle$$

$$= B \delta_{mm'} \sum_l (\delta_{lm} + \delta_{l, m+1} - \frac{1}{2})$$

$$= B \delta_{mm'} (2m + 1), \quad (A3)$$

we have

$$\hat{h}_1 = B \sum_m (2m + 1) |G_m\rangle \langle G_m |. \quad (A4)$$

The second-order perturbation reads as

$$\hat{h}_2 = \hat{P}_U \hat{H}_1 \hat{P}_U$$

$$= \frac{1}{4\Delta} \sum_{mm', l, l_1 l_2} |G_m\rangle \langle G_m| (\hat{S}_l^{+} \hat{S}_{l_1}^{+} + \hat{S}_l^{-} \hat{S}_{l_1}^{-}) |E_{l_1 l_2}\rangle$$

$$\times \langle E_{l_1 l_2}| (\hat{S}_l^{+} \hat{S}_{l_1}^{+} + \hat{S}_l^{-} \hat{S}_{l_1}^{-}) |G_{m'}\rangle \langle G_{m'} |. \quad (A5)$$

After a careful calculation, we have

$$\hat{h}_2 = \hat{P}_U \hat{H}_1 \hat{P}_U \hat{P}_V \hat{H}_1 \hat{P}_U$$

$$= \frac{1}{4\Delta} \sum_m (|G_m\rangle + |G_{m+1}\rangle) \langle G_m + G_{m+1} |. \quad (A6)$$

Combing Eqs. (A4) and (A6), we derive the effective single-particle Hamiltonian up to the second order

$$\hat{H}_{eff} = \frac{1}{4\Delta} \sum_m (|G_m\rangle + |G_{m+1}\rangle) \langle G_m + G_{m+1} |$$

$$+ B \sum_m (2m + 1) |G_m\rangle \langle G_m |$$

$$+ \Delta \sum_m |G_m\rangle \langle G_m |. \quad (A7)$$

We introduce the operator $\hat{C}_m^{+} = \hat{S}_m^{+} \hat{S}_{m+1}^{+}$, which means simultaneously flipping two adjacent spins at $m$-th and $(m + 1)$-th sites from the vacuum state $|0\rangle = |\downarrow \downarrow \ldots \downarrow\rangle$, and $\hat{C}_m = (\hat{C}_m^{+})^{\dagger}$. Therefore, the bound pairs behave as a composite particle following the Hamiltonian

$$\hat{H}_{eff} = \frac{1}{4\Delta} \sum_m (\hat{C}_m^{+} \hat{C}_{m+1} + \hat{C}_{m+1}^{+} \hat{C}_m)$$

$$+ \sum_m 2Bm \hat{C}_m \hat{C}_m^{+}, \quad (A8)$$

where the energy constant is omitted.

Comparing with free magnons, the formation of bound pairs performs BOs with the doubled frequency.

Appendix B: Two-magnon energy spectrum

To explain the interaction effects on magnon dynamics, we calculate the overlaps of initial state with the scattering and bound states in the absence of gradient magnetic field.

Since $[\hat{H}, \hat{S}^z] = 0$ with $\hat{S}^z = \sum_l \hat{S}_l^z$, the total spin excitations number is conserved and all states keep evolving in the two-magnon Hilbert space. The two-magnon Hilbert space is spanned by the basis $B^{(2)} = |l_1' l_2' \rangle = \hat{S}_l^{+} \hat{S}_l^{+} |0\rangle$ with $-L \leq l_1' < l_2' \leq L$ and the total chain length $L_t = 101$. The eigen-states can be expressed
FIG. 7. (Color online) Two-magnon energy spectrum. The two-magnon energy spectrum for $B = 0$, $L_z = 101$ and different values of $\Delta$: (a) 0, (b) −1, (c) −1.5 and (d) −5. In which, the overlaps $P_{K,r}$ between the initial state with each eigen-states are denoted by the colorbar.

as $|\Psi\rangle = \sum_{l_1 < l_2} \Psi_{l_1 l_2} |l_1 l_2\rangle$ with $\Psi_{l_1 l_2} = \langle 0 | \hat{S}_{l_2}^+ \hat{S}_{l_1}^- | \Psi \rangle$. Thus the system satisfies the following eigen-equation

$$E \Psi_{l_1 l_2} = \frac{1}{2} \left( \Psi_{l_1 l_2+1} + \Psi_{l_1 l_2-1} + \Psi_{l_1+1 l_2} + \Psi_{l_1-1 l_2} \right) + \Delta (\delta_{l_1 l_2+1} \delta_{-L L} - \delta_{l_1 l_2-1} \delta_{-L L}) \Psi_{l_1 l_2}. \quad (B1)$$

In the absence of gradient magnetic field, the Heisenberg XXZ chain has a co-translational symmetry and the center-of-mass quasi-momentum is a good quantum number under the periodic boundary condition. The motion of the two-magnon excitations consists of the motion of the center-of-mass $R = \frac{1}{2} (l_1 + l_2)$ and the relative position $r = l_1 - l_2$. Defining $\Psi_{l_1 l_2} = e^{iK R} \phi(r)$, the eigen-equation (B1) reads

$$E \phi(r) = \frac{K}{2} (\phi(r - 1) + \phi(r + 1)) + \Delta \delta_{r, \pm 1} \phi(r), \quad (B2)$$

where $J_K = \cos(\frac{K}{2})$. Under the periodic boundary conditions, we find $e^{iK R} = 1$ and $\phi(r + L_t) = e^{iK L_t/2} \phi(r)$ with the quasi-momentum $K = 2\pi \alpha / L_t$ (with $\alpha = -L, -L + 1, ..., L$). Moreover, we have $\phi(0) = 0$ and $\phi(r) = \phi(-r)$ with the commutation relations.

We give the two-magnon energy spectrum by numerically diagonalizing the Hamiltonian without a gradient magnetic field. With the nearest-neighbor ferromagnetic interaction, the two magnons are able to form BSs. When the interaction $|\Delta| > 1$, the energy spectrum shows that BSs (corresponding to the lower band) completely separate from the scattering states (SSs). After calculating the overlaps

$$P_{K,r} = |\langle \psi_{K,r} | \psi(0) \rangle|^2, \quad (B3)$$

we exactly reveal the proportion of initial state in each eigen-states $\psi_{K,r}$, see the color of energy spectrum in Fig. 7. The interaction values $\Delta$ are set as (a) 0, (b) −1, (c) −1.5 and (d) −5. The proportion in SSs makes the spins undergo independent BOs, while the proportion in BSs induces the correlated and fractional BOs. Once the initial state strongly overlaps with BSs, one can clearly observe the signature in the time-evolution of spin distributions. As the interaction increases, the overlaps with BSs become larger and the BOs of bounded magnons become dominant.

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