

Spin waves in antiferromagnetic spin chains with long-range interactions

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We study antiferromagnetic spin chains with unfrustrated long-range interactions that decay as power laws with exponent β , using the spin-wave approximation. We find for sufficiently large spin S that the Neel order is stable at $T=0$ for $\beta < 3$, and survives up to a finite Neel temperature for $\beta < 2$, validating the spin-wave approach in these regimes. We estimate the critical values of S and T for the Neel order to be stable. The spin-wave spectra are found to be gapless but have nonlinear momentum dependence at long wavelength, which is responsible for the suppression of quantum and thermal fluctuations and stabilizing the Neel state. We also show that for $\beta \leq 1$ and for a large but finite-size system size L , the excitation gap of the system approaches zero slower than L^{-1} , a behavior that is in contrast to the Lieb-Schultz-Mattis theorem.

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I. INTRODUCTION

Antiferromagnetic (AF) spin chains have attracted considerable interest of physicists in the last two decades, and continue to be a subject of active research at present. There are several reasons why they are of such strong interest. First, quantum antiferromagnetic spin chains are important examples of a larger class of strongly correlated systems, whose ground state and low-energy behavior differ from their higher-dimensional counterparts in qualitative ways. In the case of AF spin chains, quantum fluctuations destroy the Neel order in the ground state no matter how big the size of the spin is, while in higher dimensions the Neel order is stable regardless of spin size, in the absence of frustration. Second, the spin chains are of interest to physicists because they are ideal playgrounds for various types of theoretical approaches. A prominent example here is the work of Haldane,¹ who mapped the AF spin chains to quantum nonlinear σ models and predicted that the integer chains have a gap in their excitation spectra while no gap exists for half-integer chains, based on the absence or presence of a topological term in the mapping. This fundamental difference is consistent with, and to a certain degree implied in, the Lieb-Schultz-Mattis (LSM) theorem,² which states that for Heisenberg AF chains with length L and periodic condition, for half-integer spins, there exists an excited state with energy separated from the ground state that is of order $1/L$; no such theorem exists for integer chains however.

The studies of AF spin chains, and the results mentioned above, are restricted to models with short-range interactions. In this work we study AF chains with interactions that decay as power laws and without frustration:

$$H = \sum_{ij} (-1)^{i-j+1} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j, \quad (1)$$

with

$$J_{ij} = J/|i-j|^\beta, \quad (2)$$

where $J > 0$ determines the overall energy scale of the system and β is the power-law exponent that controls the decay of the interaction. The factor $(-1)^{i-j+1}$ ensures that spins

sitting on opposite sublattices have antiferromagnetic interactions and those sitting on the same sublattice have ferromagnetic interactions, thus there is no frustration. Our motivation for the study comes from the following considerations. First, such power-law long-range interactions can, in principle, be realized in experimental systems; one example of which being the Ruderman-Kittel-Kasuya-Yosida³ interaction mediated by conduction electrons that decay as power laws, with an exponent that depends on the details of the conduction-electron Fermi surface. Second, as we will show, such long-range interactions tend to suppress quantum as well as thermal fluctuations, thus increasing the range of interaction has an effect that is somewhat similar to increasing the dimensionality of the system. On the other hand, the dimensionality is discrete while the power-law exponent for the interaction can be tuned continuously, thus providing a tuning parameter for the fluctuations; it is of interest to study how the system behaves under such tuning.

Anticipating the stability of the Neel order in the presence of such long-range interactions, we study the models using the spin-wave method. We obtain the following results.

(i) We show that the Neel order is stable at zero temperature for $\beta < 3$ and sufficiently large S , justifying the usage of spin-wave method in this case. We also estimate the critical size of the spin for the Neel order to be stable, as a function of β .

(ii) In this case the spin-wave excitation spectra take the form $\omega_k \sim k^\gamma$ in the long wavelength, with $\gamma < 1$ and varying continuously with β .

(iii) Extending the spin-wave calculation to finite temperature, we show that the Neel transition temperature T_N is zero for $\beta \geq 2$ while finite for $\beta < 2$. We determine T_N as a function of S and β .

(iv) For a finite-size system with size L and periodic boundary condition, and $\beta \leq 1$, we find that the lowest excitation energy approaches zero slower than $1/L$ as L increases for both half-integer and integer spins, thus “violating” the LSM theorem. Of course the LSM theorem applies to spin chains with short-range interaction only; here we have provided explicit examples of how it is invalidated by the presence of long-range interaction.

The remainder of the paper is organized as follows. In Sec. II we discuss the application of spin-wave technique to this model. In Secs. III and IV we present and discuss the significance of our results. In Sec. V we summarize our work and discuss the implications of our results.

II. THE SPIN-WAVE APPROACH

We consider a Heisenberg antiferromagnetic chain with unfrustrated power-law long-range interaction with the Hamiltonian given by Eq. (1). The central issue we address in this work is the stability of Neel state at zero or low temperature. It is thus natural to use the spin-wave method based on the Holstein-Primakoff transformation⁴ that maps spin operators to boson operators, and check its self-consistency. The procedure is rather standard;⁵ we nevertheless include the details here for the sake of completeness and establish notation for later treatment. We divide the chain into two sublattices and represent the spin operators in terms two types of bosons: a bosons which live on A sublattice and b bosons which live on B sublattice. Up to order $1/S$, where S is the size of spin, the Holstein-Primakoff transformation for the spin operators can be written as the following:

$$\begin{aligned} S_i^z &= S - a^\dagger a, & S_i^- &= \sqrt{2S} a^\dagger [1 - a^\dagger a / (2S)]^{1/2} \simeq \sqrt{2S} a^\dagger; \\ & & & i \in \text{odd}, \\ S_i^z &= -S + b^\dagger b, & S_i^- &= \sqrt{2S} [1 - b^\dagger b / (2S)]^{1/2} b \simeq \sqrt{2S} b; \\ & & & i \in \text{even}. \end{aligned} \quad (3)$$

Using this transformation, the Hamiltonian in Eq. (1) can be separated into three terms as follows:

$$H = H_{\text{odd-even}} + H_{\text{odd-odd}} + H_{\text{even-even}},$$

where $H_{\text{odd-even}}$, $H_{\text{odd-odd}}$, and $H_{\text{even-even}}$ are defined as

$$\begin{aligned} H_{\text{odd-even}} &= \sum_{i,j}^L J_{2i-1,2j} [-S^2 + S(a_{2i-1}^\dagger a_{2i-1} + b_{2j}^\dagger b_{2j} \\ &\quad + a_{2i-1} b_{2j} + a_{2i-1}^\dagger b_{2j}^\dagger)], \\ H_{\text{odd-odd}} &= - \sum_{i<j}^L J_{2i-1,2j-1} [-S^2 + S(a_{2i-1}^\dagger a_{2i-1} \\ &\quad + a_{2j-1}^\dagger a_{2j-1} + a_{2i-1} a_{2j-1} + a_{2i-1}^\dagger a_{2j-1})], \\ H_{\text{even-even}} &= - \sum_{i<j}^L J_{2i,2j} [-S^2 + S(b_{2i}^\dagger b_{2i} + b_{2j}^\dagger b_{2j} + b_{2i} b_{2j} \\ &\quad + b_{2i}^\dagger b_{2j}^\dagger)]. \end{aligned} \quad (4)$$

We diagonalize this quadratic Hamiltonian by going to momentum space and then diagonalizing by a Bogoliubov transformation:

$$\begin{aligned} H &= \text{const} + JS \sum_k \{ [\alpha - f(k)] (a_k^\dagger a_k + b_k^\dagger b_k) \\ &\quad + g(k) (a_k^\dagger b_k^\dagger + a_k b_k) \}, \end{aligned} \quad (5)$$

where

$$\begin{aligned} \alpha &= 2 \lim_{L \rightarrow \infty} \sum_{n=1}^{L/2} \frac{1}{(2n-1)^\beta}, \\ f(k) &= 4 \lim_{L \rightarrow \infty} \sum_{n=1}^{L/2} \frac{1}{(2n)^\beta} [\cos(2nk) - 1], \\ g(k) &= 2 \lim_{L \rightarrow \infty} \sum_{n=1}^{L/2} \frac{1}{(2n-1)^\beta} \cos(2n-1)k; \end{aligned} \quad (6)$$

using the Bogoliubov transformation, the Hamiltonian (5) can be diagonalized and be written in terms of free boson operators c_k and d_k :

$$H = \text{const} + JS \sum_k \omega_k (c_k^\dagger c_k + d_k^\dagger d_k), \quad (7)$$

where

$$\omega_k = \sqrt{[\alpha - f(k)]^2 - [g(k)]^2}. \quad (8)$$

The correction to staggered magnetization is given by

$$\Delta m = \frac{1}{V} \sum_k \langle a_k^\dagger a_k \rangle = \Delta m_q + \Delta m_T(T), \quad (9)$$

where Δm_q and $\Delta m_T(T)$, which represent the quantum and thermal fluctuation corrections, respectively, are given by

$$\begin{aligned} \Delta m_q &= \int \frac{dk}{2\pi} \frac{1}{2} \left[\frac{\alpha - f(k)}{\omega_k} - 1 \right], \\ \Delta m_T(T) &= \int \frac{dk}{2\pi} \left[\frac{\alpha - f(k)}{\omega_k} \right] \frac{1}{e^{E_k/k_B T} - 1}. \end{aligned} \quad (10)$$

We will visit these equations frequently when we discuss the validity of the spin-wave approach later in the text.

It is clear that the correction to magnetization is dominated by the small k behavior of the spin-wave spectrum. We thus need to obtain the small k behavior of the expressions given in Eq. (6). To do that we express them in terms of the Bose-Einstein integral function⁶ defined as

$$\begin{aligned} F(\alpha, \nu) &= \frac{1}{\Gamma(\alpha)} \int dx \frac{x^{\alpha-1}}{e^{x+\nu} - 1} = \frac{e^{-\nu}}{1^\alpha} + \frac{e^{-2\nu}}{2^\alpha} + \frac{e^{-3\nu}}{3^\alpha} + \dots \\ &= \sum_{n=1}^{\infty} \frac{e^{-n\nu}}{n^\alpha}, \end{aligned} \quad (11)$$

and rewrite the $\cos(nk)$ term in $f(k)$ and $g(k)$ as the following:

$$\sum_n \frac{\cos(nk)}{n^\beta} = \text{Re} \left[\sum_n \frac{e^{ink}}{n^\beta} \right] = \text{Re}[F(\beta, -ik)]. \quad (12)$$

The analytical properties of $F(\alpha, v)$ near $v=0$ are known and are given by

$$F(\alpha, v) = \Gamma(1-\alpha)v^{\alpha-1} + \sum_{n=0}^{\infty} \frac{\zeta(\alpha-n)}{n!} (-v)^n, \quad (\alpha \notin \mathbb{Z}),$$

$$F(\alpha, v) = \frac{(-v)^{\alpha-1}}{(\alpha-1)!} \left[\sum_{r=1}^{\alpha-1} \frac{1}{r} - \ln(v) \right] + \sum_{n \neq \alpha-1} \frac{\zeta(\alpha-n)}{n!} (-v)^n, \quad (\alpha \in \mathbb{Z}), \quad (13)$$

where $\zeta(s)$ is the zeta function. We will use these properties in our later treatment.

III. SPIN-WAVE SPECTRA AND CORRECTIONS TO STAGGERED MAGNETIZATION

In this section we analyze Eq. (6) for different values of β to obtain the spin-wave spectra and calculate the correction to staggered magnetization, to determine the validity of the spin-wave approach.

A. $\beta \geq 3$

Equations (12) and (13) are the main ingredients to analyze Eq. (6) which can be summed up in closed forms. Up to leading order in k the relations in Eq. (6) for $\beta > 3$ read

$$\alpha = 2 \sum_{n=1}^{\infty} \frac{1}{(2n-1)^\beta} = 2(1-2^{-\beta})\zeta(\beta),$$

$$f(k) = 4 \sum_{n=1}^{\infty} \frac{1}{(2n)^\beta} [\cos(2nk) - 1]$$

$$= 2^{2-\beta} [\text{Re}(F(\beta, -2ik)) - \zeta(\beta)] \approx ck^2,$$

$$g(k) = 2 \sum_{n=1}^{\infty} \frac{1}{(2n-1)^\beta} \cos(2n-1)k$$

$$= 2 \sum_{n=1}^{\infty} \left[\frac{\cos(nk)}{n^\beta} - \frac{\cos(2nk)}{(2n)^\beta} \right] \approx \alpha - c'k^2, \quad (14)$$

where c and c' are positive constants. The same results can also be obtained by expanding the $\cos(nk)$ term to order k^2 in $f(k)$:

$$\sum_n \frac{\cos(nk) - 1}{n^\beta} \approx -k^2 \sum_n n^{2-\beta}, \quad (15)$$

in which the sum converges as long as $\beta > 3$; together with a similar expansion for $g(k)$ one reproduces Eq. (14). The spin-wave spectrum can be easily shown to be linear in k : $\omega_k \propto k$, and the $T=0$ correction to the staggered magnetization from long-wavelength spin-wave fluctuation:

$$\Delta m_q \sim \int \frac{dk}{\omega_k}, \quad (16)$$

diverges logarithmically for $\beta > 3$. This immediately indicates that the spin-wave approach is not valid for $\beta > 3$ at zero temperature. The results obtained here are essentially the same as the spin-wave calculation for nearest-neighbor interactions only.⁵

For $\beta=3$ the expansion we did above is no longer valid because the sum is divergent. We rely instead on the Bose-Einstein integral function as defined in Eq. (11) to calculate ω_k and Δm_q . After a little algebra we find $\omega_k \sim k \sqrt{|\ln(k)|}$ which leads to the correction of staggered magnetization that diverges as $\sqrt{|\ln(L)|}$, where L is the system size. We thus conclude that the quantum fluctuation destroys the Neel order, and the spin-wave approach is not valid for $\beta \geq 3$. Our results also agree with the calculation presented by Sacramento and Vieira,¹⁷ who showed the absence of a gap in $S=1$ antiferromagnetic chains for $1 < \beta < 3$.

B. $1 < \beta < 3$

We now turn our attention to the case $1 < \beta < 3$. As in $\beta=3$ case we are no longer able to expand the $\cos(nk)$ term in $f(k)$ and $g(k)$ because the coefficient of k^2 is divergent so we again take advantage of the mapping onto the Bose-Einstein integral function. In the long-wavelength regime, the relations given in Eq. (6) read

$$\alpha = 2 \sum_{n=1}^{\infty} \frac{1}{(2n-1)^\beta} = 2(1-2^{-\beta})\zeta(\beta),$$

$$f(k) = 4 \sum_{n=1}^{\infty} \frac{1}{(2n)^\beta} [\cos(2nk) - 1]$$

$$= 2^{2-\beta} [\text{Re}(F(\beta, -2ik)) - \zeta(\beta)] \approx -\phi(\beta)k^{\beta-1},$$

$$g(k) = 2 \sum_{n=1}^{\infty} \frac{1}{(2n-1)^\beta} \cos(2n-1)k$$

$$= 2 \sum_{n=1}^{\infty} \left[\frac{\cos(nk)}{n^\beta} - \frac{\cos(2nk)}{(2n)^\beta} \right] \approx \alpha - \frac{1}{2} \phi(\beta)k^{\beta-1}, \quad (17)$$

where the function $\phi(\beta)$ is given by

$$\phi(\beta) = \frac{\pi}{\Gamma(\beta)} \frac{1}{\cos[\pi(\beta-2)/2]}, \quad (18)$$

with $\Gamma(\beta)$ being the gamma function. The long-wavelength spin-wave spectrum is given by

$$\omega_k \approx \sqrt{3\alpha\phi(\beta)}k^{(\beta-1)/2}, \quad (19)$$

which is *sublinear*, and the $T=0$ correction to staggered magnetization by

$$\Delta m_q \approx \frac{1}{2\pi} \left[\sqrt{\frac{\alpha(\beta)}{3\phi(\beta)}} \frac{2}{3-\beta} \pi^{(3-\beta)/2} + \sqrt{\frac{\phi(\beta)}{3\alpha(\beta)}} \frac{2}{1+\beta} \pi^{(1+\beta)/2} - \pi \right], \quad (20)$$

which is *convergent* for $\beta < 3$. These results show that the system supports gapless excitations, the spectrum follows a sublinear power law at small momentum k , and that the Neel order at zero temperature survives, for large enough S , for $1 < \beta < 3$. Our results agree with an earlier work presented by Parreira, Bolina, and Perez⁷ who show the existence of Neel order for $\beta \geq 3$ and the presence of Neel order for $\beta < 3$ at zero temperature using rigorous proof. However, the excitation spectra were not studied in this work, nor was the critical value of S for the stability for Neel order calculated. Another support for our results at zero temperature is offered by the work of Aoki⁸ who studied the same model we are studying for the case $\beta = 2$ in one dimension (1D) and 2D using spin-wave theory. In that work he found that there exists Neel order at zero temperature in one dimension for $\beta = 2$, which is in agreement with our conclusion.

We may also estimate the critical size of the spin, S_c , above which the Neel order survives, by setting the correction to the staggered magnetization equal to the spin size: $\Delta m_q = S_c$. As $\beta \rightarrow 3$, Δm_q is dominated by long-wavelength spin-wave fluctuations, and we obtain

$$S_c(\beta) \approx \frac{1}{2\pi} \left[\sqrt{\frac{\alpha(\beta)}{3\phi(\beta)}} \frac{2}{3-\beta} \pi^{(3-\beta)/2} + \sqrt{\frac{\phi(\beta)}{3\alpha(\beta)}} \frac{2}{1+\beta} \pi^{(1+\beta)/2} - \pi \right] \approx \frac{0.41}{\sqrt{3-\beta}}, \quad (21)$$

a result we expect to be asymptotically exact in the limit $\beta \rightarrow 3$. On the other hand, we also find that the quantum correction gets suppressed very rapidly as β decreases from 3; for example, we find $S_c \approx 1/2$ for $\beta = 2.63$ and $S_c \approx 1$ for $\beta = 2.85$, suggesting that the Neel order would survive for any spin for $\beta \lesssim 2.6$.

We also calculate the correction to staggered magnetization at finite temperature. First, we discuss the case for $\beta > 2$. The thermal correction to staggered magnetization is given by

$$\Delta m_T(T) \approx \frac{k_B T}{2\pi JS} \int dk \left[\frac{k^{1-\beta}}{3\phi(\beta)} + \frac{1}{3\alpha} \right], \quad (22)$$

which diverges as $L^{\beta-2}$ for $\beta > 2$. For $\beta = 2$, it is a simple exercise to show that the spectrum behaves like $\omega_k \sim \sqrt{k}$, and the small k contribution to the thermal correction of staggered magnetization diverges as $\sqrt{|\ln(L)|}$. These results indicate that thermal fluctuations destroy the Neel order for $\beta \geq 2$ at any finite temperature. They are consistent with an extension of the Mermin-Wagner theorem that Bruno advanced,⁹ which proves the absence of Neel order for β

≥ 2 . For classical antiferromagnets in 1D, it has been shown, using Monte Carlo simulation, that there is no magnetic ordering at finite temperature.¹⁰

For $\beta < 2$ the correction to staggered magnetization is given by

$$\Delta m_T(T) \approx \frac{k_B T}{\pi JS} \left[\frac{\pi^{(2-\beta)}}{3(2-\beta)\phi(\beta)} + \frac{\pi}{3\alpha} \right]. \quad (23)$$

This *convergent* correction shows that the Neel order survives at finite temperature for $\beta < 2$. The Neel transition temperature T_N can also be estimated by applying the same rationale used to estimate the critical value of S at zero temperature. By using Eq. (23) we find

$$T_N(S, \beta) = \frac{\pi JS}{k_B} \left[\frac{\pi^{2-\beta}}{3(2-\beta)\phi(\beta)} + \frac{\pi}{3\alpha} \right]^{-1}. \quad (24)$$

In the limit $\beta \rightarrow 2$, we find that T_N vanishes linearly:

$$T_N \approx \frac{3\pi^2 JS}{k_B} (2-\beta). \quad (25)$$

We see that increasing the range of interactions (or decreasing β) in the chains has effects that are similar to increasing the dimensionality of the systems. For $\beta \geq 3$ we find the absence of Neel order at both zero and finite temperature, a genuine one-dimensional behavior. For $2 \leq \beta < 3$ we have finite Neel order at zero temperature which gets destroyed at any finite temperature, similar to the 2D situation. Finally, for $\beta < 2$ the Neel order is stable at zero and at low-enough finite temperature, a behavior expected for dimensions above 2.

In contrast to the antiferromagnetic case we are studying here, the ferromagnetic models with long-range interactions have been studied more extensively. Classical Heisenberg model with long-range ferromagnetic interactions has a phase transition at finite temperature in one dimension when the interactions decay slower than $1/r^2$. There is no phase transition at finite temperature when the interactions decay faster than $1/r^2$.¹¹ This result for the classical case in one dimension is confirmed by Monte Carlo simulation.¹² The quantum Heisenberg model with long-range interactions has also been studied using the modified spin-wave theory.^{13,14} It was shown that there exists a magnetic ordering in one dimension as long as the interactions decay slower than $1/r^2$.

C. $\beta \leq 1$

In this section we consider the case $\beta \leq 1$. The reason we separate $\beta \leq 1$ case with the rest is that there are divergences in the thermodynamic limit which require special care in their analysis. Physically, this is closely related to the fact that the ground-state energy grows faster than the system size (i.e., it becomes “superextensive”), if the local energy scale J is not rescaled according to the system size. For this reason we will not discuss the finite temperature (or thermodynamic) properties of the system, as the definition of tem-

perature becomes somewhat ambiguous; we will focus instead on the ground-state properties of the system, which is free of such ambiguity.

For the reasons mentioned we need to work explicitly with a finite system size L , defined as the number of spins per sublattice (so the total number of spins is $2L$), and treat k and L as two independent variables. For a start, the summation in α ,

$$\alpha = 2 \sum_{n=1}^{L/2} \frac{1}{(2n-1)^\beta}, \quad (26)$$

diverges for $\beta \leq 1$ if we run the summation to infinity. For large but finite L , we have

$$\alpha \approx \begin{cases} \ln(L), & \beta = 1 \\ L^{1-\beta}/(1-\beta), & \beta < 1. \end{cases}$$

Similarly,

$$f(k) = 4 \sum_{n=1}^{L/2} \frac{\cos(2nk) - 1}{(2n)^\beta}, \quad (27)$$

$$f(k) \approx \begin{cases} -2[\ln(k) + \ln(L)], & \beta = 1 \\ 2\Gamma(1-\beta)\cos[\pi(\beta-1)/2]k^{\beta-1} - 2L^{1-\beta}/(1-\beta), & \beta < 1 \end{cases}$$

and

$$g(k) = 2 \sum_{n=1}^{L/2} \frac{\cos[(2n-1)k]}{(2n-1)^\beta}, \quad (28)$$

$$g(k) \approx \begin{cases} \ln(k), & \beta = 1 \\ \Gamma(1-\beta)\cos[\pi(\beta-1)/2]k^{\beta-1}, & \beta < 1. \end{cases}$$

The spin-wave spectrum reads

$$E_k = JS\omega_k = JS\alpha \sqrt{\left(1 - \frac{f(k)}{\alpha}\right)^2 - \left(\frac{g(k)}{\alpha}\right)^2}, \quad (29)$$

$$E(k) \approx \begin{cases} 3JS \ln(L)[1 + b \ln(k)], & \beta = 1 \\ 3JSL^{1-\beta}(1 - bk^{\beta-1}), & \beta < 1, \end{cases}$$

which approach L -dependent constants as $k \rightarrow 0$. Here $b \propto 1/\ln(L)$ for $\beta = 1$ and $b \propto L^{\beta-1}$ for $\beta < 1$. Correction to staggered magnetization at zero temperature can be calculated easily using the relations derived above to yield

$$\Delta m_q \sim \begin{cases} \frac{1}{\ln(L)}, & \beta = 1 \\ \sim \frac{1}{L^{1-\beta}}, & \beta < 1, \end{cases} \quad (30)$$

suggesting that the quantum fluctuation gets completely suppressed as system size grows.

For $\beta = 0$ the calculation becomes particularly simple; the relations for α , $f(k)$, and $g(k)$ in Eq. (6) become

$$\alpha = L,$$

$$f(k) = \sum_{\delta_2} [e^{ik \cdot \delta_2} + e^{-ik \cdot \delta_2} - 2] = 2L(\delta_{k,0} - 1),$$

$$g(k) = \sum_{\delta_1} e^{ik \cdot \delta_1} = L\delta_{k,0}. \quad (31)$$

The spin-wave spectrum for $k \neq 0$ is given by

$$E_k = JSL\sqrt{(1+2)^2} = 3JSL, \quad (32)$$

which is k independent, and the correction to staggered magnetization is given by

$$\Delta m_q \sim \sum_k \frac{1}{\omega_k} \sim \frac{1}{L}. \quad (33)$$

We will compare these with an exact solution for this special case in the following section.

D. $\beta = 0$: Exact solution

The infinite range ($\beta = 0$) antiferromagnetic chain with no frustration is given by the following Hamiltonian:

$$H = J \sum_{ij}^{2L} (-1)^{i-j+1} S_i \cdot S_j, \quad (34)$$

which can be solved exactly in the following manner. We introduce

$$S_A = \sum_{i \in A} S_i, \quad S_B = \sum_{i \in B} S_i, \quad (35)$$

where $S_A(S_B)$ is the total spin operator for sublattice $A(B)$, to rewrite the Hamiltonian in the following form:

$$H = J \left[S_A \cdot S_B - (S_A^2 + S_B^2) + \left(\sum_{i \in A} (S_i)^2 + \sum_{i \in B} (S_i)^2 \right) \right]. \quad (36)$$

We define the total spin operator $S_{tot} = S_A + S_B$ to further simplify the Hamiltonian given above to become

$$H = J \left[\frac{1}{2} S_{tot}^2 - \frac{3}{2} (S_A^2 + S_B^2) + 3L/2 \right]. \quad (37)$$

The Hamiltonian in Eq. (37) can be diagonalized in the total- S basis of states given by $|(S_A, S_B); S_{tot}\rangle$, where $S_A(S_B)$ and S_{tot} are the total spin quantum numbers in sublattice $A(B)$ and in the system, respectively. Using this basis, the energy can be easily obtained as

$$E = J \left[\frac{1}{2} S_{tot}(S_{tot} + 1) - \frac{3}{2} [S_A(S_A + 1) + S_B(S_B + 1)] + 3L/2 \right]. \quad (38)$$

To minimize the energy we must have all spins aligned in each sublattice and have a minimum of S_{tot} . This means that $S_{tot} = 0$ and $S_A = S_B = LS$, where S is the spin size, will minimize the energy and give us the ground state. The momentum quantum number of the ground state is 0 (π) for even

(odd) L . The lowest-energy excited state is obtained by having $S_{tot}=1$ while still maintaining maximum S_A and S_B . The energy gap is given by

$$\Delta E = E_{ex} - E_{gs} = J. \quad (39)$$

This particular excited state has a momentum quantum number that differs from the ground state by π , which corresponds to momentum $k=0$ in the spin-wave approach, due to the doubling of the unit cell in that approach. We will say more about this in the following section. To obtain excitations with generic k , however, we must change either the S_A or S_B quantum numbers. There exist two branches of degenerate low-lying excitations, corresponding to $S_A=LS-1$ or $S_B=LS-1$ and $S_{tot}=1$, with excitation energy

$$\Delta E = E_{ex} - E_{gs} = J(1 + 3LS), \quad (40)$$

which grows linearly with system size and has no k dependence. This result agrees with the spin-wave solution obtained earlier in the limit $S \rightarrow \infty$, as expected.

IV. EXCITATIONS AT $k=0$ AND STATUS OF THE LIEB-SCHULTZ-MATTIS THEOREM

The LSM theorem² states that for half-integer spin chains with length L and short-range interaction, there exists an excited state whose momentum differs from the ground state by π , with energy that vanishes at least as fast as $1/L$ as $L \rightarrow \infty$.² Recently the theorem has been extended to spin chains with power-law long-range interaction, and it was found that the theorem remains valid for $\beta > 2$.^{15,16} The situation is unclear for $\beta \leq 2$.

In this section we check if the LSM behavior still holds for $\beta \leq 2$, using the spin-wave method. As discussed above, due to the doubling of the unit cell, the excitations whose momenta differ from the ground state by either π or 0 show up as $k=0$ excitation in the spin-wave approach. If one blindly uses the linear spin-wave results, however, one would always find $E_{k=0}=0$. But this is an artifact of the linear spin-wave approach which maps the $k=0$ modes to harmonic oscillators *without* a restoring force. Thus in order to study the excitation that is relevant to the LSM theorem, we must treat the $k=0$ modes more carefully.

To do that, we start by rewriting the Hamiltonian as given in Eq. (1) in the momentum space:

$$H = \sum_k \sum_{\delta_1} J(\delta_1) S_k^A \cdot S_{-k}^B e^{-ik \cdot \delta_1} - 2 \sum_k \sum_{\delta_2} [J(\delta_2) S_k^A \cdot S_{-k}^A e^{-ik \cdot \delta_2} + J(\delta_2) S_k^B \cdot S_{-k}^B e^{-ik \cdot \delta_2}], \quad (41)$$

where

$$S_i^{A/B} = \frac{1}{\sqrt{L}} \sum_k S_k^{A/B} e^{-ik \cdot x_i} \quad (42)$$

and $A(B)$ denotes odd (even) sublattice. Instead of applying the Holstein-Primakoff mapping for all terms in H , we separate out the $k=0$ term in H and apply Holstein-Primakoff mapping to the $k \neq 0$ terms only. Since to linear order the $k=0$ term commutes with the other terms in H , they can be

diagonalized independently. The spin-wave treatment for the $k \neq 0$ terms gives the spectra obtained earlier, excepting that k must be nonzero. On the other hand, the $k=0$ term

$$\begin{aligned} H_{k=0} &= \frac{1}{L} \sum_{\delta_1} J(\delta_1) \left(\sum_{i \in A} S_i \right) \cdot \left(\sum_{i \in B} S_i \right) \\ &\quad - \frac{1}{L} \sum_{\delta_2} J(\delta_2) \left[\left(\sum_{i \in A} S_i \right)^2 + \left(\sum_{i \in A} S_i \right)^2 \right] \\ &= \frac{1}{L} \sum_{\delta_1} J(\delta_1) S_A \cdot S_B - \frac{1}{L} \sum_{\delta_2} J(\delta_2) (S_A^2 + S_B^2) \end{aligned} \quad (43)$$

takes a form identical to the Hamiltonian for $\beta=0$ which was solved exactly in the preceding section. We can easily solve this Hamiltonian to obtain the excitation energy at momentum π measured from the ground-state momentum, or $k=0$ for the doubled unit cell:

$$\Delta E = \frac{J\alpha}{L}, \quad (44)$$

where α depends on the power-law exponent β and is given by Eq. (6). For $\beta > 1$, α is convergent in the large L limit and is given by Eq. (14). This means that the energy of the excited-state vanishes as $1/L$ as $L \rightarrow \infty$. For $\beta = 1$, α diverges as $\ln(L)$ as shown in Eq. (26) and the energy vanishes as $\ln(L)/L$. For $\beta < 1$, α diverges as $L^{1-\beta}$ as shown again in Eq. (26) and the excitation energy vanishes as $L^{-\beta}$. We thus find that the LSM behavior holds for $1 < \beta \leq 2$, despite the absence of a proof for this range of β . On the other hand, the LSM theorem is “violated” for $\beta \leq 1$. The “violation” of the LSM theorem is also observed in spin- $\frac{1}{2}$ systems with finite-range interactions in higher dimensions. It was shown that the excitation energy is bounded by $\ln(L)/L$ (Ref. 18) rather than by $1/L$ as found in one dimension.

V. SUMMARY

We have studied antiferromagnetic chains with unfrustrated long-range interactions using the spin-wave technique. We find that this approach is valid for $\beta < 3$ at zero temperature for sufficiently large size of spin, and $\beta < 2$ for sufficiently low finite temperature, due to the stability of Neel order. Within the range of validity of this approach we find that the system has a gapless excitation and the excitation spectrum follows a nontrivial k dependence. We also study how the excitation gap closes in this system in the limit $L \rightarrow \infty$, and find a behavior that is in contrast to that predicted by Lieb-Schultz-Mattis theorem for chains with short-range interactions, when $\beta \leq 1$.

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