# Spin excitations and sum rules in the Heisenberg antiferromagnet

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Various bounds for the energy of collective excitations in the Heisenberg antiferromagnet are presented and discussed using the formalism of sum rules. We show that the Feynman approximation significantly overestimates (by about 30% in the $S=\frac{1}{2}$ square lattice) the spin velocity due to the non-negligible contribution of multiple magnons to the energy-weighted sum rule. We also discuss a different, Goldstone-type bound depending explicitly on the order parameter (staggered magnetization). This bound is shown to be proportional to the dispersion of classical spin-wave theory with a $q$-independent normalization factor. Rigorous bounds for the excitation energies in the anisotropic Heisenberg model are also presented.

## I. INTRODUCTION

In the past few years a considerable number of papers have been devoted to the study of the Heisenberg model for antiferromagnetism, especially in two dimensions. This interest is mainly motivated by the need for a better understanding of the antiferromagnetic behavior of the undoped precursor insulators of the high-$T_c$ superconductors. After the pioneering works by Anderson[1] and Oguchi,[2] based on spin-wave theory, several theoretical methods have been developed to study this problem. These range from spin-wave theory up to second order in $1/2S$ to series-expansion methods from the Ising side and to Monte Carlo calculations (see the review papers, Refs. 3 and 4, for exhaustive discussions and references).

The purpose of this paper is to discuss the elementary excitations of the Heisenberg antiferromagnet at zero temperature using a sum-rule approach. Only recently systematic theoretical investigations of the dispersion of spin waves in the whole Brillouin zone have become available.[5-10] Recent experiments[11] in $La_2CuO_4$ with neutron scattering suggest that the dispersion follows the predictions of classical spin-wave theory with a proper renormalization factor. Even at low $q$, where the dispersion becomes linear, rather relevant questions still remain to be clarified in a satisfying way. Among them we recall the problem of the validity of the so-called "Feynman" or single-mode approximation for the calculation of the spin velocity and of the role of multiple magnon excitations. These questions, first discussed by Hohenberg and Brinkman many years ago in one-dimensional (1D) antiferromagnets,[12] have been recently addressed by Singh[9] in the $S=\frac{1}{2}$ square lattice. In this work we are mainly interested in the 2D case and, in general, in systems with broken symmetries.

The paper is organized as follows: In Sec. II we discuss the Feynman approach to spin excitations and we prove that it cannot reproduce the correct dispersion of spin waves at low $q$ because of the presence of multiple magnon excitations which affect the energy weighted sum rule also in the long-wavelength limit. In Sec. III we discuss a different bound for the energy of elementary excitations. This bound, first introduced by Wagner[13] many years ago, has the form of a Goldstone theorem and depends explicitly on the order parameter. It can be easily calculated through the whole Brillouin zone and in particular it exhibits the same dependence on $q$ as the one given by classical spin-wave theory (SWT), with a proper renormalization factor. In Sec. IV we present results for the anisotropic Heisenberg model. In particular we derive rigorous upper bounds for the mass gap in the easy-axis antiferromagnet and for the gapless dispersion law in the case of the easy-plane antiferromagnet.

## II. THE FEYNMAN APPROXIMATION

In the following we investigate spin excitations in the framework of the Heisenberg model for antiferromagnetism (AFM) characterized by the Hamiltonian

$$H=J\sum_{\langle ij\rangle}[s_i^z s_j^z+\lambda(s_i^x s_j^x+s_i^y s_j^y)]\ , \tag{1}$$

where $\langle ij\rangle$ denotes a sum over all nearest-neighbor pairs and $J>0$. The limits $\lambda=0$ and $\lambda=1$ correspond to the most famous Ising and isotropic Heisenberg models, respectively. At zero temperature the isotropic Heisenberg model is believed to give rise to spontaneous sublattice magnetization also in two dimensions (square lattice), though quantum fluctuations have a crucial role in reducing the value of the order parameter (actually the $S=\frac{1}{2}$ Heisenberg model has been rigorously proven to give rise to spontaneous magnetization only in three dimensions[14]). In Secs. II and III we mainly discuss the isotropic case ($\lambda=1$) and we assume the staggered magnetization to be oriented along the $z$ axis. This is also the case for the anisotropic case if $\lambda<1$. Conversely when $\lambda>1$ (see Sec. IV) the axis of (spontaneous) magnetization lies in the $x$-$y$ plane (easy plane).

In the following we will mainly consider excitations generated by the spin operator:

$$s_{\mathbf{q}}^x=\frac{1}{\sqrt{N}}\sum_i s_i^x e^{i\mathbf{q}\cdot\mathbf{r}_i}\ . \tag{2}$$

These excitations are transverse with respect to the $z$-

 

staggered magnetization axis. The most important among such excitations are spin waves (magnons) that represent the elementary excitations of the system. Rigorous upper bounds for the energy of these excitations can be obtained at zero temperature using the sum-rule method.

The most popular bound is given by the Bijl-Feynman ansatz, analog of the most famous approach employed to investigate the propagation of density excitations in Bose superfluids.[15] It is obtained by applying the spin operator (2) to the ground state of the system. One finds

$$|F\rangle=\frac{1}{\sqrt{S^{\perp}(q)}}s_{\mathbf{q}}^{x}|0\rangle \ . \tag{3}$$

In Eq. (3) $S^{\perp}(q)=\langle 0|s_{-\mathbf{q}}^{x},s_{\mathbf{q}}^{x}|0\rangle$ is the transverse structure factor entering here as a normalization factor. The excitation energy of the Feynman state is given by

$$\begin{aligned}\epsilon_F(q)&=\langle F|H|F\rangle-\langle 0|H|0\rangle\\&=\frac{1}{2}\frac{\langle 0|[s_{-\mathbf{q}}^{x}[H,s_{\mathbf{q}}^{x}]]|0\rangle}{S^{\perp}(q)}\end{aligned} \tag{4}$$

and provides, at zero temperature, a rigorous upper bound for the energy $\epsilon(q)$ of the lowest state excited by the operator $s_{\mathbf{q}}^{x}$. This can be directly shown by identifying the numerator and the denominator of Eq. (4) as the energy-weighted and non-energy-weighted moments of the transverse dynamic structure factor

$$S^{\perp}(q,\omega)=\sum_n |\langle 0|s_{\mathbf{q}}^{x}|n\rangle|^2\delta(\omega-\omega_{n0}) \ .$$

In fact, using the completeness relation, one can write

$$\begin{aligned}\int S^{\perp}(q,\omega)\omega\, d\omega&=\sum_n \langle 0|s_{-\mathbf{q}}^{x}|n\rangle|^2\omega_{n0}\\&=\tfrac{1}{2}\langle 0[s_{-\mathbf{q}}^{x}[H,s_{\mathbf{q}}^{x}]]|0\rangle\end{aligned} \tag{5}$$

and

$$\begin{aligned}\int S^{\perp}(q,\omega)d\omega&=\sum_n |\langle 0|s_{-\mathbf{q}}^{x}|n\rangle|^2\\&=\langle 0|s_{-\mathbf{q}}^{x}s_{\mathbf{q}}^{x}|0\rangle=S^{\perp}(q) \ .\end{aligned} \tag{6}$$

Note that at $T=0$ the dynamic structure factor $S^{\perp}(q,\omega)$ vanishes for $\omega<0$.

The Feynman energy (4) has been already used by several authors to study the energy of elementary excitations in the Heisenberg model.[12,5,6,9] The numerator of Eq. (4) can be easily calculated employing the commutation rules for the spin operators. The result is

$$\tfrac{1}{2}\langle 0|[s_{-\mathbf{q}}^{x}[H,s_{\mathbf{q}}^{x}]]|0\rangle=z[f_z(1-\lambda\gamma_{\mathbf{q}})+f_y(\lambda-\gamma_{\mathbf{q}})] \ . \tag{7a}$$

Analogously, for the $s_{\mathbf{q}}^{y}$ and $s_{\mathbf{q}}^{z}$ operators one finds

$$\tfrac{1}{2}\langle 0|[s_{-\mathbf{q}}^{y},[H,s_{\mathbf{q}}^{y}]]|0\rangle=z[f_z(1-\lambda\gamma_{\mathbf{q}})+f_x(\lambda-\gamma_{\mathbf{q}})] \ , \tag{7b}$$

$$\tfrac{1}{2}\langle 0|[s_{-\mathbf{q}}^{z}[H,s_{\mathbf{q}}^{z}]]|0\rangle=\lambda z(f_x+f_y)(1-\gamma_{\mathbf{q}}) \ , \tag{7c}$$

where $z$ is the number of nearest neighbors, $\gamma_{\mathbf{q}}=(1/z)\sum_\delta \cos\mathbf{q}\cdot\delta$ and we have introduced the quantities

$$\begin{aligned}f_x&=-\frac{J}{2}\langle s_i^x s_{i+\delta}^x\rangle \ ,\\f_y&=-\frac{J}{2}\langle s_i^y s_{i+\delta}^y\rangle \ ,\\f_z&=-\frac{J}{2}\langle s_i^z s_{i+\delta}^z\rangle \ .\end{aligned} \tag{8}$$

Here $\delta$ is the lattice vector connecting nearest neighbors. In the square lattice one has $\gamma_{\mathbf{q}}=\frac{1}{2}(\cos q_x+\cos q_y)$, while in the cubic lattice $\gamma_{\mathbf{q}}=\frac{1}{3}(\cos q_x+\cos q_y+\cos q_z)$, having set the lattice parameter equal to 1. It is worth noticing that the form of the energy-weighted sum rule relative to $s_{\mathbf{q}}^{z}$ differs from the one relative to $s_{\mathbf{q}}^{x}$ and $s_{\mathbf{q}}^{y}$. This follows from the fact that the Heisenberg Hamiltonian (1) is invariant for spin rotation in the $x$-$y$ plane.

In the isotropic case ($\lambda=1$), Eq. (7a) becomes

$$\tfrac{1}{2}\langle 0|[s_{-\mathbf{q}}^{x}[H,s_{\mathbf{q}}^{x}]]|0\rangle=z(f_z+f_y)(1-\gamma_{\mathbf{q}}) \ . \tag{9}$$

Note that even in the isotropic limit $\lambda=1$ the quantity $f_z$ differs from $f_y(=f_x)$ if there is spontaneous magnetization among the $z$ axis.

At small $q$ the energy-weighted sum rule (9) becomes [we consider here for simplicity the square and cubic lattices where $\gamma_{\mathbf{q}}=1-(1/z)q^2+o(q^2)$]

$$\tfrac{1}{2}\langle 0|[s_{-\mathbf{q}}^{x},[H,s_{\mathbf{q}}^{x}]]|0\rangle=(f_z+f_y)q^2 \tag{10}$$

and exhibits the typical $q^2$ dependence characterizing the most famous $f$-sum rule for density excitations.[16]

The denominator of Eq. (4) is the Fourier transform of the two-body transverse spin-correlation function. Its behavior is dominated, at low **q**, by long-range correlations associated with spin waves. Numerical results for $S^{\perp}(q)$, based on Monte Carlo calculations[5,6] and series-expansion methods,[9] are now becoming available.

From a general point of view the Feynman energy (4) is expected to provide a good estimate for the frequency of elementary excitations in Heisenberg antiferromagnets. This system can be in fact considered a relatively weakly interacting many-body system as compared, for example, to other strongly interacting quantum systems such as superfluid $^4$He, where the Feynman approximation is known to overestimate in a significant way the energy of lowest excitations at high momenta.

An important question is however to understand what happens to the Feynman approximation in the long-wavelength limit dominated by the propagation of macroscopic spin waves. While in superfluid $^4$He the Feynman ansatz is known to reproduce exactly the phonon dispersion (in terms of sum rules this means that both the energy-weighted and non-energy-weighted sum rules for the density operator are exhausted by phonons) the situation is different in the spin case. In fact the nonconservation of the spin current makes the contribution of multiple magnon excitations particularly important in the low-**q** limit. These excitations exhaust a finite fraction of the energy-weighted sum rule (EWSR) and consequently the Feynman energy (4) does not approach the correct dispersion law at small **q**. In the following we will discuss such an effect in a quantitative way with the help of available microscopic calculations of the spin-stiffness coefficient.

It is convenient to write the transverse dynamic spin-structure function in the following way:

$$S^{\perp}(q,\omega)=A(q)\delta(\omega-\omega(q))+S^{\perp}_{mm}(q,\omega)\ , \tag{11}$$

where we have separated the sharply peaked single-magnon contribution characterized by the dispersion law $\omega(q)$ and strength $A(q)$, from the smooth contribution $S^{\perp}_{mm}(q,\omega)$ arising from multiple magnon excitations $[S^{\perp}_{mm}(q,\omega)=0$ for $\omega\le\omega(q)]$.

The main results for the single magnon and multiple magnon contributions to the various moments of $S^{\perp}(q,\omega)$ at small $q$ are summarized in Table I. The main point is the $q^2$ dependence of the strength associated with multiple magnon excitations. This dependence differs from the $q^4$ dependence associated, for example, with multiple phonon excitations in Bose superfluids. The difference is due to the fact that the current is conserved in Bose superfluids because of translational invariance. In the case of spin excitations the quantity $[H,s^x_q]$, proportional to the spin current [see Eq. (15) below], is not conserved even in the low-$q$ limit and this implies a stronger $q^2$ dependence for the strength associated with multiple magnon excitations. A similar behavior is exhibited by spin excitations in normal Fermi liquids.[17] This result implies that multiple magnon excitations affect the energy-weighted sum rule with a term proportional to $q^2$.[18]

The occurrence of a $q^2$ contribution to the energy-weighted sum rule due to multiple magnon excitations is clearly exploited by the calculation of the double commutator relative to the "longitudinal" operator $s^z_{\mathbf{q}}=(1/\sqrt{N})\sum_i s^z_i e^{i\mathbf{q}\cdot\mathbf{r}_i}$ [see Eq. (7c)] for which we find, at low **q**,

$$\tfrac{1}{2}\langle 0|[s^z_{-\mathbf{q}}[H,s^z_{\mathbf{q}}]]|0\rangle=(f_x+f_y)\mathbf{q}^2\ . \tag{12}$$

This contribution, quadratic in $q$, is entirely fixed by multiple magnon excitations, since single magnons are not excited by $s^z_{\mathbf{q}}$.

The low-$q$ contribution to the transverse energy-weighted sum rule, (5) and (10), arising from single magnons is given by $\frac{1}{2}\rho_s q^2$, where $\rho_s$ is the spin-stiffness coefficient. This can be easily understood by using the hydrodynamic expression for the spin velocity:[19]

$$c^2=\frac{\rho_s}{\chi^{\perp}(0)} \tag{13}$$

where

$$\chi_{\perp}(q)=2\sum_n|\langle 0|s^x_{-\mathbf{q}}|n\rangle|^2\frac{1}{\omega_{n0}}=2\int d\omega\frac{S^{\perp}(q,\omega)}{\omega} \tag{14}$$

is the transverse magnetic susceptibility. This sum rule is expected to be entirely exhausted, at low $q$, by the one-magnon excitation. If the energy-weighted sum rule, (5) and (10), were also entirely exhausted by the one-magnon mode at low $q$, then the ratio

$$\lim_{q\to 0}\frac{1}{q^2}\frac{\sum_n|\langle 0|s^x_{-\mathbf{q}}|n\rangle|^2\omega_{n0}}{\sum_n|\langle 0|s^x_{-\mathbf{q}}|n\rangle|^2/\omega_{n0}}=\frac{2(f_z+f_y)}{\chi^{\perp}(0)}$$

should coincide with $c^2$. The comparison between the quantities $2(f_z+f_y)$ and $\rho_s$ then provides a direct and quantitative information about the contribution of multiple magnons to the energy-weighted sum rule. Both the quantities $(f_z+f_y)$ and $\rho_s$ are now available through different theoretical calculations. All the various predictions, based on spin-wave theory to second order in $1/2S$,[7,20] series expansion from the Ising side[21] and Monte Carlo calculations[5,6] agree with the value $2(f_z+f_y)=0.25$ in the $S=\frac{1}{2}$ square lattice. Vice versa the most recent estimates for $\rho_s$ (Refs. 20–22) predict values in the range 0.18–0.20. Since the non-energy-weighted sum rule (6), entering the denominator of the Feynman bound (4), is expected to be exhausted by the single magnon [see Eq. (19) below], we then conclude that the Feynman ansatz overestimates the spin velocity by about 30%. In the $S=1$ square lattice the overestimate is about 10%. In Table II we report, for completeness, the values of various thermodynamic parameters relative to the 2D Heisenberg model. These values correspond to the predictions of spin-wave theory up to $1/(2S)^2$ (Ref. 23) and are rather close to the ones given by the series-expansion method from the Ising side and by Monte Carlo calculations.

It is useful to study more explicitly the role of the spin current and its connection with the spin-stiffness coefficient and the energy-weighted sum rule. To this aim let us start from the continuity equation for the spin

TABLE I. Matrix elements $|(s^x_{\mathbf{q}})_{n0}|^2\equiv|\langle n|s^x_{\mathbf{q}}|0\rangle|^2$, excitation energies, and sum-rule contributions from one-magnon and multiple magnon excitations at $T=0$ in the isotropic Heisenberg antiferromagnet.

| | Magnon | Multiple magnons |
|---|---|---|
| $\omega$ | $cq$ | const |
| $\|(s^x_{\mathbf{q}})_{n0}\|^2$ | $\rho_s q/2c$ | $q^2$ |
| $\|(s^y_{\mathbf{g}-\mathbf{q}})_{n0}\|^2$ | $2cm^2/\rho_s q$ | const |
| $\sum_n\|(s^x_{\mathbf{q}})_{n0}\|^2/\omega_{n0}$ | $\rho_s/2c^2$ | $q^2$ |
| $\sum_n\|(s^x_{\mathbf{q}})_{n0}\|^2$ | $\rho_s q/2c$ | $q^2$ |
| $\sum_n\|(s^x_{\mathbf{q}})_{n0}\|^2\omega_{n0}$ | $\rho_s q^2/2$ | $q^2$ |
| $\sum_n\|(s^y_{\mathbf{g}-\mathbf{q}})_{n0}\|^2/\omega_{n0}$ | $m^2/2\rho_s q^2$ | const |
| $\sum_n\|(s^y_{\mathbf{g}-\mathbf{q}})_{n0}\|^2$ | $m^2c/2\rho_s q$ | const |
| $\sum_n\|(s^y_{\mathbf{g}-\mathbf{q}})_{n0}\|^2\omega_{n0}$ | $m^2c^2/2\rho_s$ | const |

TABLE II. Parameters of the isotropic 2D AFM Heisenberg model predicted by spin-wave theory up to second order in $1/(2S)^2$ (Ref. 23). The Heisenberg coupling constant $J$ has been set equal to 1 and magnetization is taken along the $z$ axis.

| | $E$ | $m$ | $\chi^{\perp}$ | $\rho_s$ | $c$ | $f_z+f_y$ | $f_z-f_y$ |
|---|---|---|---|---|---|---|---|
| $S=\frac{1}{2}$ | $-0.67$ | 0.30 | 0.061 | 0.18 | 1.7 | 0.125 | 0.04 |
| $S=1$ | $-2.33$ | 0.80 | 0.092 | 0.87 | 3.1 | 0.47 | 0.25 |

density (in the following the vector **q** will be taken along the $x$ axis):

$$[H,s_q^x]=-2iJ\frac{1}{\sqrt{N}}\sum_{\langle ij\rangle} s_i^z s_j^y(e^{iqx_i}-e^{iqx_j}) \equiv q j_{s_x}^x(q) \qquad (15)$$

defining the component of the spin current parallel to **q**. Equation (15) provides the following expression for the spin current at $\mathbf{q}=0$:

$$j_{s_x}^x(0)=-\frac{J}{\sqrt{N}}\sum_{i,\delta} s_i^z s_{i+\delta}^y \delta_x , \qquad (16)$$

where $\delta_x=x_i-x_j$ is the $x$ component of the vector connecting the nearest-neighbor pair $\langle ji\rangle$.

The key point is that the spin current (16) is not a conserved quantity (it does not commute with the Hamiltonian) and consequently, when applied to the ground state, it can give rise to excitations with nonvanishing strength. Such excitations are multiple magnon states, since spin waves with $\mathbf{q}=0$ cannot propagate.

Let us now calculate the static response relative to the current $j_{s_x}^x(q)$. Due to the equation of continuity (15), this is exactly fixed by the energy-weighted sum rule for the spin operator $s_{\mathbf{q}}^z$

$$\chi(j_{s_x}^x(q))=2\sum_n |\langle 0|j_{s_x}^x(q)|n\rangle|^2\frac{1}{\omega_{n0}} = \frac{2}{q^2}\sum_n |\langle 0|s_q^x|n\rangle|^2\omega_{n0}=2(f_z+f_y) , \qquad (17)$$

where we have taken the low-**q** limit (10) of the energy-weighted sum rule. Both spin waves and multiple magnon excitations affect this quantity at low $q$. The spin-wave contribution is fixed by the spin-stiffness coefficient (see the discussion above and Table I), while the multiple magnon contribution can be calculated through the static response of the $\mathbf{q}=0$ component (16) of the spin-current operator. In conclusion we get

$$\rho_s=2(f_z+f_y)-\chi(j_{s_x}^x(0)) . \qquad (18)$$

Result (18) for the spin-stiffness coefficient $\rho_s$ shares important analogies with the most famous expression $\rho_s=\rho-\rho_n$ for the superfluid density of a Bose liquid. In Eq. (18) the quantity $2(f_z+f_y)$ plays the role of the total density $\rho$, fixed by the model independent $f$-sum rule,[16] while the quantity $\chi(j_{s_x}^x(0))$ plays the role of the normal density $\rho_n$, defined as the low-**q** limit of the transverse current response function.[24] Note that in the case of antiferromagnetism, where the current is not conserved, we can safely take the $q\to 0$ limit of the current operator for the calculation of the multiple magnon contribution to the static current response.

It is remarkable to point out that relation (18) was obtained in an independent way by Singh and Huse[21] starting directly from the definition of the spin stiffness as helicity modulus. The full agreement between the two formal derivations provides further support to the theory of spin hydrodyamics and at the same time emphasizes the role played by multiple magnon excitations. Concerning this last point it is worth noting that in the large-$S$ limit multiple magnon excitations are absent, $\chi(j_{s_x}^x(0))=0$, and $\rho_s$ coincides with $2(f_z+f_y)$. Actually, using the results of spin-wave theory,[23] one can easily show that the multiple magnon term $\chi(j_{s_x}^x(0))$ is second order in $1/2S$, while the longitudinal sum rule (12), dominated by multiple magnons, is first order in $1/2S$. This different behavior is likely associated with the fact that longitudinal excitations are mainly two-magnon states, while the multiple magnon component of the transverse response is dominated by three-magnon states.

Another important result emerging from Table I concerns the low-**q** behavior of the transverse spin structure factor (6):

$$S^{\perp}(q)_{q\to 0}=\frac{1}{2}\frac{\rho_s}{c}q \qquad (19)$$

accounting for the fluctuations associated with the propagation of long-wavelength spin waves. The coefficient of linearity has been directly calculated by Singh[9] using the series-expansion method. The resulting estimate is in reasonable agreement with Eq. (19).

It is finally useful to stress that the results discussed in this section using the sum-rule technique emphasize in an explicit way the existence of a spontaneously broken symmetry in spin space. Different results would be obtained if one instead decided to work with an isotropic ground state, as happens, for example, in a numerical simulation in a finite system. In this case the results for the excitation energies, obtained through the evaluation of sum rules, would correspond to an average between transverse and longitudinal excitations and the information on the dispersion law of elementary modes would be consequently poorer.

## III. ORDER PARAMETER AND EXCITATION ENERGIES

The discussion of Sec. II on the behavior of the Feynman energy in the low-**q** region is based on the analysis of the spin-structure function. The existence of spin waves with linear dispersion must be, however, assumed in order to discuss such a behavior and cannot be predicted using this method, unless one exploits numerically the rather difficult low-**q** regime. For this reason it is useful to derive alternative bounds for the excitation energies which exploit more directly the long wavelength regime. Such bounds can be obtained with the help of an inequality due to Bogoliubov and point out a crucial feature characterizing antiferromagnets as well as other systems with spontaneously broken symmetries: the existence of an order parameter. This phenomenon is known to be at the origin of Goldstone modes which, in the antiferromagnetic case, take the form of spin waves with a linear dispersion at low **q**. This approach was proposed by Wagner[13] to prove the existence of Goldstone modes in an important class of physical systems. To our knowledge it has never been used to investigate the full **q** dependence of the excitation spectrum of Heisenberg antiferromagnets.

The starting point is the introduction of an upper bound for the energy $\omega(q)$ of the lowest excitation with wave vector **q**, in terms of the ratio between the energy weighted and the inverse energy-weighted sum rules relative to the operator $s^x_{\mathbf{q}}$:

$$\omega^2(q) \le \frac{\int S^{\perp}(q,\omega)\omega\, d\omega}{\int S^{\perp}(q,\omega)\frac{1}{\omega} d\omega} = \frac{\langle [s^x_{-\mathbf{q}}[H,s^x_{\mathbf{q}}]]\rangle}{\chi^{\perp}(q)} . \quad (20)$$

In Eq. (20) we have made use of Eq. (5) and used definition (14) for the transverse susceptibility.

The upper bound (20), holding at zero temperature, is stronger than the Feynman one [see Eq. (4)], being based on the inverse energy-weighted sum rule $\chi^{\perp}(q)$ rather than on the non-energy-weighted sum rule $S^{\perp}(q)$. Its determination requires however the difficult calculation of the **q** dependence of $\chi^{\perp}(q)$. In the following we will combine the bound (20) with the Bogoliubov inequality[13,25] for the static response relative to the operator $s^x_{\mathbf{q}}$

$$\chi^{\perp}(q)\langle [s^y_{\mathbf{g}-\mathbf{q}},[H,s^y_{\mathbf{q}-\mathbf{g}}]]\rangle \ge |\langle [s^x_{-\mathbf{q}},s^y_{\mathbf{q}-\mathbf{g}}]\rangle|^2 . \quad (21)$$

This inequality introduces the "conjugate" operator $s^y_{\mathbf{q}-\mathbf{g}}$ where **g** is the antiferromagnetic vector fixed by the condition $e^{i\mathbf{g}\cdot\mathbf{R}}=1$ when **R** connects sites in the same sublattice and $-1$ when it connects sites in different sublattices.

Using inequality (20) and (21) we then obtain the useful rigorous result[26]

$$\omega^2(q) \le \frac{\langle [s^x_{-\mathbf{q}},[H,s^x_{\mathbf{q}}]]\rangle \langle [s^y_{\mathbf{g}-\mathbf{q}},[H,s^y_{\mathbf{q}-\mathbf{g}}]]\rangle}{|\langle [s^x_{-\mathbf{q}},s^y_{\mathbf{q}-\mathbf{g}}]\rangle|^2} . \quad (22)$$

A major advantage of inequality (22) as compared to the Feynman bound (4), is that it involves commutators both in the numerator and denominator. In particular the quantity

$$\langle [s^x_{-\mathbf{q}},s^y_{\mathbf{q}-\mathbf{g}}]\rangle = i\left\langle \frac{1}{N}\sum_i s^z_i e^{i\mathbf{g}\cdot\mathbf{r}_i}\right\rangle \equiv im \quad (23)$$

coincides with the staggered magnetization (assumed here along the $z$ axis), i.e., with the order parameter of the problem, and is independent of $q$.

The full $q$ dependence of the bound (22) is then entirely fixed by the double commutators entering the numerator. Such commutators have been already calculated in Sec. II [see Eq. (7)]. Noting that $\gamma_{\mathbf{q}-\mathbf{g}}=-\gamma_{\mathbf{q}}$ we find the following result:

$$\omega(q) \le \frac{2z(f_z+f_y)}{m}\sqrt{1-\gamma^2_{\mathbf{q}}} = \frac{2(f_z+f_y)}{mSJ}\omega^{\mathrm{SW}}(q) , \quad (24)$$

where $\omega^{\mathrm{SW}}(q)=zJS\sqrt{1-\gamma^2_{\mathbf{q}}}$ is the dispersion law of classical spin-wave (SW) theory[1] and we have used the property $f_x=f_y$.

The following remarks are in order here.

(i) The rigorous bound (24) exhibits a linear behavior in $q$ for $q\to 0$, provided the order parameter is different from zero (Goldstone theorem). Furthermore this bound is symmetric by exchange of **q** with **g**$-$**q** and hence predicts the vanishing of elementary excitations also at the staggered wave vector **g**.

(ii) The $q$ dependence of this bound is entirely contained in the classical law $\omega^{\mathrm{SW}}(q)$, the coefficient of proportionality being independent of $q$. In particular from Eq. (24) we obtain the bound

$$c \le \frac{2(f_z+f_y)}{SmJ}c^{\mathrm{SW}} = 2\sqrt{2z}\frac{(f_z+f_y)}{m} \quad (25)$$

for the spin velocity in terms of the quantities $(f_z+f_y)$ and $m$ ($c^{\mathrm{SW}}=\sqrt{2z}SJ$ is the prediction of classical SW theory). Using the numerical results of Table I for $(f_z+f_y)$ and $m$ we find $c\le 1.6c^{\mathrm{SW}}$ in the $S=\frac{1}{2}$ square lattice. The bound (25) overestimates by $\sim 30\%$ the value of the spin velocity calculated through Eq. (13) ($c=1.2c^{\mathrm{SW}}$). In the $S=1$ square lattice result (25) yields $c\le 1.2c^{\mathrm{SW}}$, while Eq. (13) gives $c=1.1c^{\mathrm{SW}}$. At small $q$ the quality of the new bound is hence similar to the one of the Feynman approximation. From a conceptual point of view it has the advantage of exploiting directly the low-$q$ behavior with the only assumption of the existence of a broken symmetry. It is also interesting to remark that, using the result of second-order spin-wave theory,[23] the bound (25) for the spin velocity coincides with the exact value (13) up to first-order terms in $1/2S$. Deviations from the exact value are associated with multiple magnon effects [terms in $1/(2S)^2$].

The dispersion of magnon excitations in the $S=\frac{1}{2}$ square lattice Heisenberg model has been the object of a recent Monte Carlo calculation.[5] The authors of Ref. 8 have fitted their results with the law $\omega(q)\sim 1.2\omega^{\mathrm{SW}}(q)$ (similar results have been very recently found also by the authors of Ref. 10), consistently with the value of the spin velocity obtained from Eq. (13). The upper bound (24) is then found to overestimate the magnon dispersion by the same amount ($\sim 30\%$) in the whole Brillouin zone. In Fig. 1 we report the prediction of the Goldstone-type bound (24) together with the fit to the results of Ref. 8 and the predictions of the Feynman approximation taken from Ref. 9. It is interesting to remark that the Feynman approximation is much more accurate near the maximum of the dispersion curve rather than in the low-$q$ region where, according to the discussion of Sec. II, it overestimates the linear dispersion by $\sim 30\%$.

(iii) Inequality (24) becomes an identity in the large-$S$ limit ($f_z=\frac{1}{2}S^2$, $f_x=f_y=0$, $m=S$) where it coincides

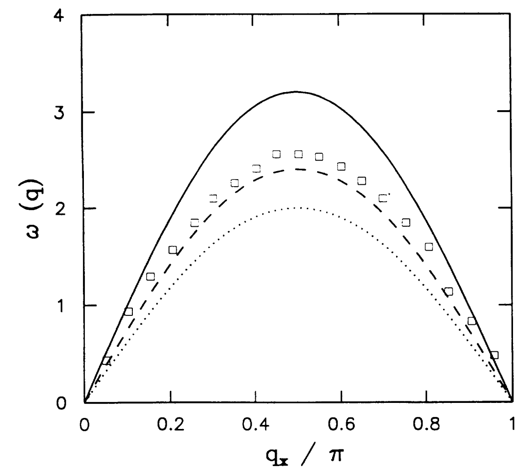


FIG. 1. Dispersion of spin excitations in the $S=\frac{1}{2}$ square lattice ($q_x=q_y$). The long-dashed line corresponds to the $\omega(q)=1.2\omega^{\rm SW}(q)$ fit to the Monte Carlo results of Refs. 8 and 10; the squares (taken from Ref. 9) correspond the Feynman bound (4), while the full line to the Goldstone-type bound (24). The prediction of classical spin-wave theory $\omega(q)=\omega^{\rm SW}(q)$ is also reported (dashed line).

with the prediction of classical spin-wave theory.[1]

The Bogoliubov inequality (21) can be used to provide directly a bound for the transverse susceptibility $\chi^{\perp}(q)$. Using the relation $\gamma_{\mathbf{q}-\mathbf{g}}=-\gamma_{\mathbf{q}}$ one finds

$$\chi^{\perp}(q)\geq\frac{m^2}{2z(f_z+f_y)(1+\gamma_{\mathbf{q}})} . \tag{26}$$

At $q=0$ Eq. (26) yields

$$\chi^{\perp}(0)\geq\frac{m^2}{4z(f_z+f_y)} , \tag{27}$$

while near the staggered vector $\mathbf{g}$ one finds the typical divergent behavior

$$\chi^{\perp}(|\mathbf{g}-\mathbf{q}|)\geq\frac{m^2}{2(f_z+f_y)q^2} \tag{28}$$

characterizing the transverse staggered susceptibility.

Once more these inequalities become identities if one works with spin-wave theory up to first order in $1/2S$. Deviations from the exact results for these formulas are the direct consequence of the role of multiple magnon excitations.

It is finally useful to complete the analysis of Sec. II concerning the contribution to the various sum rules given by the single-magnon and multiple magnon excitations in the region of the staggered vector $\mathbf{g}$. The results are reported in Table I. We note that single magnons exhaust the transverse structure factor and susceptibility sum rules characterized by typical infrared divergencies. The result for the spin-structure factor near the staggered vector can be obtained with the help of the sum rule (23)

$$\sum_n [\langle 0|s^x_{-\mathbf{q}}|n\rangle\langle n|s^y_{\mathbf{q}-\mathbf{g}}|0\rangle-\langle 0|s^y_{\mathbf{q}-\mathbf{g}}|n\rangle\langle n|s^x_{-\mathbf{q}}|0\rangle]$$
$$=\langle [s^x_{-\mathbf{q}},s^y_{\mathbf{q}-\mathbf{g}}|\rangle=im . \tag{29}$$

In fact, since the magnon matrix element $\langle 0|s^x_{-\mathbf{q}}|n\rangle$ behaves like $\sqrt{q}$ at low $\mathbf{q}$ [see Table I and Eq. (19)], it follows that the sum rule (29) can be satisfied only by a divergent behavior of the magnon matrix element $\langle n|s^y_{\mathbf{q}-\mathbf{g}}|0\rangle$ (multiple magnon excitations give rise to higher-order contributions) according to the equation

$$\langle n|s^y_{\mathbf{q}-\mathbf{g}}|0\rangle=\langle 0|s^y_{\mathbf{q}-\mathbf{g}}|n'\rangle=\frac{i}{2}\frac{m}{\langle 0|s^x_{-\mathbf{q}}|n\rangle} \tag{30}$$

holding for $q\to 0$. Here $|n\rangle$ and $|n'\rangle$ are single-magnon states with opposite wave vector and we have assumed, without any loss of generality, the matrix element $\langle 0|s^x_{-\mathbf{q}}|n\rangle=\langle n'|s^x_{-\mathbf{q}}|0\rangle$ to be real. The magnon contribution (30) dominates the divergent behavior of the spin-structure factor near the staggered vector that then takes the form

$$S^{\perp}(|\mathbf{g}-\mathbf{q}|)_{q\to 0}=\frac{cm^2}{2\rho_s q} . \tag{31}$$

The above results are consistent with the rigorous inequality[27]

$$S^{\perp}(q)S^{\perp}(|\mathbf{g}-\mathbf{q}|)\geq\tfrac{1}{4}m^2 \tag{32}$$

following from the uncertainty principle and holding for any value of $q$ and for any antiferromagnetic system. According to results (19) and (31), the uncertainty principle inequality becomes an identity in the $q\to 0$ limit. The coefficient of the $1/q$ law (31) has been recently calculated in the $S=\frac{1}{2}$ square lattice by Singh[9] using the series-expansion method from the Ising side. His prediction turns out to be larger by ($\sim 20\%$) than the value predicted by Eq. (31). This discrepancy remains to be understood.

Result (31) can be used to study the quality of the Feynman energy (4) near the staggered vector $\mathbf{g}$. One finds

$$\omega_F(|\mathbf{g}-\mathbf{q}|)_{q\to 0}=\frac{4z(f_z+f_y)\chi^{\perp}(0)}{m^2}cq , \tag{33}$$

where we have used expression (13) for the spin velocity $c$. Result (33) overestimates the spin velocity by $\sim 30\%$ in the $S=\frac{1}{2}$ square lattice. The enhancement coincides with the ratio between the left- and right-hand sides of inequality (27) for the transverse susceptibility and follows from the multiple magnon contribution to the energy-weighted sum rule.

## IV. RESULTS FOR THE ANISOTROPIC HEISENBERG MODEL

The energy-weighted sum rule (7) for the Heisenberg model has an interesting behavior at low $q$ in the anisotropic case ($\lambda\neq 1$). In fact at $q=0$, Eqs. (7a) and (7b) become

$$\lim_{q\to 0}\tfrac{1}{2}\langle 0|[s^x_{-\mathbf{q}},[H,s^x_{\mathbf{q}}]]|0\rangle=z(1-\lambda)(f_z-f_y) \tag{34a}$$

and

$$\lim_{q\to 0}\tfrac{1}{2}\langle 0|[s^y_{-\mathbf{q}},[H,s^y_{\mathbf{q}}]]|0\rangle=z(1-\lambda)(f_z-f_x) . \tag{34b}$$

Conversely the EWSR relative to $s^z_{\mathbf{q}}$ vanishes with $q$, since the Heisenberg Hamiltonian (1) conserves the $z$ component of the spin operator.

Note that the quantities $f_z - f_y$ and $f_z - f_x$ must be positive for $\lambda < 1$ and negative for $\lambda > 1$. This is a rigorous stability criterium imposed by the positivity of the energy-weighted sum rules (34).

Result (34) can be used to derive a rigorous upper bound for the mass gap when $\lambda < 1$. In fact in this case Eq. (22) yields

$$\omega(q=0) \leq \frac{2z}{m_z}\sqrt{(f_z^2 - f_y^2)}\sqrt{1-\lambda^2}\ , \tag{35}$$

where we have explicitly specified that the magnetization is along the $z$ axis (easy axis) and used the property $\gamma_{\mathbf{g}} = -1$.

This upper bound exhibits the typical nonanalytic $\sqrt{1-\lambda^2}$ behavior predicted by SWT near $\lambda = 1$. In the $S = \frac{1}{2}$ square lattice the coefficient of proportionality of the upper bound (35) is equal to 1.9, compared to the value 1.3 obtained in Ref. 28 using the series-expansion method.

Using the Bogoliubov inequality (21) it is also possible to obtain the rigorous bound

$$\chi^{\perp}(\mathbf{g}) \geq \frac{m_z^2}{2z(f_z - f_y)(1-\lambda)} \tag{36}$$

for the transverse staggered susceptibility.

Both results (35) and (36) apply only to the case $\lambda < 1$. It is also interesting to discuss the behavior of the system beyond the isotropic point $\lambda = 1$ where one expects the spontaneous magnetization to occur in the $x$-$y$ plane (easy plane). In the following we assume the magnetization axis to coincide with the $x$ axis. One can find in this case a rigorous Goldstone-type upper bound similar to Eq. (24). This bound is obtained starting from inequality (22), by replacing the operator $s^x_{\mathbf{q}}$ with $s^z_{\mathbf{q}}$ (the replacement follows from the new direction of the magnetization axis):

$$\omega^2(q) \leq \frac{\langle [s^z_{-\mathbf{q}}, [H, s^z_{\mathbf{q}}]]\rangle \langle [s^y_{\mathbf{g}-\mathbf{q}}, [H, s^y_{\mathbf{q}-\mathbf{g}}]]\rangle}{|\langle [s^z_{-\mathbf{q}}, s^y_{\mathbf{q}-\mathbf{g}}]\rangle|^2}\ . \tag{37}$$

Using results (7) for the corresponding double commutators and the identity

$$\langle [s^z_{-\mathbf{q}}, s^y_{\mathbf{q}-\mathbf{g}}]\rangle = -i\left\langle \frac{1}{N}\sum_i s_i^x e^{i\mathbf{g}\cdot\mathbf{r}_i}\right\rangle \equiv -im_x$$

(staggered magnetization along the $x$ axis), we obtain

$$\omega^2(q) \leq \frac{4\lambda z^2}{m_x^2}(f_x + f_y)(1-\gamma_{\mathbf{q}}) \times [f_z(1+\lambda\gamma_{\mathbf{q}}) + f_x(\lambda + \gamma_{\mathbf{q}})] \tag{38}$$

yielding a linear dispersion for $\omega(q)$ at small $q$ (the occurrence of gapless spin excitations for the easy-plane antiferromagnet has been recently pointed out in Ref. 29). It is worth noticing, however, that, differently from Eq. (24) holding in the isotropic case, the bound (38) is not symmetric by change of $\mathbf{q}$ with $\mathbf{g}-\mathbf{q}$ and in particular it is not gapless at the staggered point $\mathbf{g}$. This reflects the fact that this system, characterized by an anisotropy of the Hamiltonian in the $z$ direction and by a spontaneous staggered magnetization along the $x$ axis, exhibits two different branches in the excitation spectrum: one excited by the operator $s^z_{\mathbf{q}}$ and for which Eqs. (37) and (38) provide a rigorous upper bound, and one excited by the operator $s^y_{\mathbf{q}}$. The bound for the second branch is easily obtained by replacing, in Eq. (37), the operator $s^z_{\mathbf{q}}$ with $s^y_{\mathbf{q}}$ and $s^y_{\mathbf{g}-\mathbf{q}}$ with $s^z_{\mathbf{g}-\mathbf{q}}$. This corresponds to replacing $\mathbf{q}$ with $\mathbf{g}-\mathbf{q}$ and hence, in Eq. (38), $\gamma_{\mathbf{q}}$ with $-\gamma_{\mathbf{q}}$. Notice that this second branch is gapless at the staggered vector $\mathbf{g}$.

Equation (38) provides a rigorous upper bound for the spin velocity holding for an arbitrary value of $\lambda$ (larger than 1 of course):

$$c \leq \frac{2}{m_x}\sqrt{z\lambda(1+\lambda)}\sqrt{(f_x + f_y)(f_x + f_z)}\ . \tag{39}$$

Result (39) coincides with result (26) in the $\lambda \to 1$ limit and provides a nontrivial result also in the $\lambda \to \infty$ limit ($XY$ model).

Another interesting result can be obtained for the behavior of the derivative of the energy with respect to the transverse coupling constant $\lambda$. This behavior is important because it characterizes the nature of the phase transition at the isotropic point. The derivative can be calculated starting from the general Feynman formula

$$\frac{dE(\lambda)}{d\lambda} = -z(f_x + f_y)\ , \tag{40}$$

which straightforwardly follows from the form of the Heisenberg Hamiltonian (1) and definitions (8) for $f_x$ and $f_y$. When $\lambda \to 1^-$ one has $f_x^- = f_y^- \neq f_z^-$, while when $\lambda \to 1^+$ one has $f_x^+ = f_z^-$ and $f_z^+ = f_y^+ = f_y^-$. This finally yields

$$\frac{dE(\lambda)^-}{d\lambda} = -2zf_y^-\ ,\qquad \frac{dE(\lambda)^+}{d\lambda} = -z(f_z^- + f_y^-)\ . \tag{41}$$

Using the values for $f_z$ and $f_y$ reported in Table II (corresponding to spontaneous magnetization along the $z$ axis and hence to $f_z^-$ and $f_y^-$, respectively) we find $dE(\lambda)^-/d\lambda = -0.32$ and $dE(\lambda)^+/d\lambda = -0.50$. These values are in excellent agreement with the results obtained in Ref. 30 through a direct Monte Carlo calculation of the energy as a function of the coupling constant $\lambda$.

## V. CONCLUSIONS

In this work we have derived several new results concerning the propagation of elementary excitations in the Heisenberg antiferromagnet. In particular:

(1) We have proven that the Feynman approximation does not yield the correct dispersion of long-wavelength spin waves, due to the role of multiple magnon excitations which contribute to the energy-weighted sum rule (EWSR) even in the low-$q$ limit. Physically this behavior originates from the fact that the spin current is not conserved. Actually the multiple magnon contribution to

the EWSR is fixed by the static spin current polarizability $\chi(j^x_{s_x}(0))$ [see Eq. (18)]. Due to this effect, second order in $1/2S$, the Feynman approximation turns out to overestimate the spin velocity in the $S=\frac{1}{2}$ square lattice by about 30%.

(2) We have derived (Sec. III) a Goldstone-type bound for the energy of spin excitations. This rigorous bound depends explicitly on the order parameter (staggered magnetization) and is proportional to the classical dispersion of spin-wave theory with a $q$-independent normalization factor. It consequently vanishes at $\mathbf{q}=0$ as well as at the staggered wave vector $\mathbf{q}=\mathbf{g}$. This bound is shown to have an accuracy similar to the one of the Feynman approximation.

(3) We have obtained useful results also for the anisotropic case (Sec. IV). In particular for the easy-axis antiferromagnet we have derived a rigorous bound for the mass gap. Vice versa the upperbound in the easy-plane antiferromagnet is proven to be gapless in agreement with the general statement of the Goldstone theorem. We have also explicitly calculated the discontinuity of the derivative of the energy with respect to the transverse coupling constant at the isotropic point.

A more systematic investigation of the structure of elementary excitations in the anisotropic case (including the $XY$ model) will be presented in a future paper.

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$$E=4(f_z+2f_y)=-2JS^2[1+0.316/2S+0.025/(2S)^2]\ ,$$

$$m=S[1-0.393/2S]\ ,$$

$$\chi^{\perp}=1/8J[1-0.551/2S+0.065/(2S)^2],$$

$$\rho_s=JS^2[1-0.235/2S-0.041/(2S)^2]\ ,$$

$$2(f_z+f_y)=JS^2[1-0.235/2S+0.242/(2S)^2]\ .$$

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