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LETTER TO THE EDITOR

Bounds for correlation functions of the Heisenberg antiferromagnet

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Abstract. We present rigorous lower bounds for spin correlations of the quantum Heisenberg antiferromagnet under the assumption of long range order, at zero as well as non-zero temperatures in the form of a crossover function. These are obtained by combining a recent inequality giving lower bounds to correlation functions with infrared upper bounds for the static susceptibility. The functional forms of the lower bounds are identical with upper (infrared) bounds for the correlation functions implying that the nature of divergence of the correlations near the antiferromagnetic zone boundary is determined. The form agrees with the prediction of the theory of spin waves. We also present a generalized inequality in quantum statistical mechanics that contains the previously known cases as special cases.

An interesting recent paper by Pitaevskii and Stringari [1] introduces a new inequality in quantum statistical mechanics, that has several features that are complementary to the well known inequality of Bogoliubov [2]. This inequality helps in establishing the absence of long ranged order (LRO) in the ground state of several generic one-dimensional many body problems possessing a continuous symmetry group, such as the Heisenberg antiferomagnet (SU(2)), the interacting Bose gas (U(1)) and the crystal (translation group). This is the zero temperature analogue of the Hohenberg–Mermin–Wagner theorem [3]. We find that the inequality can be supplemented by infrared bounds available for the quantum Heisenberg antiferromagnet (HAFM), available from the work of Dyson, Lieb and Simon (DLS) [4], and together we obtain lower bounds for the correlation functions under the assumption of LRO. These bounds have the same functional form as the upper bounds available from [4], and imply that if the model has LRO then the singular part of the correlation functions is determined. The assumption of LRO is known to be true for all spin in three dimensions [5, 6], and hence we have an interesting rigorous result in this case. The form of the correlation function agrees with the results of the hydrodynamic theory of spin waves [7] at non-zero temperature and with the Anderson–Kubo theory of spin waves at zero temperature [8].

Let us first consider the inequality in question. The work of [1] showing that an inequality distinct from that of [2] can be constructed, raises the question: how many such 'independent' inequalities exist? We provide an answer: an infinite number of such inequalities can be written down. We derive a generalization of which the inequalities of [1] and [2] are special cases. Of course only a few may be actually useful in physical applications. Firstly let us define a spectral function depending on two (non-Hermitian in general) operators a and b with $\mathscr{Z}$ the partition function:

$$p_{a,b}(\omega)=\frac{1}{\mathscr{Z}}(1+\exp(-\beta\omega))\sum\exp(-\beta\varepsilon_\nu)\langle\nu|a|\mu\rangle\langle\mu|b|\nu\rangle\delta(\varepsilon_\mu-\varepsilon_\nu-\omega). \quad (1)$$

It is readily seen that

$$p_{a^\dagger,a}(\omega)\geqslant 0 \quad (2)$$

which is the most fundamental property of the spectral function, and also $p_{a,b}(-\omega)=p_{b,a}(\omega)=p^*_{a^\dagger,b^\dagger}(\omega)$. Let us also note the following properties of the function p: (1) $p_{a+b,c}(\omega)=p_{a,c}(\omega)+p_{b,c}(\omega)$, (2) $p_{\alpha a,b}(\omega)=\alpha p_{a,b}(\omega)$ where $\alpha=$ constant. The pointwise (in ω) nature of (2) is at the root of the generalization set out here. We can in fact use the above properties to define a scalar product satisfying the Cauchy–Schwartz inequality

$$|p_{a^\dagger,b}(\omega)|^2\leqslant p_{a^\dagger,a}(\omega)\,p_{b^\dagger,b}(\omega). \quad (3)$$

The function p is expected to be 'smooth' in the thermodyanamic limit, but for a finite sized system, will consist of a series of delta functions and the manipulations carried out out here require the theory of generalized functions for justification, which we will not attempt here [9]. We will assume that the functions are sufficiently smooth here. Given (3), we see that for any two complex functions, $f_{a^\dagger}(\omega)$, $f_b(\omega)$, labelled by the two operators a and b, the integral

$$\left|\int \mathrm{d}\omega\, f_{a^\dagger}(\omega)f_b(\omega)\,p_{a^\dagger,b}(\omega)\right|^2\leqslant\left\{\int \mathrm{d}\omega\,|f_{a^\dagger}(\omega)f_b(\omega)|\sqrt{p_{a^\dagger,a}(\omega)\,p_{b^\dagger,b}(\omega)}\right\}^2. \quad (4)$$

Using the Cauchy–Schwartz inequality, we conclude

$$\left|\int \mathrm{d}\omega\, f_{a^\dagger}(\omega)f_b(\omega)\,p_{a^\dagger,b}(\omega)\right|^2\leqslant\int \mathrm{d}\omega\,|f_{a^\dagger}(\omega)|^2 p_{a^\dagger,a}(\omega)\int \mathrm{d}\omega\,|f_b(\omega)|^2 p_{b^\dagger,b}(\omega). \quad (5)$$

Various choices of the filter functions f generate the different inequalities, the inequality of Bogoliubov [2] is obtained by setting $f_{a^\dagger}(\omega)=f_b(\omega)=\sqrt{\tanh(\beta\omega/2)/\omega}$, and that of Pitaevskii and Stringari [1] by setting $f_{a^\dagger}(\omega)=\tanh(\beta\omega)$, $f_b(\omega)=1$. It is clear that the first [2] gives a large weight to frequencies less than $k_B T$ and suppresses higher frequencies, whereas the second [1] favours the opposite regime for one of the operators. More general functions can be readily imagined, for example we can take $f_{a^\dagger}(\omega)=\alpha_1+\alpha_2\tanh(\beta\omega/2)$ and $f_b(\omega)=1$ with complex α_i to generate generalized commutators that arise in parafermionic theories. For completeness, we note the results of convolution with the following frequently needed filter functions with the notation $\langle f(\omega)\rangle_{a,b}\equiv\int \mathrm{d}\omega\, f(\omega)\,p_{a,b}(\omega)$,

$$\langle 1\rangle_{a,b}=\langle\{a,b\}\rangle \qquad \langle\tanh(\beta\omega/2)\rangle_{a,b}=\langle[a,b]\rangle \quad (6)$$

$$\langle\omega\tanh(\beta\omega/2)\rangle_{a,b}=\langle[[a,H],b]\rangle \qquad \langle\omega^{-1}\tanh(\beta\omega/2)\rangle_{a,b}=\beta(a,b) \quad (7)$$

where the Duhamel two point function is defined as

$$(a,b)=(k_B T)\frac{1}{\mathscr{Z}}\sum\frac{(\exp(-\beta\varepsilon_\nu)-\exp(-\beta\varepsilon_\mu))}{(\varepsilon_\mu-\varepsilon_\nu)}\langle\nu|a|\mu\rangle\langle\mu|b|\nu\rangle$$

and $\langle A\rangle$ stands for the thermal average.

We now cast the inequality of [1] into a more useful form involving equilibrium quantities. With $f_{a^\dagger}(\omega)=\tanh(\beta\omega)$, $f_b(\omega)=1$ we write

$$|\langle[a^\dagger, b]\rangle|^2 \leqslant \langle\{b^\dagger, b\}\rangle\langle\tanh^2(\beta\omega/2)\rangle_{a^\dagger,a}. \tag{8}$$

Now we bound the second term in the RHS of (8) and begin by writing

$$\int_{-\infty}^{+\infty} d\omega \tanh^2(\beta\omega/2)\, p_{a^\dagger,a}(\omega) = \int_0^{+\infty} d\omega \tanh^2(\beta\omega/2)\{p_{a^\dagger,a}(\omega)+p_{a,a^\dagger}(\omega)\}.$$

We next use the concavity of $\tanh(x)$ in $[0,\infty)$ to obtain an upper bound (Jensen's inequality [10])

$$\langle\tanh^2(\beta\omega/2)\rangle_{a^\dagger,a} \leqslant \Phi \tanh\left(\beta\frac{\langle\omega\tanh(\beta\omega/2)\rangle_{a^\dagger,a}}{2\Phi}\right) \tag{10}$$

where

$$\Phi = \langle|\tanh(\beta\omega/2)|\rangle_{a^\dagger,a}. \tag{11}$$

From the Cauchy-Schwartz inequality we have

$$0 \leqslant \Phi \leqslant \sqrt{\langle\omega\tanh(\beta\omega/2)\rangle_{a^\dagger,a}\langle\omega^{-1}\tanh(\beta\omega/2)\rangle_{a^\dagger,a}}. \tag{12}$$

Since $\tanh(x)/x$ is monotonically decreasing in the interval $[0,\infty)$, we maximize the RHS of (10) subject to the constraint (12) giving

$$\langle\tanh^2(\beta\omega/2)\rangle_{a^\dagger,a} \leqslant \sqrt{\langle[[a^\dagger,H],a]\rangle\beta(a^\dagger,a)}\,\tanh\left(\frac{\beta}{2}\sqrt{\frac{\langle[[a^\dagger,H],a]\rangle}{\beta(a^\dagger,a)}}\right). \tag{13}$$

Combining inequalities (8) and (13), we find the final inequality

$$\langle\{b^\dagger,b\}\rangle \geqslant \frac{|\langle[a^\dagger,b]\rangle|^2}{\sqrt{\langle[[a^\dagger,H],a]\rangle\beta(a^\dagger,a)}}\coth\left(\frac{\beta}{2}\sqrt{\frac{\langle[[a^\dagger,H],a]\rangle}{\beta(a^\dagger,a)}}\right). \tag{14}$$

It is possible to show that the inequlaity (14) continues to hold if either or both of $\langle[[a^\dagger,H],a]\rangle$ or $\beta(a^\dagger,a)$ are replaced by their respective upper bounds by using the fact that $y^{-1/2}\coth(y^{\sigma/2})$ with $\sigma=\pm1$ is a monotonically decreasing function of y. At $T=0\,°K$, the coth function is replaced by unity and for $T\neq 0°K$, we can degrade the inequality by using $\coth(x)\geqslant(1/x)$ to write it in a form that is used in the theorems concerning absence of LRO [3]. The above form of (14), interpolates usefully between the two.

We now apply this general inequality to the Heisenberg antiferromagnet on a hypercubic lattice in d dimensions. Let $|\Lambda|$ stand for the number of sites in the lattice, and Λ^* the dual lattice. We denote $g_q^\alpha \equiv \langle S_q^\alpha S_{-q}^\alpha\rangle$, with

$$S_q^\alpha = \frac{1}{\sqrt{\Lambda}}\sum_{r\in\Lambda^*} S_r^\alpha \exp(-\mathrm{i}q\cdot r) \tag{15}$$

We choose [1] $b=S_{q+Q}^y$ and $a=S_q^x$, where $Q=\pi(1,\ldots)$; whence $[a^\dagger,b]=i|\Lambda|^{-1/2}S_Q^z$. If we assume that LRO exists along the x axis then $\langle S_Q^z\rangle=|\Lambda|^{1/2}m_0$, where m_0 is the staggered magnetization; thus $|\langle[a^\dagger,b]\rangle|=m_0$. The double commutator is readily evaluated using translation invariance as

$$\langle[[S_q^x,H],S_{-q}^x]\rangle = 2c_xE_q^- \tag{16}$$

where

$$c_x = -\sum_{\beta \neq x} \langle S_0^\beta S_\delta^\beta \rangle \tag{17}$$

with $\delta =$ *nearest neighbour* and

$$E_q^\pm = \sum_{i=1}^{d} (1 \pm \cos(qi)). \tag{18}$$

Upper bounds for the positive constant c_x are easily found from lower bounds to the internal energy; details may be found in [4].

For the Heisenberg antiferromagnet we are in the fortunate position of having the infrared bounds on the Duhamel function due to DLS:

$$\beta(S_q^x, S_{-q}^x) \leqslant \frac{1}{2E_q^+}. \tag{19}$$

We can thus bound the correlation function from below under the assumption of LRO. Towards this end we define the function G

$$G(q) \equiv \sqrt{\frac{E_q^-}{4E_q^+}} \coth(\beta\sqrt{c_x E_q^+ E_q^-}) \tag{20}$$

The lower bound for g_q^x can now be found by substituting in (14), shifting $q = Q + q'$ and using $E_{q+Q}^\pm = E_q^\mp$

$$g_q^x \geqslant m_0^2 G(q)/c_x \tag{21}$$

whereas the upper bound from DLS is

$$g_q^x \leqslant G(q). \tag{22}$$

Putting these together we find

$$G(q) \geqslant g_q^x \geqslant m_0^2 G(q)/c_x. \tag{23}$$

The final inequality (23) shows that the transverse spin correlation diverges as $1/|q - Q|$ at $T = 0°$ and as $k_B T/|q - Q|^2$ at finite temperatures when the system possesses LRO. This provides rigorous support to the theory of spin waves in this system, which is based on hydrodynamic reasoning at $T \neq 0°$ [7], and on an expansion in inverse powers of S, the spin, at $T = 0°$ [8]. It is remarkable that the Gaussian domination estimate of the Duhamel two point function [4], upon which our bounds rest, obtains the exponents of divergence exactly in these cases ([11]).

In the case of one dimension where the Heisenberg antiferromagnet cannot have LRO at any temperature, by virtue of the incompatibility of these bounds with the sum rule $\Sigma_{q,\alpha} g_q^\alpha = |\Lambda| S(S+1)$, there is a considerable body of numerical and approximate analytical work at $T = 0$ K summarized in [12], which suggests for large separation that $g(r) \sim (-1)^r (\log(r))^{1/2}/r$, which means that the bound overestimates the divergence near Q significantly. This is not unreasonable since the bounds do not take any simplifying factors special to one-dimension into account.

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[9] For a finite system, we imagine the function $p(\omega)$ to be smoothed by multiplying by a smearing function and integrating over a small energy range containing several discrete levels of the finite system. The functions $f_{a'}(\omega)$ should be sufficiently smooth on this energy scale.

[10] Hardy G, Littlewood J E and Pólya G 1934 *Inequalities* (Cambridge: Cambridge University Press)

[11] In the limit of large dimensionality, the Néel state is easily seen to be the exact gound state. In fact, the spontaneous magnetization is known to converge to that in the classical Néel state [6]. The Néel state that is picked out in the present case, is one with long ranged order in the Z direction, as opposed to the rotationally invariant one implicit in [6], and hence m_0^2 is expected to be S^2, rather than $S^2/3$. Also the tranverse term in c_x vanishes in this limit and hence we expect $c_x = S^2$. Therefore inequality (23) would imply for large dimensions: $g_q^x = G(q)$.

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