An Upper Bound for the Energy Spectrum of Hard-Core Bosonic Lattice Gases

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April 10, 2019

Abstract

This document combines derivations and explanations of current proofs of an upper bound for the spin-wave spectrum of antiferromagnets in quantum Heisenberg moidel. The connection between antiferromagnets and lattice gases consisting of hard-core bosons is discussed in motivation section.

1 Motivation

One can consider a gas of hard-core bosons in a crystal lattice. Term *hard-core* here refers to the fact that two or more of these particles cannot occupy the same lattice site. Thus said, each lattice site can be either occupied by a single boson or remain empty. The ground state energy spectrum is given by:

$$\varepsilon_0(\boldsymbol{q}) = \inf \text{ spec } \mathcal{H}|_{\boldsymbol{p}=\boldsymbol{q}}, \tag{1}$$

where $\mathcal{H}$ is the Hamiltonian of the system, $\boldsymbol{p}$ is some conserved parameter, which in this case is represented by the momentum $\boldsymbol{q}$. Thus said, the ground state energy is the infimum of system energies of states with fixed momentum $\boldsymbol{q}$. One can obtain an upper bound for (1) by using so-called Bijl-Feynman ansatz (single mode approximation). This upper bound can be written down in a form:

$$\varepsilon_0(\boldsymbol{q}) \lesssim \frac{|\boldsymbol{q}|^2}{S(\boldsymbol{q})}, \tag{2}$$

where $S(\boldsymbol{q}) \propto |\boldsymbol{q}|$ is called a structure factor.

One may notice the similarity between the bosonic problem and a spin-$\frac{1}{2}$ quantum Heisenberg model for antiferromagnets, for which the upper bound was proved by several papers, including [1] and better, as claimed, [2] and [3]. The idea of mapping problems to one another is relatively simple: the existence of the particle in the lattice site i refers to the value of spin $S_i = +\frac{1}{2}$, whereas the empty site refers to $S_i = -\frac{1}{2}$ value of spin. More accurately, $\hat{S}_+$ and $\hat{S}_-$ operators are linked with bosonic creation and annihilation operators respectively. If one considers the anisotropy parameter $\Delta = 0$ in quantum Heisenberg model, the Hamiltonian has the following representation (only nearest neighbor interaction is taken into account):

$$\hat{\mathcal{H}} = \sum_{i,j:|\boldsymbol{r}_i - \boldsymbol{r}_j|=1} (\hat{S}_x^{(i)} \hat{S}_x^{(j)} + \hat{S}_y^{(i)} \hat{S}_y^{(j)}), \tag{3}$$

which can be rewritten in terms of $\hat{S}_+$ and $\hat{S}_-$ operators and then mapped to the following bosonic Hamiltonian:

$$\hat{\mathcal{H}}_B = \sum_{i,j:|\boldsymbol{r}_i - \boldsymbol{r}_j|=1} (\hat{a}_i^\dagger \hat{a}_j + \hat{a}_j^\dagger \hat{a}_i). \tag{4}$$

One may notice, that terms in Hamiltonian (4) refer to the movement of boson between lattice sites i and j. If one considers also the $\hat{S}_z$ term, by making $\Delta \neq 0$, in the relation for antiferromagnet Hamiltonian (3), the corresponding bosonic term will refer to the nearest-neighbor interaction between bosons.
To sum up: in case if one understands the proof of an upper bound for the spin-wave energy spectrum for the antiferromagnetic Heisenberg model, the same type of upper bound may be claimed for the ground state energy of interacting hard-core bosons in a lattice.

2 Uncertainty principle for non-Hermitian operators

The results presented in this section were originally obtained by Lev Pitaevskii and Sandro Stringari in [4]. Main goal of this section is to present the inequality yielding, at low temperature, relevant information on the fluctuations of physical quantities. The resulting inequality can be applied both to Hermitian and non-Hermitian operators and can be consequently regarded as a natural generalization of the Heisenberg uncertainty principle. Its determination is based on the use of the Cauchy-Schwarz inequality for auxiliary operators related to the physical operators through a linear transformation. The inequality is later used in Section 3 to calculate the upper bound for spin-wave structure factor.

2.1 Zero-temperature limit

Let us define a scalar product between the two operators A and B as:

$$(A, B) = \left\langle \{A^\dagger, B\} \right\rangle, \tag{5}$$

where $\{A^\dagger, B\} = A^\dagger B + B A^\dagger$ and $\langle ... \rangle$ means the statistical average. This definition satisfies all the requirements for a scalar product, thus the Cauchy-Schwarz inequality can be used:

$$|(u,v)|^2 \leq (u,u) \cdot (v,v) \Longrightarrow \left\langle \{A^\dagger, A\} \right\rangle \cdot \left\langle \{B^\dagger, B\} \right\rangle \geq \left| \left\langle \{A^\dagger, B\} \right\rangle \right|^2. \tag{6}$$

One can show that this inequality holds even if the anticommutator is replaced by q-commutator:

$$[A^\dagger, B]_q = A^\dagger B + q B A^\dagger; \quad |q| \leq 1. \tag{7}$$

One can first prove the statement (6) for the ordinary commutator in the simplest case, where the average is taken on the ground state of the system (zero-temperature limit). Given the physical operator C, one can define an auxiliary operator $\tilde{C}$ satisfying the following properties:

$$\langle n | \tilde{C} | 0 \rangle = \langle n | C | 0 \rangle \quad \text{and} \quad \langle 0 | \tilde{C} | n \rangle = - \langle 0 | C | n \rangle, \tag{8}$$

and hence:

$$\langle n | \tilde{C}^\dagger | 0 \rangle = - \langle n | C^\dagger | 0 \rangle \quad \text{and} \quad \langle 0 | \tilde{C}^\dagger | n \rangle = \langle 0 | C^\dagger | n \rangle, \tag{9}$$

where states $|n\rangle$ form a complete set of states of the system and operators satisfy the condition $\langle 0 | C | 0 \rangle = \langle 0 | \tilde{C} | 0 \rangle = 0$. One can now write down explicitly the average of an anticommutator $\{A^\dagger, B\}$ in the form:

$$\langle 0 | \{A^\dagger, B\} | 0 \rangle = \sum_n \Big(\langle 0 | A^\dagger | n \rangle \langle n | B | 0 \rangle + \langle 0 | B | n \rangle \langle n | A^\dagger | 0 \rangle \Big) \tag{10}$$

and straightforwardly check the following identities:

$$\langle 0 | \{A^\dagger, \tilde{B}\} | 0 \rangle = \langle 0 | [A^\dagger, B] | 0 \rangle \quad \text{and} \quad \langle 0 | [\tilde{B}^\dagger, \tilde{B}] | 0 \rangle = \langle 0 | \{B^\dagger, B\} | 0 \rangle, \tag{11}$$

but due to the Cauchy-Schwarz inequality:

$$\left\langle \{A^\dagger, A\} \right\rangle \left\langle \{B^\dagger, B\} \right\rangle = \left\langle \{A^\dagger, A\} \right\rangle \left\langle \{\tilde{B}^\dagger, \tilde{B}\} \right\rangle \geq \left| \{A^\dagger, \tilde{B}\} \right|^2 = \left| \left\langle [A^\dagger, B] \right\rangle \right|^2. \tag{12}$$

2.2 Finite temperatures

One can consider a system at a temperature different than zero in statistical equilibrium. In this case, the definition of the auxiliary operator $\tilde{C}$ should be generalized the following way:

$$\langle n|\, \tilde{C}\, |m\rangle = \frac{\rho_m - \rho_n}{\rho_m + \rho_n} \langle n|\, C\, |m\rangle\,, \tag{13}$$

where $\rho_n = Z^{-1}\exp(-\beta E_n)$ is the statistical weight relative to the state $|n\rangle$, E_n is the eigenvalue of the grand canonical Hamiltonian $\mathcal{H} - \mu N$ and $Z = \sum_n \exp(-\beta E_n)$ is the partition function. By writing the statistical average of the anticommutator $\{A^\dagger, B\}$ in the form:

$$\begin{aligned}\left\langle\{A^\dagger, B\}\right\rangle = \left\langle A^\dagger B + BA^\dagger\right\rangle = Z^{-1}\sum_m \exp(-\beta E_m)\,\langle m|\, A^\dagger B\, |m\rangle + \\ + Z^{-1}\sum_n \exp(-\beta E_n)\,\langle n|\, BA^\dagger\, |n\rangle = Z^{-1}\sum_{m,n}(\exp(-\beta E_m) + \exp(-\beta E_n))\,\langle m|\, A^\dagger\, |n\rangle\,\langle n|\, B\, |m\rangle\,.\end{aligned} \tag{14}$$

One straightforwardly finds the following identities:

$$\begin{aligned}\left\langle\{A^\dagger, \tilde{B}\}\right\rangle &= Z^{-1}\sum_{m,n}(\exp(-\beta E_m) + \exp(-\beta E_n))\,\langle m|\, A^\dagger\, |n\rangle\,\langle n|\, \tilde{B}\, |m\rangle = \\ &= Z^{-1}\sum_{m,n}(\exp(-\beta E_m) + \exp(-\beta E_n))\,\langle m|\, A^\dagger\, |n\rangle\,\frac{\rho_m - \rho_n}{\rho_m + \rho_n}\,\langle n|\, B\, |m\rangle = \\ &= Z^{-1}\sum_{m,n}(\exp(-\beta E_m) - \exp(-\beta E_n))\,\langle m|\, A^\dagger\, |n\rangle\,\langle n|\, \tilde{B}\, |m\rangle = \left\langle[A^\dagger, B]\right\rangle,\end{aligned} \tag{15}$$

$$\begin{aligned}\left\langle\{\tilde{B}^\dagger, \tilde{B}\}\right\rangle &= Z^{-1}\sum_{m,n}(\exp(-\beta E_m) + \exp(-\beta E_n))\,\langle m|\, \tilde{B}^\dagger\, |n\rangle\,\langle n|\, \tilde{B}\, |m\rangle = \\ &= Z^{-1}\sum_{m,n}(\exp(-\beta E_m) + \exp(-\beta E_n))\frac{\rho_m - \rho_n}{\rho_m + \rho_n}\,\langle m|\, B^\dagger\, |n\rangle\,\frac{\rho_m - \rho_n}{\rho_m + \rho_n}\,\langle n|\, B\, |m\rangle = \\ &= Z^{-1}\sum_{m,n}\frac{(\rho_m - \rho_n)^2}{\rho_m + \rho_n}\,\langle m|\, B^\dagger\, |n\rangle\,\langle n|\, B\, |m\rangle\,.\end{aligned} \tag{16}$$

Given the fact that:

$$\begin{aligned}\int \tanh(\beta\omega/2)\delta(\omega - E_n + E_m)d\omega &= \tanh\!\left(\frac{\beta}{2}(E_n - E_m)\right) = \\ &= \frac{\exp\!\left(\frac{\beta}{2}(E_n - E_m)\right) - \exp\!\left(-\frac{\beta}{2}(E_n - E_m)\right)}{\exp\!\left(\frac{\beta}{2}(E_n + E_m)\right) - \exp\!\left(-\frac{\beta}{2}(E_n - E_m)\right)} = \frac{\rho_m - \rho_n}{\rho_m + \rho_n},\end{aligned} \tag{17}$$

one finally obtains:

$$\begin{aligned}\left\langle\{\tilde{B}^\dagger, \tilde{B}\}\right\rangle &= \int Z^{-1}\sum_{m,n}(\rho_m - \rho_n)\,\langle m|\, B^\dagger\, |n\rangle\,\langle n|\, B\, |m\rangle \tanh(\beta\omega/2)\delta(\omega - E_n + E_m)d\omega = \\ &= \int d\omega A_{B^\dagger,B}(\omega)\tanh(\beta\omega/2),\end{aligned} \tag{18}$$

where:

$$A_{A^\dagger,B}(\omega) = Z^{-1}\sum_{m,n}(\exp(-\beta E_m) - \exp(-\beta E_n))\,\langle m|\, A^\dagger\, |n\rangle\,\langle n|\, B\, |m\rangle\,\delta(\omega - E_n + E_m). \tag{19}$$

One can now prove the following identities:

$$\left\langle\{A^\dagger, A\}\right\rangle = Z^{-1}\sum_{m,n}(\exp(-\beta E_m) + \exp(-\beta E_n))\,\langle m|\, A^\dagger\, |n\rangle\,\langle n|\, A\, |m\rangle = \int d\omega A_{A^\dagger,A}(\omega)\coth(\beta\omega/2), \tag{20}$$

$$\left\langle\{\tilde{B}^\dagger,\tilde{B}\}\right\rangle = Z^{-1}\sum_{m,n}(\exp(-\beta E_m)+\exp(-\beta E_n))\langle m|\tilde{B}^\dagger|n\rangle\langle n|\tilde{B}|m\rangle = \int d\omega A_{B^\dagger,B}(\omega)\tanh(\beta\omega/2), \tag{21}$$

$$\left\langle\{A^\dagger,\tilde{B}\}\right\rangle = \sum_{m,n}(\rho_m+\rho_n)\langle m|A^\dagger|n\rangle\langle n|\tilde{B}|m\rangle = \sum_{m,n}(\rho_m-\rho_n)\langle m|A^\dagger|n\rangle\langle n|B|m\rangle = \int d\omega A_{A^\dagger,B}(\omega). \tag{22}$$

Applying the Cauchy-Schwarz inequality to $\left\langle\{A^\dagger,B\}\right\rangle$, which defines the scalar product as it was mentioned before, one can obtain general non-trivial result:

$$\left\langle\{A^\dagger,A\}\right\rangle\cdot\left\langle\{\tilde{B}^\dagger,\tilde{B}\}\right\rangle \geq \left|\left\langle\{A^\dagger,\tilde{B}\}\right\rangle\right|^2, \tag{23}$$

$$\int d\omega A_{A^\dagger,A}(\omega)\coth(\beta\omega/2)\cdot\int d\omega A_{B^\dagger,B}(\omega)\tanh(\beta\omega/2) \geq \left|\int d\omega A_{A^\dagger,B}(\omega)\right|^2. \tag{24}$$

The result for zero temperature (12) might be obtained directly by implying:

$$\lim_{\beta\to\infty}\coth(\beta\omega/2) = \lim_{\beta\to\infty}\tanh(\beta\omega/2) = 1. \tag{25}$$

Using (24) one may obtain the Bogoliubov inequality as well. See Appendix A for details.

3 Lower bound for correlation function (structure factor)

The results presented in this section were originally obtained by B. Sriram Shastry in [7]. The goal of this section is to provide a lower bound for the structure factor (or correlation function) of the Heisenberg antiferromagnet.

The spectral function depending on two (non-Hermitian in general) operators a and b with Z being the partition function can be defined the following way:

$$\rho_{a,b}(\omega) = \frac{1}{Z}\big(1+\exp(-\beta\omega)\big)\sum_{\mu,\nu}\exp(-\beta\varepsilon_\nu)\langle\nu|a|\mu\rangle\langle\mu|b|\nu\rangle\,\delta(\varepsilon_\mu-\varepsilon_\nu-\omega). \tag{26}$$

Note: this spectral function is related to spectral function (19) through:

$$\rho_{a,b}(\omega)\tanh(\beta\omega/2) = A_{a,b}(\omega).$$

It can be easily proved that:

$$\rho_{a^\dagger,a}(\omega) = \frac{1}{Z}\big(1+\exp(-\beta\omega)\big)\sum_{\mu,\nu}\exp(-\beta\varepsilon_\nu)\langle\nu|a^\dagger|\mu\rangle\langle\mu|a|\nu\rangle\,\delta(\varepsilon_\mu-\varepsilon_\nu-\omega) =$$
$$= \frac{1}{Z}\big(1+\exp(-\beta\omega)\big)\sum_{\mu,\nu}\exp(-\beta\varepsilon_\nu)\big|\langle\mu|a|\nu\rangle\big|^2\delta(\varepsilon_\mu-\varepsilon_\nu-\omega)\geq 0, \tag{27}$$

which is the most fundamental property of the spectral function and also:

$$\rho_{a,b}(-\omega) = \rho_{b,a}(\omega) = \rho^*_{a^\dagger,b^\dagger}(\omega), \tag{28}$$

$$\rho_{a+b,c}(\omega) = \rho_{a,c}(\omega)+\rho_{b,c}(\omega), \tag{29}$$

$$\rho_{\alpha a,b}(\omega) = \alpha\rho_{a,b}(\omega),\ \text{where } \alpha \text{ - constant.} \tag{30}$$

The above properties prove that the spectral function may be used to define a scalar product, which satisfies the Cauchy-Schwarz inequality:

$$a^\dagger\cdot b \equiv \int d\omega f_{a^\dagger}(\omega)f_b(\omega)\rho_{a^\dagger,b}(\omega), \tag{31}$$

$$\left|\int d\omega f_{a^\dagger}(\omega) f_b(\omega)\rho_{a^\dagger,b}(\omega)\right|^2 \le \int d\omega \left|f_{a^\dagger}(\omega)\right|^2 \rho_{a^\dagger,a}(\omega) \int d\omega \left|f_b(\omega)\right|^2 \rho_{b^\dagger,b}(\omega). \tag{32}$$

Various choices of filter functions f generate the different inequalities:

1. Bogoliubov inequality: $f_{a^\dagger}(\omega) = f_b(\omega) = \sqrt{\tanh(\beta\omega/2)}$ gives a large weight to frequencies less than $k_B T$ and suppresses higher frequencies.
2. Pitaevskii and Stringari inequality: $f_{a^\dagger}(\omega) = \tanh(\beta\omega/2)$; $f_b(\omega) = 1$ favors the opposite regime for one of the operators.

Note: the original paper [7] has a mistake in the transition to Pitaevskii and Stringari inequality. One can calculate the results of convolution with the following frequently needed filter functions:

$$\langle f(\omega)\rangle_{a,b} = \int d\omega f(\omega)\rho_{a,b}(\omega), \tag{33}$$

$$\begin{gathered}\langle 1\rangle_{a,b} = \langle\{a,b\}\rangle\,,\ \langle\tanh(\beta\omega/2)\rangle_{a,b} = \langle[a,b]\rangle\,,\\ \langle\omega\tanh(\beta\omega/2)\rangle_{a,b} = \langle[[a,\mathcal{H}],b]\rangle\,,\ \left\langle\omega^{-1}\tanh(\beta\omega/2)\right\rangle_{a,b} = \beta(a,b),\end{gathered} \tag{34}$$

where the Duhamel two-point function is defined as:

$$(a,b) = (k_B T)\frac{1}{Z}\sum_{\mu,\nu}\frac{(\exp(-\beta\varepsilon_\nu) - \exp(-\beta\varepsilon_\mu))}{(\varepsilon_\mu - \varepsilon_\nu)}\langle\nu|\,a\,|\mu\rangle\langle\mu|\,b\,|\nu\rangle\,, \tag{35}$$

and $\langle A\rangle$ stands for the thermal average.
With $f_{a^\dagger}(\omega) = \tanh(\beta\omega/2)$ and $f_b(\omega) = 1$ from the Cauchy-Schwarz inequality one can write down the following:

$$\left|\int d\omega\tanh(\beta\omega/2)\rho_{a^\dagger,b}(\omega)\right|^2 \le \int d\omega\left|\tanh(\beta\omega/2)\right|^2\rho_{a^\dagger,a}(\omega)\int d\omega\rho_{b^\dagger,b}(\omega), \tag{36}$$

$$\left|\left\langle[a^\dagger,b]\right\rangle\right|^2 \le \left\langle\{b^\dagger,b\}\right\rangle\left\langle\left(\tanh(\beta\omega/2)\right)^2\right\rangle_{a^\dagger,a}. \tag{37}$$

One can now bound the second term in the r.h.s. of (37):

$$\int_{-\infty}^{+\infty} d\omega\left(\tanh(\beta\omega/2)\right)^2\rho_{a^\dagger,a}(\omega) = \int_0^{+\infty} d\omega\left(\tanh(\beta\omega/2)\right)^2\left(\rho_{a^\dagger,a}(\omega) + \rho_{a,a^\dagger}(\omega)\right), \tag{38}$$

by using the concavity of $\tanh(x)$ in $[0,+\infty)$ and Jensen's inequality for a concave function φ:

$$\varphi\left(\frac{\sum_i a_i x_i}{\sum_i a_i}\right) \ge \frac{\sum_i a_i\varphi(x_i)}{\sum_i a_i}, \tag{39}$$

together with the notations:

$$\sum_i a_i \equiv \left\langle\left|\tanh(\beta\omega/2)\right|\right\rangle_{a^\dagger,a} = \int_0^{+\infty} d\omega\left|\tanh(\beta\omega/2)\right|\rho_{a^\dagger,a}(\omega), \tag{40}$$

$$\varphi(x_i) \equiv \tanh(\beta\omega/2). \tag{41}$$

The resulting bound is given by:

$$\frac{1}{\Phi}\int_0^{+\infty} d\omega\left|\tanh(\beta\omega/2)\right|\tanh(\beta\omega/2)\rho_{a^\dagger,a}(\omega) \le \tanh\left(\frac{1}{\Phi}\int_0^{+\infty} d\omega\left|\tanh(\beta\omega/2)\right|\frac{\beta\omega}{2}\rho_{a^\dagger,a}(\omega)\right), \tag{42}$$

$$\left\langle \left(\tanh(\beta\omega/2) \right)^2 \right\rangle_{a^\dagger,a} \le \Phi \tanh\left(\beta \frac{\langle \omega \tanh(\beta\omega/2) \rangle_{a^\dagger,a}}{2\Phi} \right), \tag{43}$$

where:

$$\Phi = \left\langle \left| \tanh(\beta\omega/2) \right| \right\rangle_{a^\dagger,a}. \tag{44}$$

The Cauchy-Schwarz inequality gives:

$$0 \le \Phi = \int_{-\infty}^{+\infty} d\omega \left| \tanh(\beta\omega/2) \right| \rho_{a^\dagger,a}(\omega) \le \sqrt{\langle \omega \tanh(\beta\omega/2) \rangle_{a^\dagger,a} \langle \omega^{-1} \tanh(\beta\omega/2) \rangle_{a^\dagger,a}}. \tag{45}$$

Given the fact that $\frac{\tanh(x)}{x}$ is monotonically decreasing in the interval $[0, +\infty)$, one can maximize the r.h.s of (43) with the bound given by (45):

$$\left\langle \left(\tanh(\beta\omega/2) \right)^2 \right\rangle_{a^\dagger,a} \le \sqrt{\langle [[a^\dagger, \mathcal{H}], a] \rangle_{a^\dagger,a} \beta(a^\dagger, a)} \tanh\left(\frac{\beta}{2} \sqrt{\frac{\langle [[a^\dagger, \mathcal{H}], a] \rangle_{a^\dagger,a}}{\beta(a^\dagger, a)}} \right). \tag{46}$$

Inserting (46) into previously obtained (37):

$$\left| \left\langle [a^\dagger, b] \right\rangle \right|^2 \le \left\langle \{b^\dagger, b\} \right\rangle \sqrt{\langle [[a^\dagger, \mathcal{H}], a] \rangle_{a^\dagger,a} \beta(a^\dagger, a)} \tanh\left(\frac{\beta}{2} \sqrt{\frac{\langle [[a^\dagger, \mathcal{H}], a] \rangle_{a^\dagger,a}}{\beta(a^\dagger, a)}} \right), \tag{47}$$

and finally:

$$\left\langle \{b^\dagger, b\} \right\rangle \ge \frac{\left| \left\langle [a^\dagger, b] \right\rangle \right|^2}{\sqrt{\langle [[a^\dagger, \mathcal{H}], a] \rangle_{a^\dagger,a} \beta(a^\dagger, a)}} \coth\left(\frac{\beta}{2} \sqrt{\frac{\langle [[a^\dagger, \mathcal{H}], a] \rangle_{a^\dagger,a}}{\beta(a^\dagger, a)}} \right). \tag{48}$$

One can 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^* for the dual lattice. One denotes the structure factor $g^\alpha_{\boldsymbol{q}} = \left\langle S^\alpha_{\boldsymbol{q}} S^\alpha_{-\boldsymbol{q}} \right\rangle$ using the Fourier transform:

$$S^\alpha_{\boldsymbol{q}} = \frac{1}{\sqrt{|\Lambda|}} \sum_{\boldsymbol{r} \in \Lambda} S^\alpha_{\boldsymbol{r}} \exp(-i \boldsymbol{q} \cdot \boldsymbol{r}). \tag{49}$$

Note: the original paper [7] has $\boldsymbol{r} \in \Lambda^*$, which seems confusing as sites coordinates should be elements of the real lattice, not the dual one.
One can choose $\boldsymbol{Q} = (\pi, ..., \pi)$, $a = S^y_{\boldsymbol{q}}$ and $b = S^z_{\boldsymbol{q}+\boldsymbol{Q}}$, then:

$$[a^\dagger, b] = \frac{1}{\Lambda} \left[\sum_{\boldsymbol{r} \in \Lambda} S^y_{\boldsymbol{r}} \exp(i \boldsymbol{q} \cdot \boldsymbol{r}), \sum_{\boldsymbol{r}' \in \Lambda} S^z_{\boldsymbol{r}'} \exp(-i (\boldsymbol{q} + \boldsymbol{Q}) \cdot \boldsymbol{r}') \right] = i \left(\sqrt{|\Lambda|} \right)^{-1} S^x_{\boldsymbol{Q}}. \tag{50}$$

If one assumes that long ranged order (LRO) exists along the x-axis, then $\left\langle S^x_{\boldsymbol{Q}} \right\rangle = \sqrt{|\Lambda|} \mathcal{M}_0$, where $\mathcal{M}_0$ is the staggered magnetization, thus $\left| \left\langle [a^\dagger, b] \right\rangle \right| = \mathcal{M}_0$. The double commutator is readily evaluated using the translation and rotation invariance as:

$$\left\langle [[S^y_{-\boldsymbol{q}}, \mathcal{H}], S^y_{\boldsymbol{q}}] \right\rangle = 2 c_y E^-_{\boldsymbol{q}}, \tag{51}$$

where $c_y = -\sum_{\beta \neq y} \left\langle S^\beta_0 S^\beta_\delta \right\rangle$ with δ - the nearest neighbor and $E^\pm_{\boldsymbol{q}} = \sum_{i=0}^{d} (1 \pm \cos(q_i))$.
Thus, the correlation function can be bounded from below under the assumption of LRO. One can define the function:

$$G(\boldsymbol{q}) \equiv \sqrt{\frac{E^-_{\boldsymbol{q}}}{4 E^+_{\boldsymbol{q}}}} \coth\left(\beta \sqrt{c_y E^+_{\boldsymbol{q}} E^-_{\boldsymbol{q}}} \right). \tag{52}$$

The lower bound for the correlation function $g^z_{\boldsymbol{q}}$ can now be found by substituting $\boldsymbol{Q}$, a and b in (48), shifting $\boldsymbol{q} = \boldsymbol{Q} + \boldsymbol{q}'$ and using the fact that $E^{\pm}_{\boldsymbol{q}+\boldsymbol{Q}} = E^{\mp}_{\boldsymbol{q}}$:

$$\left\langle \{S^z_{-\boldsymbol{q}-\boldsymbol{Q}}, S^z_{\boldsymbol{q}+\boldsymbol{Q}}\} \right\rangle \geq \frac{\left| \left\langle i\left(\sqrt{|\Lambda|}\right)^{-1} S^x_{\boldsymbol{Q}} \right\rangle \right|^2}{\sqrt{\left\langle [[S^y_{-\boldsymbol{q}}, \mathcal{H}], S^y_{\boldsymbol{q}}] \right\rangle \beta (S^y_{-\boldsymbol{q}}, S^y_{\boldsymbol{q}})}} \coth\left(\frac{\beta}{2} \sqrt{\frac{\left\langle [[S^y_{-\boldsymbol{q}}, \mathcal{H}], S^y_{\boldsymbol{q}}] \right\rangle}{\beta (S^y_{-\boldsymbol{q}}, S^y_{\boldsymbol{q}})}} \right), \tag{53}$$

$$\left\langle \{S^z_{-\boldsymbol{q}-\boldsymbol{Q}}, S^z_{\boldsymbol{q}+\boldsymbol{Q}}\} \right\rangle \geq \frac{m_0^2}{\sqrt{2c_y E^-_{\boldsymbol{q}} \beta \frac{1}{2\beta E^+_{\boldsymbol{q}}}}} \coth\left(\frac{\beta}{2} \sqrt{\frac{2c_y E^-_{\boldsymbol{q}}}{\beta \frac{1}{2\beta E^+_{\boldsymbol{q}}}}} \right), \tag{54}$$

$$\left\langle \{S^z_{-\boldsymbol{q}-\boldsymbol{Q}}, S^z_{\boldsymbol{q}+\boldsymbol{Q}}\} \right\rangle \geq m_0^2 \sqrt{\frac{E^+_{\boldsymbol{q}}}{c_y E^-_{\boldsymbol{q}}}} \coth\left(\beta \sqrt{c_y E^-_{\boldsymbol{q}} E^+_{\boldsymbol{q}}} \right), \tag{55}$$

$$\left\langle \{S^z_{-\boldsymbol{q}'}, S^z_{\boldsymbol{q}'}\} \right\rangle \geq m_0^2 \sqrt{\frac{E^-_{\boldsymbol{q}'}}{c_y E^+_{\boldsymbol{q}'}}} \coth\left(\beta \sqrt{c_y E^+_{\boldsymbol{q}'} E^-_{\boldsymbol{q}'}} \right), \tag{56}$$

$$g^z_{\boldsymbol{q}} \geq m_0^2 G(\boldsymbol{q}) / \sqrt{c_y}. \tag{57}$$

Inequality (57) is used in Section 4 and is extended for the case of anisotropic model. One may notice that in transition from (53) to (54) and upper bound for the Duhamel two-point function is used. This bound is proved in Appendix B.

4 An upper bound for spectrum

The results presented in this section were originally derived by Tsuomu Momoi in [1]. This section proves an upper bound for the spin-wave spectrum in quantum Heisenberg model for antiferromagnets.

In quantum Heisenberg model for an XXZ antiferromagnet on the d-dimensional $L \times ... \times L$ hypercubic lattice $\Lambda \subset \mathbb{Z}^d$ $(d \geq 2)$ the Hamiltonian is defined by:

$$\mathcal{H}_\Lambda = J \sum_{\langle i,j \rangle \in \Lambda} \left(S^x_i S^x_j + S^y_i S^y_j + \Delta S^z_i S^z_j \right), \tag{58}$$

where $0 \leq \Delta \leq 1$ and the summation runs over the nearest neighbor sites. The system size of Λ is $N = L^d$. One can consider the system under the small staggered magnetic field. The Hamiltonian of such a system:

$$\mathcal{H}_\Lambda(B) = \mathcal{H}_\Lambda - B \mathcal{M}_\Lambda, \tag{59}$$

where:

$$\mathcal{M}_\Lambda = \sum_{i \in A} S^x_i - \sum_{i \in B} S^x_i. \tag{60}$$

Note: A and B - respectively, sets of spins directing up and down (sublattices).

One can now consider $|\Phi_{GS,B}\rangle$ to be a ground state of the Hamiltonian (59). The staggered magnetization in a thermodynamic limit under infinitesimally small field B is given by:

$$m_s = \lim_{B \searrow 0} \lim_{\Lambda \nearrow \infty} \frac{1}{N} \langle \Phi_{GS,B} | \mathcal{M}_\Lambda | \Phi_{GS,B} \rangle. \tag{61}$$

As the excited state, the following one is considered (this excitation is called magnon):

$$|\psi_B(\boldsymbol{k})\rangle = \frac{S^z_{\boldsymbol{k}} |\Phi_{GS,B}\rangle}{\left\| S^z_{\boldsymbol{k}} |\Phi_{GS,B}\rangle \right\|}, \tag{62}$$

where:

$$S^z_{\boldsymbol{k}} = \frac{1}{\sqrt{N}} \sum_i S^z_i \exp(-i\boldsymbol{k} \cdot \boldsymbol{r}_i),\ \boldsymbol{k} = (k_1, ..., k_d), \tag{63}$$

$$\left\| S^z_{\boldsymbol{k}} |\Phi_{GS,B}\rangle \right\| = \sqrt{\langle \Phi_{GS,B}| S^z_{-\boldsymbol{k}} S^z_{\boldsymbol{k}} |\Phi_{GS,B}\rangle}. \tag{64}$$

When the spins lie in the XY-plane, the operation of S^z_i flips the spin in the site i. The excitation energy of $|\psi_B(\boldsymbol{k})\rangle$ is given by:

$$\varepsilon(\boldsymbol{k}) = \lim_{B\searrow 0} \lim_{\Lambda \nearrow \infty} \Big[\langle \psi_B(\boldsymbol{k})| \mathcal{H}_\Lambda(B) |\psi_B(\boldsymbol{k})\rangle - \langle \Phi_{GS,B}| \mathcal{H}_\Lambda(B) |\Phi_{GS,B}\rangle \Big]. \tag{65}$$

Note: shorter version of derivations, explicitly implying $\beta \to \infty$ is available in Appendix C.
One can choose the momentum $\boldsymbol{k}$ as $\boldsymbol{k} \neq \boldsymbol{0}, \boldsymbol{k} = (\pi, ..., \pi)$ and $k_m = \frac{2\pi}{L} l_m$, $l_m \in [0, L-1]$, thus making the states $|\Phi_{GS,B}\rangle$ and $|\psi_B(\boldsymbol{k})\rangle$ orthogonal as eigenstates of the transverse momentum operator with different eigenvalues. This trial state is called in the literature the Bijl-Feynman single mode approximation.

Theorem If the ground state has a Neél order, i.e., if $m_s > 0$, the energy spectrum $\varepsilon(\boldsymbol{k})$ is bounded as:

$$\varepsilon(\boldsymbol{k}) \leq \frac{2dJ(\rho_x + \rho_y)}{m_s^2} \sqrt{\rho_x(1 + \Delta\gamma_{\boldsymbol{k}}) + \rho_z(\Delta + \gamma_{\boldsymbol{k}})} \sqrt{1 - \gamma_{\boldsymbol{k}}}, \tag{66}$$

where:

$$\rho_\alpha = -\lim_{B\searrow 0} \lim_{\Lambda \nearrow \infty} \frac{1}{Nd} \langle \Phi_{GS,B}| \sum_{\langle i,j\rangle \in \Lambda} S^\alpha_i S^\alpha_j |\Phi_{GS,B}\rangle,\ \alpha = \{x, y, z\}, \tag{67}$$

and:

$$\gamma_{\boldsymbol{k}} = \frac{1}{d} \sum_{i=1}^{d} \cos(k_i). \tag{68}$$

□ The excitation energy of $|\psi_B(\boldsymbol{k})\rangle$ is given by:

$$\begin{aligned}
&\langle \psi_B(\boldsymbol{k})| \mathcal{H}_\Lambda(B) |\psi_B(\boldsymbol{k})\rangle - \langle \Phi_{GS,B}| \mathcal{H}_\Lambda(B) |\Phi_{GS,B}\rangle = \\
&= \frac{\langle \Phi_{GS,B}| S^z_{-\boldsymbol{k}} \mathcal{H}_\Lambda(B) S^z_{\boldsymbol{k}} |\Phi_{GS,B}\rangle}{\left\| S^z_{\boldsymbol{k}} |\Phi_{GS,B}\rangle \right\|^2} - \langle \Phi_{GS,B}| \mathcal{H}_\Lambda(B) |\Phi_{GS,B}\rangle = \\
&= \frac{\langle \Phi_{GS,B}| S^z_{-\boldsymbol{k}} \mathcal{H}_\Lambda(B) S^z_{\boldsymbol{k}} |\Phi_{GS,B}\rangle - \langle \Phi_{GS,B}| \mathcal{H}_\Lambda(B) |\Phi_{GS,B}\rangle \langle \Phi_{GS,B}| S^z_{-\boldsymbol{k}} S^z_{\boldsymbol{k}} |\Phi_{GS,B}\rangle}{\langle \Phi_{GS,B}| S^z_{-\boldsymbol{k}} S^z_{\boldsymbol{k}} |\Phi_{GS,B}\rangle}.
\end{aligned} \tag{69}$$

The states $|\pm\rangle = S^z_{\pm\boldsymbol{k}} |\Phi_{GS,B}\rangle$ has the same energy $\langle \pm| \mathcal{H}_\Lambda(B) |\pm\rangle$ as Hamiltonian remains constant during the coordinate inversion, but the states transform to one another. Thus said:

$$\begin{aligned}
&[[S^z_{-\boldsymbol{k}}, \mathcal{H}_\Lambda(B)], S^z_{\boldsymbol{k}}] = [S^z_{-\boldsymbol{k}} \mathcal{H}_\Lambda(B) - \mathcal{H}_\Lambda(B) S^z_{-\boldsymbol{k}}, S^z_{\boldsymbol{k}}] = \\
&= S^z_{-\boldsymbol{k}} \mathcal{H}_\Lambda(B) S^z_{\boldsymbol{k}} - \mathcal{H}_\Lambda(B) S^z_{-\boldsymbol{k}} S^z_{\boldsymbol{k}} - S^z_{\boldsymbol{k}} S^z_{-\boldsymbol{k}} \mathcal{H}_\Lambda(B) + S^z_{\boldsymbol{k}} \mathcal{H}_\Lambda(B) S^z_{-\boldsymbol{k}},
\end{aligned} \tag{70}$$

$$\begin{aligned}
&\langle \Phi_{GS,B}| [[S^z_{-\boldsymbol{k}}, \mathcal{H}_\Lambda(B)], S^z_{\boldsymbol{k}}] |\Phi_{GS,B}\rangle = \\
&= 2\Big(\langle \Phi_{GS,B}| S^z_{-\boldsymbol{k}} \mathcal{H}_\Lambda(B) S^z_{\boldsymbol{k}} |\Phi_{GS,B}\rangle - \langle \Phi_{GS,B}| \langle \Phi_{GS,B}| \mathcal{H}_\Lambda(B) |\Phi_{GS,B}\rangle S^z_{-\boldsymbol{k}} S^z_{\boldsymbol{k}} |\Phi_{GS,B}\rangle \Big).
\end{aligned} \tag{71}$$

The excitation energy now has the following representation:

$$\langle \psi_B(\boldsymbol{k})| \mathcal{H}_\Lambda(B) |\psi_B(\boldsymbol{k})\rangle - \langle \Phi_{GS,B}| \mathcal{H}_\Lambda(B) |\Phi_{GS,B}\rangle = \frac{\langle \Phi_{GS,B}| [[S^z_{-\boldsymbol{k}}, \mathcal{H}_\Lambda(B)], S^z_{\boldsymbol{k}}] |\Phi_{GS,B}\rangle}{\langle \Phi_{GS,B}| S^z_{-\boldsymbol{k}} S^z_{\boldsymbol{k}} |\Phi_{GS,B}\rangle}. \tag{72}$$

One can explicitly insert (58) with $\Delta = 1$ (isotropic model) into (72) and evaluate the commutators step-by step:

$$[[S^z_\mu, S^x_i], S^z_\nu] = i\delta_{i\mu}[S^y_i, S^z_\nu] = -\delta_{i\mu}\delta_{i\nu}S^x_i, \tag{73}$$

$$\langle\Phi_{GS,B}|\,\frac{1}{N}\left[\left[\sum_\mu S^z_\mu \exp(-i\boldsymbol{k}\cdot\boldsymbol{r}_\mu), -B\Big(\sum_{i\in A} S^x_i - \sum_{i\in B} S^x_i\Big)\right], \sum_\nu S^z_\nu \exp(i\boldsymbol{k}\cdot\boldsymbol{r}_\nu)\right]|\Phi_{GS,B}\rangle = \\ = \frac{B}{N}\langle\Phi_{GS,B}|\,\mathcal{M}_\Lambda\,|\Phi_{GS,B}\rangle, \tag{74}$$

$$[[S^z_\mu, S^z_i S^z_j], S^z_\nu] = 0, \tag{75}$$

$$\langle\Phi_{GS,B}|\,\frac{1}{N}\left[\left[\sum_\mu S^z_\mu \exp(-i\boldsymbol{k}\cdot\boldsymbol{r}_\mu), J\sum_{\langle i,j\rangle\in\Lambda}\Delta S^z_i S^z_j\right], \sum_\nu S^z_\nu \exp(i\boldsymbol{k}\cdot\boldsymbol{r}_\nu)\right]|\Phi_{GS,B}\rangle = 0, \tag{76}$$

$$[S^z_\mu, S^x_i S^x_j] = S^z_\mu S^x_i S^x_j - S^x_i S^x_j S^z_\mu = (S^x_i S^z_\mu + i\delta_{i\mu}S^y_i)S^x_j - S^x_i(S^z_\mu S^x_j - i\delta_{j\mu}S^y_j) = \\ = i\delta_{i\mu}S^y_i S^x_j + i\delta_{j\mu}S^x_i S^y_j, \tag{77}$$

$$[S^y_i S^x_j, S^z_\nu] = S^y_i S^x_j S^z_\nu - S^z_\nu S^y_i S^x_j = S^y_i(S^z_\nu S^x_j - i\delta_{j\nu}S^y_j) - (S^y_i S^z_\nu - i\delta_{i\nu}S^x_i)S^x_j = \\ = -i\delta_{j\nu}S^y_i S^y_j + i\delta_{i\nu}S^x_i S^x_j, \tag{78}$$

$$[S^x_i S^y_j, S^z_\nu] = S^x_i S^y_j S^z_\nu - S^z_\nu S^x_i S^y_j = S^x_i(S^z_\nu S^y_j + i\delta_{j\nu}S^x_j) - (S^x_i S^z_\nu + i\delta_{i\nu}S^y_i)S^y_j = \\ = i\delta_{j\nu}S^x_i S^x_j - i\delta_{i\nu}S^y_i S^y_j, \tag{79}$$

$$[[S^z_\mu, S^x_i S^x_j], S^z_\nu] = i\delta_{i\mu}(-i\delta_{j\nu}S^y_i S^y_j + i\delta_{i\nu}S^x_i S^x_j) + i\delta_{j\mu}(i\delta_{j\nu}S^x_i S^x_j - i\delta_{i\nu}S^y_i S^y_j) = \\ = S^x_i S^x_j(-\delta_{i\mu}\delta_{i\nu} - \delta_{j\mu}\delta_{j\nu}) + S^y_i S^y_j(\delta_{i\mu}\delta_{j\nu} + \delta_{j\mu}\delta_{i\nu}), \tag{80}$$

$$\exp(-i\boldsymbol{k}\cdot\boldsymbol{r}_\mu)[[S^z_\mu, S^x_i S^x_j], S^z_\nu]\exp(i\boldsymbol{k}\cdot\boldsymbol{r}_\nu) = -2S^x_i S^x_j + 2S^y_i S^y_j\cos(\boldsymbol{k}\cdot(\boldsymbol{r}_\nu - \boldsymbol{r}_\mu)), \tag{81}$$

$$\langle\Phi_{GS,B}|\,\frac{1}{N}\left[\left[\sum_\mu S^z_\mu \exp(-i\boldsymbol{k}\cdot\boldsymbol{r}_\mu), J\sum_{\langle i,j\rangle\in\Lambda} S^x_i S^x_j\right], \sum_\nu S^z_\nu \exp(i\boldsymbol{k}\cdot\boldsymbol{r}_\nu)\right]|\Phi_{GS,B}\rangle = \\ = -2\frac{J}{N}\langle\Phi_{GS,B}|\sum_{\langle i,j\rangle\in\Lambda} S^x_i S^x_j\,|\Phi_{GS,B}\rangle + 2\frac{J}{N}\gamma_{\boldsymbol{k}}\langle\Phi_{GS,B}|\sum_{\langle i,j\rangle\in\Lambda} S^y_i S^y_j\,|\Phi_{GS,B}\rangle. \tag{82}$$

After calculating the commutators, (72) transforms to:

$$\langle\psi_B(\boldsymbol{k})|\,\mathcal{H}_\Lambda(B)\,|\psi_B(\boldsymbol{k})\rangle - \langle\Phi_{GS,B}|\,\mathcal{H}_\Lambda(B)\,|\Phi_{GS,B}\rangle = \\ = \frac{2J(1-\gamma_{\boldsymbol{k}})\langle\Phi_{GS,B}| - \sum_{\langle i,j\rangle\in\Lambda}\left(S^x_i S^x_j + S^y_i S^y_j\right)|\Phi_{GS,B}\rangle + B\langle\Phi_{GS,B}|\,\mathcal{M}_\Lambda\,|\Phi_{GS,B}\rangle}{2N\langle\Phi_{GS,B}|\,S^z_{-\boldsymbol{k}}S^z_{\boldsymbol{k}}\,|\Phi_{GS,B}\rangle}. \tag{83}$$

For the excitation energy in the thermodynamic limit:

$$\lim_{B\searrow 0}\lim_{\Lambda\nearrow\infty}\varepsilon(\boldsymbol{k}) = \frac{2Jd(\rho_x + \rho_y)(1-\gamma_{\boldsymbol{k}})}{2S^z_\perp(\boldsymbol{k})}, \tag{84}$$

where $S^z_\perp(\boldsymbol{k})$ denotes the structure factor of the Neél order ground state:

$$S^z_\perp(\boldsymbol{k}) = \lim_{B\searrow 0}\lim_{\Lambda\nearrow\infty} \langle\Phi_{GS,B}|\, S^z_{-\boldsymbol{k}} S^z_{\boldsymbol{k}}\, |\Phi_{GS,B}\rangle\,, \tag{85}$$

which describes the correlations of spins transverse to the magnetic field.
Note: here the excitation energy of spin-waves was calculated. By definition (1) it is greater or equal than the ground state energy, thus the upper bound for $\varepsilon(\boldsymbol{k})$ is also valid for $\varepsilon_0(\boldsymbol{k})$.
To bound the structure factor for the Heisenberg model from below, one can use the Shastry inequality (57):

$$2S^z_\perp(\boldsymbol{k}) \geq \frac{m_s^2\sqrt{1-\gamma_{\boldsymbol{k}}}}{\sqrt{\rho_x+\rho_z}\sqrt{1+\gamma_{\boldsymbol{k}}}}. \tag{86}$$

Note: notations here are slightly different from the ones used in Section 3.
This bound can be extended to the anisotropic model ($\Delta \neq 0$) by recalculating the commutation relation (51):

$$[[S^z_{\boldsymbol{q}}, \mathcal{H}_\Lambda(B)], S^z_{-\boldsymbol{q}}] = 2(\rho_x(1+\Delta\gamma_{\boldsymbol{q}}) + \rho_z(\Delta+\gamma_{\boldsymbol{q}})), \tag{87}$$

$$2S^z_\perp(\boldsymbol{k}) \geq \frac{m_s^2\sqrt{1-\gamma_{\boldsymbol{k}}}}{\sqrt{\rho_x(1+\Delta\gamma_{\boldsymbol{k}})+\rho_z(\Delta+\gamma_{\boldsymbol{k}})}}. \tag{88}$$

Using equations (88) and (84), one can finally obtain (66).

■

The expectation value $\varepsilon(\boldsymbol{k})$ can be bounded from below as well. The transverse structure factor $S^z_\perp(\boldsymbol{k})$ is bounded from above in the form given by:

$$2S^z_\perp(\boldsymbol{k}) \leq \left[\frac{(\rho_x+\rho_y)(1-\gamma_{\boldsymbol{k}})}{\Delta(1+\gamma_{\boldsymbol{k}})}\right]^{1/2}, \tag{89}$$

which is the corollary from an upper bound (151). For discussion on how the structure factor is connected with the Duhamel two-point function as well as the proof of an upper bound for DTF, see Appendix B. Using (89) one can obtain:

$$\varepsilon(\boldsymbol{k}) \geq 2dJ\sqrt{\Delta(\rho_x+\rho_y)(1-\gamma^2_{\boldsymbol{k}})}. \tag{90}$$

Appendices

A Bogoliubov inequality

In case if one defines the scalar product through:

$$(A, C) = \int \frac{d\omega}{\omega} A_{A^\dagger,C}(\omega), \tag{91}$$

then from the Cauchy-Schwarz inequality:

$$\int \frac{d\omega}{\omega} A_{A^\dagger,A}(\omega) \cdot \int \frac{d\omega}{\omega} A_{C^\dagger,C}(\omega) \geq \left| \int \frac{d\omega}{\omega} A_{A^\dagger,C}(\omega)\right|^2. \tag{92}$$

If one also uses the fact that $\coth(x) \geq \frac{1}{x}$ for $x > 0$:

$$A_{A^\dagger,A}(\omega)\coth(\beta\omega/2) \geq \left(\frac{\beta\omega}{2}\right)^{-1} A_{A^\dagger,A}(\omega), \tag{93}$$

then the following inequality may be obtained:

$$\frac{\beta}{2}\left\langle\{A^{\dagger},A\}\right\rangle \geq \int \frac{d\omega}{\omega}A_{A^{\dagger},A}(\omega). \tag{94}$$

Using the energy weighted sum rule:

$$\left\langle[A^{\dagger},[\mathcal{H},B]]\right\rangle = \left\langle[A^{\dagger},\mathcal{H}B-B\mathcal{H}]\right\rangle = \left\langle A^{\dagger}\mathcal{H}B - A^{\dagger}B\mathcal{H} - \mathcal{H}BA^{\dagger} + B\mathcal{H}A^{\dagger}\right\rangle, \tag{95}$$

$$\left\langle A^{\dagger}\mathcal{H}B\right\rangle = Z^{-1}\sum_{m,n}\exp(-\beta E_m)\langle m|A^{\dagger}|n\rangle\langle n|\mathcal{H}B|m\rangle =$$
$$= Z^{-1}\sum_{m,n}E_n\exp(-\beta E_m)\langle m|A^{\dagger}|n\rangle\langle n|B|m\rangle, \tag{96}$$

$$\left\langle -A^{\dagger}B\mathcal{H}\right\rangle = -Z^{-1}\sum_{m,n}\exp(-\beta E_m)\langle m|A^{\dagger}|n\rangle\langle n|B\mathcal{H}|m\rangle =$$
$$= Z^{-1}\sum_{m,n}(-E_m)\exp(-\beta E_m)\langle m|A^{\dagger}|n\rangle\langle n|B|m\rangle, \tag{97}$$

$$\left\langle -\mathcal{H}BA^{\dagger}\right\rangle = -Z^{-1}\sum_{m,n}\exp(-\beta E_m)\langle m|\mathcal{H}B|n\rangle\langle n|A^{\dagger}|m\rangle =$$
$$= Z^{-1}\sum_{m,n}(-E_n)\exp(-\beta E_n)\langle m|A^{\dagger}|n\rangle\langle n|B|m\rangle, \tag{98}$$

$$\left\langle B\mathcal{H}A^{\dagger}\right\rangle = Z^{-1}\sum_{m,n}\exp(-\beta E_m)\langle m|B\mathcal{H}|n\rangle\langle n|A^{\dagger}|m\rangle =$$
$$= Z^{-1}\sum_{m,n}E_m\exp(-\beta E_n)\langle m|A^{\dagger}|n\rangle\langle n|B|m\rangle, \tag{99}$$

$$\left\langle[A^{\dagger},[\mathcal{H},B]]\right\rangle = Z^{-1}\sum_{m,n}(\exp(-\beta E_m)(E_n-E_m)+\exp(-\beta E_n)(E_m-E_n))\cdot$$
$$\cdot\langle m|A^{\dagger}|n\rangle\langle n|B|m\rangle = \int d\omega\omega A_{A^{\dagger},B}(\omega). \tag{100}$$

One can now calculate (using $C=[\mathcal{H},B]$):

$$\left\langle[B^{\dagger},[\mathcal{H},B]]\right\rangle = \int d\omega\omega A_{B^{\dagger},B}(\omega), \tag{101}$$

$$A_{C^{\dagger},C}(\omega) = Z^{-1}\sum_{m,n}(\exp(-\beta E_m)-\exp(-\beta E_n))\langle m|C^{\dagger}|n\rangle\langle n|C|m\rangle\delta(\omega-E_n+E_m) =$$
$$= Z^{-1}\sum_{m,n}(\exp(-\beta E_m)-\exp(-\beta E_n))\langle m|B^{\dagger}E_n-E_mB^{\dagger}|n\rangle\langle n|E_nB-E_mB|m\rangle\delta(\omega-E_n+E_m) =$$
$$= \omega^2 A_{B^{\dagger},B}(\omega), \tag{102}$$

$$\int\frac{d\omega}{\omega}A_{C^{\dagger},C}(\omega) = \left\langle[B^{\dagger},[\mathcal{H},B]]\right\rangle, \tag{103}$$

$$\int\frac{d\omega}{\omega}A_{A^{\dagger},C}(\omega) = \int d\omega A_{A^{\dagger},B}(\omega) = \left\langle[A^{\dagger},B]\right\rangle. \tag{104}$$

Finally, using (92) one obtains:

$$\frac{\beta}{2}\left\langle\{A^{\dagger},A\}\right\rangle\left\langle[B^{\dagger},[\mathcal{H},B]]\right\rangle \geq \left|\left\langle[A^{\dagger},B]\right\rangle\right|^2, \tag{105}$$

or in the form used in literature (Bogoliubov inequality):

$$\left\langle\{A^{\dagger},A\}\right\rangle\left\langle[B^{\dagger},[\mathcal{H},B]]\right\rangle \geq \frac{2}{\beta}\left|\left\langle[A^{\dagger},B]\right\rangle\right|^2. \tag{106}$$

B Upper bound for Duhamel two-point function and it's relation to structure factor

The results presented in this section were originally obtained by Freeman J. Dyson, Elliot H. Lieb and Barry Simon in [5]. This section gives a commentary on the connection between the structure factor and Duhamel two-point function as well as proves the upper bound for the latter.

B.1 Classic Heisenberg model and transition to quantum case

The existence of phase transitions in a variety of classical spin systems, including certain classic Heisenberg models, is proved in [6]. However, while latter deal directly with infinite volume expectations, it is useful to rephrase the result in terms of the finite volume statements.
Let Λ be a parallelepiped in the simple ν-dimensional cubic lattice $\mathbb{Z}^\nu$ of the form:

$$\Lambda = \{\boldsymbol{\alpha} : 0 \leq \alpha_1 \leq L_1 - 1, ..., 0 \leq \alpha_\nu \leq L_\nu - 1\}. \tag{107}$$

In the classical model one has a "spin" $\boldsymbol{S}_{\boldsymbol{\alpha}}$ for each $\boldsymbol{\alpha} \in \Lambda$, where $\boldsymbol{S}$ has three components $S^{(j)}$. The classical spins are normalized by:

$$\boldsymbol{S}_{\boldsymbol{\alpha}} \cdot \boldsymbol{S}_{\boldsymbol{\alpha}} \equiv \sum_j \left(S^{(j)}_{\boldsymbol{\alpha}}\right)^2 = 1 \tag{108}$$

and distributed according to the isotropic spherical distribution $d\lambda(\boldsymbol{S})$. The basic Hamiltonian is:

$$\mathcal{H} = -\sum_{\boldsymbol{\alpha},i} \boldsymbol{S}_{\boldsymbol{\alpha}} \cdot \boldsymbol{S}_{\boldsymbol{\alpha}+\boldsymbol{\delta}_i}, \tag{109}$$

where $\boldsymbol{\delta}_i$ is the unit vector with i-th component equal to one (nearest neighbor). $\mathcal{H}$ has periodic boundary conditions. Using the normalization condition (108), one can rewrite the Hamiltonian in form:

$$\mathcal{H} = -\sum_{\boldsymbol{\alpha},i} \boldsymbol{S}_{\boldsymbol{\alpha}} \cdot \boldsymbol{S}_{\boldsymbol{\alpha}+\boldsymbol{\delta}_i} = \frac{1}{2}\big(\nu|\Lambda| - \sum_i \sum_{\boldsymbol{\alpha}} \boldsymbol{S}_{\boldsymbol{\alpha}} \cdot \boldsymbol{S}_{\boldsymbol{\alpha}}\big) + \frac{1}{2}\big(\nu|\Lambda| - \sum_i \sum_{\boldsymbol{\alpha}} \boldsymbol{S}_{\boldsymbol{\alpha}+\boldsymbol{\delta}_i} \cdot \boldsymbol{S}_{\boldsymbol{\alpha}+\boldsymbol{\delta}_i}\big) - \\ - \sum_{\boldsymbol{\alpha},i} \boldsymbol{S}_{\boldsymbol{\alpha}} \cdot \boldsymbol{S}_{\boldsymbol{\alpha}+\boldsymbol{\delta}_i} = \text{const} + \frac{1}{2}\sum_{\boldsymbol{\alpha},i}\big(\boldsymbol{S}_{\boldsymbol{\alpha}} - \boldsymbol{S}_{\boldsymbol{\alpha}+\boldsymbol{\delta}_i}\big)^2. \tag{110}$$

The partition function Z is defined by:

$$Z = \int \exp\big(-\beta\mathcal{H}(\boldsymbol{S})\big) \prod_{\boldsymbol{\alpha}\in\Lambda} d\lambda(\boldsymbol{S}_{\boldsymbol{\alpha}}) \tag{111}$$

and thermal excitations by:

$$\langle f(\boldsymbol{S})\rangle_{\Lambda,\beta} = Z^{-1} \int f(\boldsymbol{S}) \exp\big(-\beta\mathcal{H}(\boldsymbol{S})\big) \prod_{\boldsymbol{\alpha}\in\Lambda} d\lambda(\boldsymbol{S}_{\boldsymbol{\alpha}}). \tag{112}$$

The basic result of [6] claims that for sufficiently large β:

$$\lim_{\Lambda\nearrow\infty} \left\langle \sum_{j=1}^{3} \Big(|\Lambda|^{-1} \sum_{\boldsymbol{\alpha}\in\Lambda} S^{(j)}_{\boldsymbol{\alpha}}\Big)^2 \right\rangle_{\Lambda,\beta} \neq 0. \tag{113}$$

One can introduce the Fourier variables $\hat{\boldsymbol{S}}_{\boldsymbol{p}}$ by:

$$\hat{\boldsymbol{S}}_{\boldsymbol{p}} = |\Lambda|^{-1/2} \sum_{\boldsymbol{\alpha}\in\Lambda} \exp(-i\boldsymbol{p}\cdot\boldsymbol{\alpha})\boldsymbol{S}_{\boldsymbol{\alpha}}, \tag{114}$$

where $\boldsymbol{p}$ runs through the dual lattice Λ^*, i.e. $p_j = \frac{2\pi}{L_j} l_j$. The inverse transform is defined by:

$$\boldsymbol{S}_{\boldsymbol{\alpha}} = |\Lambda|^{-1/2} \sum_{\boldsymbol{p}} \exp(i\boldsymbol{p}\cdot\boldsymbol{\alpha}) \hat{\boldsymbol{S}}_{\boldsymbol{p}}, \tag{115}$$

$$\boldsymbol{S}_{\boldsymbol{\alpha}} = |\Lambda|^{-1/2} \sum_{\boldsymbol{p}} \exp(i\boldsymbol{p}\cdot\boldsymbol{\alpha}) |\Lambda|^{-1/2} \sum_{\boldsymbol{\gamma}\in\Lambda} \exp(-i\boldsymbol{p}\cdot\boldsymbol{\gamma}) \boldsymbol{S}_{\boldsymbol{\gamma}} = \sum_{\boldsymbol{p}} \sum_{\boldsymbol{\gamma}\in\Lambda} |\Lambda|^{-1} \boldsymbol{S}_{\boldsymbol{\gamma}} |\Lambda| \delta_{\boldsymbol{\gamma},\boldsymbol{\alpha}} = \boldsymbol{S}_{\boldsymbol{\alpha}}. \tag{116}$$

The Plancherel sum rule gives:

$$\sum_{\boldsymbol{p}} \hat{\boldsymbol{S}}_{\boldsymbol{p}} \cdot \hat{\boldsymbol{S}}_{-\boldsymbol{p}} = \sum_{\boldsymbol{p}} \Big[|\Lambda|^{-1/2} \sum_{\boldsymbol{\alpha}\in\Lambda} \exp(-i\boldsymbol{p}\cdot\boldsymbol{\alpha}) \boldsymbol{S}_{\boldsymbol{\alpha}} \Big] \cdot \Big[|\Lambda|^{-1/2} \sum_{\boldsymbol{\gamma}\in\Lambda} \exp(i\boldsymbol{p}\cdot\boldsymbol{\gamma}) \boldsymbol{S}_{\boldsymbol{\gamma}} \Big] =$$
$$= \sum_{\boldsymbol{\alpha},\boldsymbol{\gamma}} \delta_{\boldsymbol{\alpha},\boldsymbol{\gamma}} \boldsymbol{S}_{\boldsymbol{\alpha}} \cdot \boldsymbol{S}_{\boldsymbol{\gamma}} = |\Lambda|. \tag{117}$$

In terms of these Fourier variables Hamiltonian $\mathcal{H}$ has the form:

$$\begin{aligned}
\mathcal{H} &= -\sum_{\boldsymbol{\alpha},i} \boldsymbol{S}_{\boldsymbol{\alpha}} \cdot \boldsymbol{S}_{\boldsymbol{\alpha}+\boldsymbol{\delta}_i} = -\frac{1}{2} \sum_{\boldsymbol{\alpha},|\boldsymbol{\delta}|=1} \boldsymbol{S}_{\boldsymbol{\alpha}} \cdot \boldsymbol{S}_{\boldsymbol{\alpha}+\boldsymbol{\delta}} = \\
&= -\frac{1}{2} \sum_{\boldsymbol{\alpha},\boldsymbol{\delta}} \left[\sum_{\boldsymbol{p}} |\Lambda|^{-1/2} \exp(i\boldsymbol{p}\cdot\boldsymbol{\alpha}) \hat{\boldsymbol{S}}_{\boldsymbol{p}} \right] \cdot \left[\sum_{\boldsymbol{p}'} |\Lambda|^{-1/2} \exp\big(i\boldsymbol{p}'\cdot(\boldsymbol{\alpha}+\boldsymbol{\delta})\big) \hat{\boldsymbol{S}}_{\boldsymbol{p}'} \right] = \\
&= -\frac{1}{2} |\Lambda|^{-1} \sum_{\boldsymbol{p},\boldsymbol{p}'} \hat{\boldsymbol{S}}_{\boldsymbol{p}} \cdot \hat{\boldsymbol{S}}_{\boldsymbol{p}'} \sum_{\boldsymbol{\alpha},\boldsymbol{\delta}} \exp\big(i\boldsymbol{p}\cdot\boldsymbol{\alpha} + i\boldsymbol{p}'\cdot(\boldsymbol{\alpha}+\boldsymbol{\delta})\big) = -\frac{1}{2} \sum_{\boldsymbol{p}} \sum_{\boldsymbol{\delta}} \exp(-i\boldsymbol{p}\cdot\boldsymbol{\delta}) \hat{\boldsymbol{S}}_{\boldsymbol{p}} \cdot \hat{\boldsymbol{S}}_{-\boldsymbol{p}} = \\
&= -\frac{1}{2} \Big(2\nu|\Lambda| - \sum_{\boldsymbol{p}} \sum_{\boldsymbol{\delta}} \hat{\boldsymbol{S}}_{\boldsymbol{p}} \cdot \hat{\boldsymbol{S}}_{-\boldsymbol{p}} \Big) - \sum_{\boldsymbol{p}} \sum_{\boldsymbol{\delta}} \exp(-i\boldsymbol{p}\cdot\boldsymbol{\delta}) \hat{\boldsymbol{S}}_{\boldsymbol{p}} \cdot \hat{\boldsymbol{S}}_{-\boldsymbol{p}} = \text{const} + \sum_{\boldsymbol{p}} E_{\boldsymbol{p}} \hat{\boldsymbol{S}}_{\boldsymbol{p}} \cdot \hat{\boldsymbol{S}}_{-\boldsymbol{p}},
\end{aligned} \tag{118}$$

where:

$$E_{\boldsymbol{p}} = \frac{1}{2} \sum_{\boldsymbol{\delta}} \big(1 - \exp(-i\boldsymbol{p}\cdot\boldsymbol{\delta}) \big) = \nu - \sum_{i=1}^{\nu} \cos(p_i). \tag{119}$$

For small $|\boldsymbol{p}|$:

$$E_{\boldsymbol{p}} \sim |\boldsymbol{p}|^2/2. \tag{120}$$

In terms of Fourier variables the [6] result is:

$$\lim_{\Lambda\to\infty} |\Lambda|^{-1} g_{\boldsymbol{p}=\boldsymbol{0}} \neq 0, \tag{121}$$

where:

$$g_{\boldsymbol{p}} = \left\langle \hat{\boldsymbol{S}}_{\boldsymbol{p}} \cdot \hat{\boldsymbol{S}}_{-\boldsymbol{p}} \right\rangle. \tag{122}$$

Due to the Plancherel rule (117) (or the normalization condition for spins (108)):

$$|\Lambda|^{-1} \sum_{\boldsymbol{p}} g_{\boldsymbol{p}} = 1. \tag{123}$$

Hence the [6] proof gives:

$$g_{\boldsymbol{p}} \leq \frac{3}{2\beta E_{\boldsymbol{p}}};\ \boldsymbol{p} \neq \boldsymbol{0}. \tag{124}$$

Note: the physical interpretation of this fact is that the average energy $E_{\boldsymbol{p}} \langle \boldsymbol{S}_{\boldsymbol{p}} \cdot \boldsymbol{S}_{-\boldsymbol{p}} \rangle$ per mode is dominated by its equiparticion value of $\frac{kT}{2}$ per each degree of freedom.
The bound (124) implies that:

$$\lim_{\Lambda\to\infty} |\Lambda|^{-1} \sum_{\boldsymbol{p}\neq\boldsymbol{0}} g_{\boldsymbol{p}} \leq \frac{3}{2\beta} G_{\nu}(0), \tag{125}$$

where:

$$G_\nu(0) = (2\pi)^{-\nu} \int\limits_{|p_i|\le\pi} (E_{\boldsymbol p})^{-1} d^\nu \boldsymbol p. \tag{126}$$

Note: the Fourier integral was obtained as a limiting case of the Fourier sum.
For $\nu \ge 3$, $G_\nu(0)$ is finite as $E_{\boldsymbol p} \sim |\boldsymbol p|^2$. The bound is now defined by:

$$\begin{aligned} &\lim_{\Lambda\to\infty} |\Lambda|^{-1} g_{\boldsymbol p=\boldsymbol 0} \neq 0 \\ &\lim_{\Lambda\to\infty} |\Lambda|^{-1} \sum_{\boldsymbol p} g_{\boldsymbol p} = 1 \qquad \Longrightarrow \qquad \frac{3}{2\beta} G_\nu(0) < 1 \qquad \Longrightarrow \qquad \beta > \frac{3}{2} G_\nu(0) \equiv \beta_{FSS} \\ &\lim_{\Lambda\to\infty} |\Lambda|^{-1} \sum_{\boldsymbol p\neq\boldsymbol 0} g_{\boldsymbol p} \le \frac{3}{2\beta} G_\nu(0) \end{aligned} \tag{127}$$

Note: the bound and the Plancherel sum rule force the macroscopic occupation of $\boldsymbol p = \boldsymbol 0$ mode. This is kind of spin-wave Bose-condensation. The above discussion can be transfered from antiferromagnetic to ferromagnetic case by substituting $\boldsymbol p$ with $(\pi, ..., \pi) - \boldsymbol p$.
To explain the problems one needs to overcome in extending the [6] result to the quantum case, one should first describe a model. Let S be a fixed number chosen from $\frac{1}{2}, 1, \frac{3}{2}, ...$ Each lattice site $\boldsymbol\alpha \in \Lambda$ has associated with it $(2S+1)$-dimensional space $\mathscr{H}_{\boldsymbol\alpha} \simeq \mathbb{C}^{2S+1}$ and three self-adjoined operators $\boldsymbol S_{\boldsymbol\alpha}$ obeying the usual commutation relations:

$$[S^j_{\boldsymbol\alpha}, S^{(k)}_{\boldsymbol\alpha}] = i\varepsilon_{jkl} S^{(l)}_{\boldsymbol\alpha}. \tag{128}$$

However, the normalization condition (108) is replaced by:

$$\boldsymbol S^2_{\boldsymbol\alpha} = S(S+1), \tag{129}$$

since $\dim \mathscr{H}_{\boldsymbol\alpha} = 2S+1$. In volume Λ the basic Hilbert space is:

$$\mathscr{H}_\Lambda = \bigotimes_{\boldsymbol\alpha\in\Lambda} \mathscr{H}_{\boldsymbol\alpha} \simeq \mathbb{C}^{(2S+1)|\Lambda|}. \tag{130}$$

Now, partition function and thermal expectations are given by:

$$Z = \mathrm{Tr}_{\mathscr{H}_\Lambda}[\exp(-\beta \mathcal{H}_\Lambda)], \tag{131}$$

$$\langle \mathcal{A} \rangle_{\Lambda,\beta} = Z^{-1}\, \mathrm{Tr}_{\mathscr{H}_\Lambda}[\mathcal{A} \exp(-\beta \mathcal{H}_\Lambda)]. \tag{132}$$

Due to commutation relations:

$$[S^{(j)}_{\boldsymbol\alpha}, S^{(k)}_{\boldsymbol\beta}] = i\delta_{\boldsymbol\alpha,\boldsymbol\beta} \varepsilon_{jkl} S^{(l)}_{\boldsymbol\alpha}. \tag{133}$$

For Fourier transformed operators one obtains:

$$\begin{aligned} [\hat S^{(j)}_{\boldsymbol p}, \hat S^{(k)}_{\boldsymbol q}] &= \Big[|\Lambda|^{-1/2} \sum_{\boldsymbol\alpha\in\Lambda} \exp(-i\boldsymbol p\cdot\boldsymbol\alpha) S^{(j)}_{\boldsymbol\alpha}, |\Lambda|^{-1/2} \sum_{\boldsymbol\gamma\in\Lambda} \exp(-i\boldsymbol q\cdot\boldsymbol\gamma) S^{(k)}_{\boldsymbol\gamma} \Big] = \\ &= |\Lambda|^{-1} \sum_{\boldsymbol\alpha,\boldsymbol\gamma} \exp(-i\boldsymbol p\cdot\boldsymbol\alpha - i\boldsymbol q\cdot\boldsymbol\gamma)[S^{(j)}_{\boldsymbol\alpha}, S^{(k)}_{\boldsymbol\gamma}] = |\Lambda|^{-1} \sum_{\boldsymbol\alpha,\boldsymbol\gamma} \exp(-i\boldsymbol p\cdot\boldsymbol\alpha - i\boldsymbol q\cdot\boldsymbol\gamma) i\delta_{\boldsymbol\alpha,\boldsymbol\gamma} \varepsilon_{jkl} S^{(l)}_{\boldsymbol\alpha} = \\ &= |\Lambda|^{-1/2} i\varepsilon_{jkl} \hat S^{(l)}_{\boldsymbol p+\boldsymbol q}, \end{aligned} \tag{134}$$

$$[\hat S^{(j)}_{\boldsymbol p}, (\hat S^{(j)}_{\boldsymbol p})^*] = [\hat S^{(j)}_{\boldsymbol p}, \hat S^{(j)}_{-\boldsymbol p}] = 0 \quad \Longrightarrow \quad g_{\boldsymbol p} = \big\langle \hat{\boldsymbol S}_{\boldsymbol p} \cdot \hat{\boldsymbol S}_{-\boldsymbol p} \big\rangle = g_{-\boldsymbol p}. \tag{135}$$

The relation for Hamiltonian $\mathcal{H}$ in terms of Fourier variables matches the classic result (118).
The Plancherel sum rule (117) in quantum case is replaced by:

$$|\Lambda|^{-1} \sum_{\boldsymbol p} g_{\boldsymbol p} = S(S+1). \tag{136}$$

The problem is that in quantum case the bound for the structure factor can't hold. If the bound was true:

$$g_{\boldsymbol{p}} \leq \frac{3}{2\beta}\frac{1}{E_{\boldsymbol{p}}}, \tag{137}$$

$$\beta \to \infty,\ \Lambda \text{ - fixed and finite} \implies \quad g_{\boldsymbol{p}} \to 0, \tag{138}$$

but on the other hand, when $\beta \to \infty$:

$$\boldsymbol{S}_{\boldsymbol{\alpha}} \cdot \boldsymbol{S}_{\boldsymbol{\gamma}} \to \begin{cases} S^2 & \text{, if } \boldsymbol{\alpha} \neq \boldsymbol{\gamma} \\ S(S+1) & \text{, if } \boldsymbol{\alpha} = \boldsymbol{\gamma} \end{cases} \implies \quad g_{\boldsymbol{p}} \neq 0. \tag{139}$$

It is believed that:

$$g_{\boldsymbol{p}} \leq \sqrt{\frac{3}{2}} S \coth\left(\sqrt{\frac{2}{3}} S\beta E_{\boldsymbol{p}}\right) \tag{140}$$

is true for the ferromagnet. For antiferromagnet $g_{\boldsymbol{p}}$ should be replaced with Duhamel two-point function $b_{\boldsymbol{p}}$.

B.2 Duhamel two-point function

For quantum systems in finite volume with the partition function $Z = \mathrm{Tr}[\exp(-\beta\mathcal{H})]$, one can define the Duhamel two-point function (DTF) by:

$$(A,B) = Z^{-1}\int_0^1 \mathrm{Tr}\Big[\exp(-x\beta\mathcal{H})A\exp(-(1-x)\beta\mathcal{H})B\Big]dx. \tag{141}$$

The name of the function comes from the fact that $\frac{1}{2}\mu^2(A,A)Z$ is the second-order term in a perturbation expansion for $\mathrm{Tr}[\exp(-\beta\mathcal{H}+\mu A)]$, first derived by Duhamel. This leads to the second definition:

$$(A,B)Z = \frac{\partial^2}{\partial\mu\partial\lambda}\mathrm{Tr}[\exp(-\beta\mathcal{H}+\mu A+\lambda B)]. \tag{142}$$

From both the definitions it is obvious that:

$$(A,B) = Z^{-1}\frac{\partial^2}{\partial\mu\partial\lambda}\mathrm{Tr}[\exp(-\beta\mathcal{H}+\mu A+\lambda B)] = \frac{\partial^2}{\partial\mu\partial\lambda}\mathrm{Tr}[\exp(-\beta\mathcal{H}+\mu B+\lambda A)] = (B,A), \tag{143}$$

$$\begin{aligned}(A,B) &= Z^{-1}\int_0^1 \mathrm{Tr}\Big[\exp(-x\beta\mathcal{H})A\exp(-(1-x)\beta\mathcal{H})B\Big]dx = \\ &= Z^{-1}\int_1^0 \mathrm{Tr}\Big[\exp(-(1-y)\beta\mathcal{H})A\exp(-y\beta\mathcal{H})B\Big]dy = \\ &= Z^{-1}\int_0^1 \mathrm{Tr}\Big[\exp(-y\beta\mathcal{H})B\exp(-(1-y)\beta\mathcal{H})A\Big]dy = (B,A).\end{aligned} \tag{144}$$

In particular, if $A = A_r + iA_i$, then:

$$(A^*,A) = (A_r - iA_i, A_r + iA_i) = (A_r,A_r) + (A_i,A_i). \tag{145}$$

If $\langle B\rangle_\mu = \left[\operatorname{Tr}[\exp(-\beta\mathcal{H}+\mu A)]\right]^{-1}\operatorname{Tr}[B\exp(-\beta\mathcal{H}+\mu A)]$, then:

$$\begin{aligned}\frac{\partial\langle B\rangle_\mu}{\partial\mu}\bigg|_{\mu=0} &= \frac{\partial}{\partial\mu}\left[\frac{\operatorname{Tr}[B\exp(-\beta\mathcal{H}+\mu A)]}{\operatorname{Tr}[\exp(-\beta\mathcal{H}+\mu A)]}\right] = \\ &= \frac{\operatorname{Tr}[AB\exp(-\beta\mathcal{H}+\mu A)]}{\operatorname{Tr}[\exp(-\beta\mathcal{H}+\mu A)]} - \frac{\operatorname{Tr}[A\exp(-\beta\mathcal{H}+\mu A)]\operatorname{Tr}[B\exp(-\beta\mathcal{H}+\mu A)]}{\left(\operatorname{Tr}[\exp(-\beta\mathcal{H}+\mu A)]\right)^2} = \\ &= \frac{\operatorname{Tr}[AB\exp(-\beta\mathcal{H}+\mu A)]}{\operatorname{Tr}[\exp(-\beta\mathcal{H}+\mu A)]} - \langle A\rangle\langle B\rangle = (A,B) - \langle A\rangle\langle B\rangle = \left(A-\langle A\rangle, B-\langle B\rangle\right). \end{aligned} \tag{146}$$

For quantum systems DTF substitutes the thermal two-point function:

$$\langle A,B\rangle = Z^{-1}\operatorname{Tr}[AB\exp(-\beta\mathcal{H})]. \tag{147}$$

Note: unlike (A,B), $\langle A,B\rangle$ is not symmetric A and B.
If $\mathcal{H}$ has a complete set of eigenfunctions φ_i with $\mathcal{H}\varphi_i = \varepsilon_i\varphi_i$ and $a_{ij} = \left(\varphi_i, A\varphi_j\right)$ and $b_{ij} = \left(\varphi_i, B\varphi_j\right)$,then:

$$(A,B) = Z^{-1}\int_0^1 \sum_{i,j} a_{ij}b_{ji}\exp(-x\beta\varepsilon_i)\exp(-(1-x)\beta\varepsilon_j)dx = \sum_{i,j}\frac{a_{ij}b_{ji}\left(\exp(-\beta\varepsilon_i)-\exp(-\beta\varepsilon_j)\right)}{\beta Z(\varepsilon_j-\varepsilon_i)}. \tag{148}$$

B.3 Upper bound for Duhamel two-point function

For each lattice site $\boldsymbol{\alpha}$ one can choose a copy of $\mathscr{H}_{\boldsymbol{\alpha}}$ of the same Hilbert space and copies of $n+1$ basic operators denoted by $S_{\boldsymbol{\alpha}}^{(1)},...,S_{\boldsymbol{\alpha}}^{(n)},\tilde{A}_{\boldsymbol{\alpha}}$.The basic Hamiltonian in Λ is:

$$\mathcal{H} = \sum_{\alpha\in\Lambda}\left(\tilde{A}_{\boldsymbol{\alpha}} - \sum_{m=1}^{\nu}\sum_{j=1}^{n} S_{\boldsymbol{\alpha}}^{(j)}S_{\boldsymbol{\alpha}+\boldsymbol{\delta}_m}^{(j)}\right) = \sum_{\alpha\in\Lambda}\left(A_{\boldsymbol{\alpha}} + \frac{1}{2}\sum_{m=1}^{\nu}\left(\boldsymbol{S}_{\boldsymbol{\alpha}} - \boldsymbol{S}_{\boldsymbol{\alpha}+\boldsymbol{\delta}_m}\right)^2\right), \tag{149}$$

where $A_\alpha = \tilde{A}_\alpha - \nu\boldsymbol{S}_{\boldsymbol{\alpha}}^2$. The Fourier transformed operator $\hat{\boldsymbol{S}}_{\boldsymbol{p}}$ was defined previously by (114) and:

$$b_{\boldsymbol{p}}^{(j)} = (\hat{S}_{\boldsymbol{p}}^{(j)}, \hat{S}_{-\boldsymbol{p}}^{(j)}) \tag{150}$$

is the Duhamel two-point function.
Theorem 1 For Hamiltonians of the form (149) in boxes Λ of sides $L_1\times...\times L_\nu$ with each an L_j even integer and such that Theorem 2 holds:

$$b_{\boldsymbol{p}}^{(j)} \le \frac{1}{2\beta E_{\boldsymbol{p}}}, \tag{151}$$

where $E_{\boldsymbol{p}}$ is given by (119).
Theorem 2 Let $\mathcal{H}$ be a Hamiltonian of the form (149) in which all the matrices are real. Let $\{\boldsymbol{h}_i(\boldsymbol{\alpha}) : \boldsymbol{\alpha}\in\Lambda, i=1,...,\nu\}$ be $\nu|\Lambda|$ vectors in $\mathbb{R}^n$. Let $\partial_j\boldsymbol{h}_i \equiv \boldsymbol{h}_i(\boldsymbol{\alpha}+\boldsymbol{\delta}_j) - \boldsymbol{h}_i(\boldsymbol{\alpha})$ and $\sigma(\boldsymbol{h}) = \sum_{\boldsymbol{\alpha}}\boldsymbol{h}(\boldsymbol{\alpha})\cdot\boldsymbol{S}_{\boldsymbol{\alpha}}$. Let Λ be $L_1,...,L_\nu$ with each L_i even. Then:

$$\frac{\operatorname{Tr}\left[\exp\left(-\beta\mathcal{H}+\sigma\left(\sum_i\partial_i\boldsymbol{h}_i\right)\right)\right]}{\operatorname{Tr}[\exp(-\beta\mathcal{H})]} \le \exp\left(\frac{||\boldsymbol{h}||^2}{2\beta}\right), \tag{152}$$

where $||\boldsymbol{h}||^2 = \sum_{i,\boldsymbol{\alpha}}|\boldsymbol{h}_i(\boldsymbol{\alpha})|^2$.
□ (of Theorem 1, given Theorem 2)

From (152) by substituting $\boldsymbol{h}_i \to \lambda \boldsymbol{h}_i$, subtracting 1 from both sides, dividing by λ^2 and taking limit $\lambda \to 0$:

$$\frac{\operatorname{Tr}\Big[\exp\Big(-\beta\mathcal{H} + \sigma\big(\sum_i \partial_i \lambda \boldsymbol{h}_i\big)\Big)\Big]}{\operatorname{Tr}[\exp(-\beta\mathcal{H})]} - 1 \le \exp\left(\frac{\|\lambda \boldsymbol{h}\|^2}{2\beta}\right) - 1, \tag{153}$$

$$\lim_{\lambda\to 0}\left(\frac{\operatorname{Tr}\Big[\exp\Big(-\beta\mathcal{H} + \sigma\big(\sum_i \partial_i \lambda \boldsymbol{h}_i\big)\Big)\Big] - \operatorname{Tr}[\exp(-\beta\mathcal{H})]}{\lambda^2 \operatorname{Tr}[\exp(-\beta\mathcal{H})]}\right) \le \lim_{\lambda\to 0}\left(\frac{1}{\lambda^2}\exp\left(\frac{\lambda^2\|\boldsymbol{h}\|^2}{2\beta}\right) - \frac{1}{\lambda^2}\right). \tag{154}$$

For the r.h.s. of (154):

$$\lim_{\lambda\to 0}\left(\frac{1}{\lambda^2}\exp\left(\frac{\lambda^2\|\boldsymbol{h}\|^2}{2\beta}\right) - \frac{1}{\lambda^2}\right) = \lim_{\lambda\to 0}\frac{\|\boldsymbol{h}\|^2}{2\beta}\int_0^1 \exp\left(\frac{\lambda^2\|\boldsymbol{h}\|^2}{2\beta}\right)dx = \frac{\|\boldsymbol{h}\|^2}{2\beta}. \tag{155}$$

For the l.h.s of (154), using the notation $A = \sigma(\sum_i \partial_i \boldsymbol{h}_i)$:

$$\begin{aligned}
&\lim_{\lambda\to 0}\left(\frac{\operatorname{Tr}\Big[\exp\Big(-\beta\mathcal{H} + \sigma\big(\sum_i \partial_i \lambda \boldsymbol{h}_i\big)\Big)\Big] - \operatorname{Tr}[\exp(-\beta\mathcal{H})]}{\lambda^2 \operatorname{Tr}[\exp(-\beta\mathcal{H})]}\right) = \\
&= \lim_{\lambda\to 0}\left(\frac{1}{\lambda^2}\Big[Z^{-1}\operatorname{Tr}[\exp(-\beta\mathcal{H} + \lambda A)] - 1\Big]\right) = \lim_{\lambda\to 0}\left(\frac{1}{Z\lambda^2}\Big[\operatorname{Tr}[\exp(-\beta\mathcal{H} + \lambda A)] - \operatorname{Tr}[\exp(-\beta\mathcal{H})]\Big]\right) = \\
&= \lim_{\lambda\to 0}\left(\frac{1}{Z\lambda^2}\Big[\operatorname{Tr}[\exp(-\beta\mathcal{H})] + \frac{\lambda^2}{2}(A,A)Z - \operatorname{Tr}[\exp(-\beta\mathcal{H})]\Big]\right) = (A,A)/2.
\end{aligned} \tag{156}$$

Finally, one obtains the following inequality:

$$\left(\Big(\sigma\big(\sum_i \partial_i \boldsymbol{h}_i\big)\Big)^*, \sigma\big(\sum_i \partial_i \boldsymbol{h}_i\big)\right) \le \beta^{-1}\sum_{i,\boldsymbol{\alpha}} |\boldsymbol{h}_i(\boldsymbol{\alpha})|^2. \tag{157}$$

Note: for complex-valued $\boldsymbol{h}$ it also works due to (145).
One can fix $\boldsymbol{p} \ne \boldsymbol{0}$ and $j \in \{1, ..., n\}$ and choose:

$$[\boldsymbol{h}_i(\boldsymbol{\alpha})]_k = \delta_{j,k}|\Lambda|^{-1/2}\big(\exp(i\boldsymbol{p}\cdot(\boldsymbol{\alpha} - \boldsymbol{\delta}_i)) - \exp(i\boldsymbol{p}\cdot\boldsymbol{\alpha})\big). \tag{158}$$

Then:

$$\begin{aligned}
&\sum_{i,\boldsymbol{\alpha}} |\boldsymbol{h}_i(\alpha)|^2 = \sum_{i,\boldsymbol{\alpha},k} \delta_{j,k}|\Lambda|^{-1}\big(\exp(i\boldsymbol{p}\cdot(\boldsymbol{\alpha} - \boldsymbol{\delta}_i)) - \exp(i\boldsymbol{p}\cdot\boldsymbol{\alpha})\big)^2 = \\
&= \sum_{i,\boldsymbol{\alpha}} |\Lambda|^{-1}\exp(2i\boldsymbol{p}\cdot\boldsymbol{\alpha})\big(\exp(-i\boldsymbol{p}\cdot\boldsymbol{\delta}_i) - 1)\big)^2 = \sum_i \big(\exp(-i\boldsymbol{p}\cdot\boldsymbol{\delta}_i) - 1)\big)^2 \cdot \sum_{\boldsymbol{\alpha}} |\Lambda|^{-1}\exp(2i\boldsymbol{p}\cdot\boldsymbol{\alpha}) = 2E_{\boldsymbol{p}},
\end{aligned} \tag{159}$$

while:

$$\begin{aligned}
&\Big[\sum_i \partial_i \boldsymbol{h}_i(\boldsymbol{\alpha})\Big]_k = \delta_{j,k}|\Lambda|^{-1/2}\sum_i \big(\exp(i\boldsymbol{p}\cdot\boldsymbol{\alpha}) - \exp(i\boldsymbol{p}\cdot(\boldsymbol{\alpha} + \boldsymbol{\delta}_i)) - \exp(i\boldsymbol{p}\cdot(\boldsymbol{\alpha} - \boldsymbol{\delta}_i)) + \exp(i\boldsymbol{p}\cdot\boldsymbol{\alpha})\big) = \\
&= 2\delta_{j,k}|\Lambda|^{-1/2}\exp(i\boldsymbol{p}\cdot\boldsymbol{\alpha})\sum_{|\boldsymbol{\delta}|=1}\big(1 - \exp(i\boldsymbol{p}\cdot\boldsymbol{\delta})\big) = \delta_{j,k}|\Lambda|^{-1/2}(2E_{\boldsymbol{p}})\exp(i\boldsymbol{p}\cdot\boldsymbol{\alpha}).
\end{aligned} \tag{160}$$

Finally, (157) becomes:

$$4E_{\boldsymbol{p}}^2\Big(\sigma_{\boldsymbol{p}}^{(j)}, \sigma_{-\boldsymbol{p}}^{(j)}\Big) \le (2E_{\boldsymbol{p}})\beta^{-1}. \tag{161}$$

■

Lemma Let $\mathscr{H}_1$ be a finite dimensional vector space and let $\mathscr{H} = \mathscr{H}_1 \otimes \mathscr{H}_1$. If $A, B, \ldots$ are operators on $\mathscr{H}_1$, one can use the symbols $A, B, \ldots$ for the operators $A\otimes 1, B\otimes 1, \ldots$ and the symbols $\tilde{A}, \tilde{B}, \ldots$ for $1\otimes A, 1\otimes B, \ldots$ Then for any self-adjoint operators $A, B, C_1, \ldots, C_l$ with real matrix representations and real numbers $h_1, \ldots, h_l$:

$$\left(\mathrm{Tr}\left[\exp\left(A+\tilde{B}-\sum_{i=1}^{l}\left(C_i-\tilde{C}_i-h_i\right)^2\right)\right]\right)^2 \leq$$
$$\leq \mathrm{Tr}\left[\exp\left(A+\tilde{A}-\sum_{i=1}^{l}\left(C_i-\tilde{C}_i\right)^2\right)\right]\mathrm{Tr}\left[\exp\left(B+\tilde{B}-\sum_{i=1}^{l}\left(C_i-\tilde{C}_i\right)^2\right)\right]. \quad (162)$$

□ If one uses the notation:

$$\alpha = \mathrm{Tr}\left[\exp\left(A+\tilde{B}-\sum_{i=1}^{l}\left(C_i-\tilde{C}_i-h_i\right)^2\right)\right], \quad (163)$$

then, using the Trotter product formula:

$$\alpha = \lim_{n\to\infty}\alpha_n, \quad (164)$$

where:

$$\alpha_n = \mathrm{Tr}\left[\left\{\exp(A/n)\exp\left(\tilde{B}/n\right)\exp\left(-\left(C_1-\tilde{C}_1-h_1\right)^2/n\right)\ldots\right\}^n\right]. \quad (165)$$

Using the operator identity:

$$\exp\left(-D^2\right) = (4\pi)^{-1/2}\int\exp(ikD)\exp\left(-k^2/4\right)dk, \quad (166)$$

one may obtain:

$$\alpha_n = (4\pi)^{-nl/2}\int \mathrm{Tr}\left[\exp(A/n)\exp\left(\tilde{B}/n\right)\exp\left(ik_1(C_1-\tilde{C}_1)/\sqrt{n}+\ldots\right)\right]\cdot$$
$$\cdot\exp\left(-\boldsymbol{k}^2/4\right)\exp\left(-ik_1h_1/\sqrt{n}-\ldots\right)d^{nl}\boldsymbol{k}. \quad (167)$$

Operators can be thought of as matrices, which are real due to the initial assumption. Then:

$$\mathrm{Tr}\left[\exp(A/n)\exp\left(\tilde{B}/n\right)\exp\left(ik_1(C_1-\tilde{C}_1)/\sqrt{n}+\ldots\right)\right] =$$
$$= \mathrm{Tr}\left[\exp(A/n)\exp\left(ik_1C_1/\sqrt{n}+\ldots\right)\right]\left(\mathrm{Tr}\left[\exp(B/n)\exp\left(ik_1C_1/\sqrt{n}+\ldots\right)\right]\right)^*. \quad (168)$$

Note: the reality of matrices is used to take the complex conjugate without reversing the order of the factors, also the fact that for any of the two operators D and F, $\tilde{D}$ and F commute, used here.
Using the Cauchy-Schwarz inequality on $d^{nl}\boldsymbol{k}$ integration and (168) with $A = B$ one obtains:

$$|\alpha_n|^2 = \alpha_n^*\alpha_n = (4\pi)^{-nl/2}\int d^{nl}\boldsymbol{k}\,\mathrm{Tr}\left[\exp(A/n)\exp\left(\tilde{B}/n\right)\exp\left(-ik_1(C_1-\tilde{C}_1)/\sqrt{n}-\ldots\right)\right]\cdot$$
$$\cdot\exp\left(-\boldsymbol{k}^2/4\right)\exp\left(ik_1h_1/\sqrt{n}+\ldots\right)\times(4\pi)^{-nl/2}\int d^{nl}\boldsymbol{k}\cdot$$
$$\cdot\mathrm{Tr}\left[\exp(A/n)\exp\left(\tilde{B}/n\right)\exp\left(ik_1(C_1-\tilde{C}_1)/\sqrt{n}+\ldots\right)\right]\exp\left(-\boldsymbol{k}^2/4\right)\exp\left(-ik_1h_1/\sqrt{n}-\ldots\right) =$$
$$= (A,B) \leq (A,A)\cdot(B,B) =$$
$$= \left[(4\pi)^{-nl/2}\int d^{nl}\boldsymbol{k}\,\mathrm{Tr}\left[\exp(A/n)\exp\left(\tilde{A}/n\right)\exp\left(ik_1(C_1-\tilde{C}_1)/\sqrt{n}+\ldots\right)\right]\exp\left(-\boldsymbol{k}^2/4\right)\right]\times$$
$$\times\left[(4\pi)^{-nl/2}\int d^{nl}\boldsymbol{k}\cdot\mathrm{Tr}\left[\exp(B/n)\exp\left(\tilde{B}/n\right)\exp\left(ik_1(C_1-\tilde{C}_1)/\sqrt{n}-\ldots\right)\right]\exp\left(-\boldsymbol{k}^2/4\right)\right]. \quad (169)$$

■

□ (of Theorem 2)
One can define:

$$Z\big(\{\boldsymbol{h}_i(\boldsymbol{\alpha})\}\big) = \mathrm{Tr}\Bigg[\exp\Bigg(-\sum_{\boldsymbol{\alpha}\in\Lambda}\Big\{\beta A_{\boldsymbol{\alpha}} + \frac{\beta}{2}\sum_{m=1}^{\nu}\big[\boldsymbol{S}_{\boldsymbol{\alpha}} - \boldsymbol{S}_{\boldsymbol{\alpha}+\boldsymbol{\delta}_m} + \beta^{-1}\boldsymbol{h}_m(\boldsymbol{\alpha})\big]^2\Big\}\Bigg)\Bigg], \tag{170}$$

then:

$$Z\big(\{\boldsymbol{h}_i(\boldsymbol{\alpha})\}\big) = \mathrm{Tr}\Bigg[\exp\Bigg(-\beta\mathcal{H} + \sigma\big(\sum_i \partial_i \boldsymbol{h}_i\big) - \frac{1}{2\beta}\sum_{\boldsymbol{\alpha}\in\Lambda}\sum_{m=1}^{\nu}\big(\boldsymbol{h}_m(\boldsymbol{\alpha})\big)^2\Bigg)\Bigg], \tag{171}$$

$$Z(\{0\}) = \mathrm{Tr}[\exp(-\beta\mathcal{H})]. \tag{172}$$

In these notations (152) is equivalent to:

$$Z\big(\{\boldsymbol{h}_i(\boldsymbol{\alpha})\}\big) \le Z(\{0\}), \tag{173}$$

for all real $\{\boldsymbol{h}_i(\boldsymbol{\alpha})\}$. Since Z is continuous in all the h's and goes to zero if any $\boldsymbol{h}_i(\boldsymbol{\alpha}) \to \infty$, it takes its maximum value Z_0 at some set of h's, one can denote as $\{\bar{\boldsymbol{h}}_i(\boldsymbol{\alpha})\}$. If this maximum value is taken at more than one point, one can choose the set of h's with the largest number of h's equal to zero.
One must now show that $\bar{\boldsymbol{h}}_i(\boldsymbol{\alpha})$ for all $\boldsymbol{\alpha}, i$. If this is not true, by relabeling the following set is obtained:

$$\bar{\boldsymbol{h}}_i(\boldsymbol{\alpha}) \ne \boldsymbol{0} \quad \text{for} \quad i = 1 \quad \text{and} \quad \boldsymbol{\alpha} = (L-1, 0, ..., 0). \tag{174}$$

Let $\mathscr{H}_1$ be the tensor product of all the $\mathscr{H}_{\boldsymbol{\gamma}}$, such that $\boldsymbol{\gamma} = (\gamma_1, ..., \gamma_\nu)$ with $0 \le \gamma_1 \le \frac{1}{2}L_1 - 1$ and $\gamma_2, ..., \gamma_\nu$ arbitrary. Then $\mathscr{H}_\Lambda = \mathscr{H}_1 \otimes \mathscr{H}_1$ in such a way that $\tilde{\boldsymbol{S}}_{\boldsymbol{\gamma}} = \boldsymbol{S}_{\boldsymbol{\gamma}}$, where $\tilde{\gamma}_2 = \gamma_2, ..., \tilde{\gamma}_\nu = \gamma_\nu$ and $\tilde{\gamma}_1 = L_1 - 1 - \gamma_1$. Using this representation:

$$Z\big(\{\boldsymbol{h}_i(\boldsymbol{\alpha})\}\big) = \mathrm{Tr}\Bigg[\exp\Bigg(D + \tilde{D} - \sum_{i=1}^{l}\big(C_i - \tilde{C}_i - y_i\big)^2\Bigg)\Bigg], \tag{175}$$

where D is all "interactions" between $\mathscr{H}_1$ spins, C_i - between spins at sites $(0, \gamma_2, ..., \gamma_\nu)$ and $(\frac{1}{2}L_1 - 2, \gamma_2, ..., \gamma_\nu)$, y's corresponding to the h's to the factor of β. Using Lemma one concludes that:

$$\big[Z\big(\{\boldsymbol{h}_i(\boldsymbol{\alpha})\}\big)\big]^2 \le Z\big(\{\boldsymbol{h}_i^{(1)}(\boldsymbol{\alpha})\}\big)Z\big(\{\boldsymbol{h}_i^{(2)}(\boldsymbol{\alpha})\}\big), \tag{176}$$

where $\{\boldsymbol{h}_i^{(1)}(\boldsymbol{\alpha})\}$ (or $\{\boldsymbol{h}_i^{(2)}(\boldsymbol{\alpha})\}$) is a set of $\{\boldsymbol{h}_i(\boldsymbol{\alpha})\}$ invariant under $\gamma \to \tilde{\gamma}$ reflection and equal to the $\{\bar{\boldsymbol{h}}_i(\boldsymbol{\alpha})\}$ on the $\mathscr{H}_1$ (or $\tilde{\mathscr{H}_1}$) and zero on the bonds between $\mathscr{H}_1$ and $\tilde{\mathscr{H}_1}$.
Note: basically, what one does here is the separation of the real lattice in two parts and calculation of an upper bound (176) for the total value of Z function. One only needs $\{\boldsymbol{h}_i(\boldsymbol{\alpha})\}$ invariant under $\gamma \to \tilde{\gamma}$ reflection, because other terms will cancel out.
Now, on the one hand, either $\{\boldsymbol{h}_i^{(1)}(\boldsymbol{\alpha})\}$ or $\{\boldsymbol{h}_i^{(2)}(\boldsymbol{\alpha})\}$ must contain strictly more zero elements than $\{\bar{\boldsymbol{h}}_i(\boldsymbol{\alpha})\}$ (due to the definition). On the other hand, since $Z\big(\{\bar{\boldsymbol{h}}_i(\boldsymbol{\alpha})\}\big) = Z_0$ and $Z\big(\{\boldsymbol{h}_i(\boldsymbol{\alpha})\}\big) \le Z_0$, by inserting $\{\boldsymbol{h}_i(\boldsymbol{\alpha})\} = \{\bar{\boldsymbol{h}}_i(\boldsymbol{\alpha})\}$ into (176), one obtains:

$$Z_0^2 \le Z\big(\{\boldsymbol{h}_i^{(1)}(\boldsymbol{\alpha})\}\big)Z\big(\{\boldsymbol{h}_i^{(2)}(\boldsymbol{\alpha})\}\big). \tag{177}$$

So, set $\{\boldsymbol{h}_i^{(1)}(\boldsymbol{\alpha})\} + \{\boldsymbol{h}_i^{(2)}(\boldsymbol{\alpha})\}$ has more zero elements than $\{\bar{\boldsymbol{h}}_i(\boldsymbol{\alpha})\}$ and defines maximum. This contradicts with the definition of $\{\bar{\boldsymbol{h}}_i(\boldsymbol{\alpha})\}$.

■

C Zero temperature derivations

One can directly use the zero-temperature inequality (12) to obtain the (86). In order to do that one needs to rewrite the anticommutation relation $\{a^\dagger, a\}$ in a way done in [7]:

$$\begin{aligned}\Big\langle\{a^\dagger, a\}\Big\rangle = \sum_n \Big(\langle 0| a |n\rangle \langle n| a^\dagger |0\rangle + \langle 0| a^\dagger |n\rangle \langle n| a |0\rangle \Big) \le \\ \le \sum_n \sqrt{\varepsilon_n}\sqrt{\varepsilon_n^{-1}} \Big| \langle 0| a |n\rangle \langle n| a^\dagger |0\rangle + \langle 0| a^\dagger |n\rangle \langle n| a |0\rangle \Big| = \\ = \sum_n \sqrt{\varepsilon_n}\sqrt{\varepsilon_n^{-1}} \sqrt{\langle 0| a |n\rangle \langle n| a^\dagger |0\rangle + \langle 0| a^\dagger |n\rangle \langle n| a |0\rangle}^2 .\end{aligned} \tag{178}$$

Here and further in this section the expectation value should be taken considering only the ground state of the system. After implying the Cauchy-Schwarz inequality for summation:

$$\begin{aligned}\sum_n \sqrt{\varepsilon_n}\sqrt{\varepsilon_n^{-1}} \sqrt{\langle 0| a |n\rangle \langle n| a^\dagger |0\rangle + \langle 0| a^\dagger |n\rangle \langle n| a |0\rangle}^2 \le \\ \le \sqrt{\sum_n \varepsilon_n \Big(\langle 0| a |n\rangle \langle n| a^\dagger |0\rangle + \langle 0| a^\dagger |n\rangle \langle n| a |0\rangle \Big)} \sqrt{\sum_n \varepsilon_n^{-1} \Big(\langle 0| a |n\rangle \langle n| a^\dagger |0\rangle + \langle 0| a^\dagger |n\rangle \langle n| a |0\rangle \Big)}.\end{aligned} \tag{179}$$

The value under first square root is the expectation value of double commutator:

$$\begin{aligned}\Big\langle[[a^\dagger, \mathcal{H}], a]\Big\rangle = \Big\langle a^\dagger \mathcal{H} a - \mathcal{H} a^\dagger a - a a^\dagger \mathcal{H} + a \mathcal{H} a^\dagger \Big\rangle = \langle 0| a^\dagger \mathcal{H} a + a \mathcal{H} a^\dagger |0\rangle = \\ = \sum_n \varepsilon_n \Big(\langle 0| a |n\rangle \langle n| a^\dagger |0\rangle + \langle 0| a^\dagger |n\rangle \langle n| a |0\rangle \Big).\end{aligned} \tag{180}$$

While the second expectation value is a second order perturbation term in the expansion:

$$\begin{aligned}\sum_n \varepsilon_n^{-1} \Big(\langle 0| a |n\rangle \langle n| a^\dagger |0\rangle + \langle 0| a^\dagger |n\rangle \langle n| a |0\rangle \Big) = \langle 0| a \frac{\mathbb{I} - |0\rangle\langle 0|}{\mathcal{H}} a^\dagger |0\rangle + \langle 0| a^\dagger \frac{\mathbb{I} - |0\rangle\langle 0|}{\mathcal{H}} a |0\rangle = \\ = \frac{\partial^2}{\partial\lambda\partial\mu} \operatorname{Tr}\Big[\mathcal{H} + \lambda a + \mu a^\dagger\Big].\end{aligned} \tag{181}$$

The last expression may be rewritten as Bogoliubov inner product (or Duhamel two-point function as referred in this document), for which the bound is proved by the (151). Finally, considering $\boldsymbol{Q} = (\pi, ..., \pi)$, $a = S^y_{\boldsymbol{q}}$ and $b = S^z_{\boldsymbol{q}+\boldsymbol{Q}}$ and using (12) and (178) one can obtain (86).

References

[1] Tsutomu Momoi. An Upper Bound for the Spin-Wave Spectrum of the Heisenberg Antiferromagnet. *Journal of the Physical Society of Japan*, 63:2507, July 1994.

[2] Sandro Stringari. Spin excitations and sum rules in the heisenberg antiferromagnet. *Phys. Rev. B*, 49:6710–6717, March 1994.

[3] Tohru Koma. Maximum Spontaneous Magnetization and Nambu-Goldstone Mode. *arXiv e-prints*, page arXiv:1712.09018, December 2017.

[4] Lev Pitaevskii and Sandro Stringari. Uncertainty principle, quantum fluctuations, and broken symmetries. *Journal of Low Temperature Physics*, 85(5):377–388, December 1991.

[5] Freeman J. Dyson, Elliott H. Lieb, and Barry Simon. Phase transitions in quantum spin systems with isotropic and nonisotropic interactions. *Journal of Statistical Physics*, 18(4):335–383, April 1978.

[6] Jürg Fröhlich, Barry Simon, and Thomas Spencer. Infrared bounds, phase transitions and continuous symmetry breaking. *Comm. Math. Phys.*, 50(1):79–95, 1976.

[7] B Sriram Shastry. Bounds for correlation functions of the heisenberg antiferromagnet. *Journal of Physics A: Mathematical and General*, 25(5):L249–L253, March 1992.