Mermin-Wagner theorem analogous treatment of the long-range order in La_2CuO_4-type compound spin models

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The analysis of the high-T_C superconductor parent compound La_2CuO_4 phase diagram shows that in the tetragonal phase of this system spontaneous magnetization at any finite temperature equals zero, whereas in the orthorhombic phase long-range order exists up to a certain temperature greater than zero. In this paper, such behavior is demonstrated exactly for the spin model which describes this compound, by making use of the Bogoliubov's inequality. We may therefore conclude that the results of Mermin and Wagner can also be extended to some 3*d*-isotropic magnetic lattices. The situation for the $YBa_2Cu_3O_6$-type model is also discussed.

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I. INTRODUCTION

The exact relations, either equalities or inequalities are rather rare, yet invaluable tools in theoretical physics, since they represent an important test of correctness of any approximate approach. Among them, Mermin-Wagner theorem (MWT)[1] with its broad applicability has been used in statistical physics for almost 40 years to test the results concerning the phase transitions in various magnetic systems. Based on the so-called Bogoliubov's inequality, it relates the possible existence of the spontaneous magnetization to the dimensionality of the system. It is still the subject of detailed analysis.[2–4]

During our study[5] of the magnetism in the spin model describing high-T_C superconductor parent compound La_2CuO_4 (Figs. 3 and 6 in Ref. 5), we had come to some interesting results concerning the existence of the spontaneous magnetization in that system. Namely, though in general the three-dimensional systems have finite Néel temperature [due to the convergency of the integral in Eq. (12) in Ref. 1], we obtained that in the isotropic tetragonal La_2CuO_4 Néel temperature vanishes. At first, we inferred it to be most likely the consequence of the application of Tyablikov's decoupling[6] of the system of equations for Green's functions. Similar conclusion was also drawn by Ref. 7. Nevertheless, we found out later that these conclusions can be proven directly (using Bogoliubov's inequality) for this type of structure and we intend to present our results here, since some previous attempts to extend MWT results to more complex three-dimensional magnetic lattices seem to be inconclusive.[8] For that reason, we offer a somewhat extended derivation of our results.

II. BOGOLIUBOV'S INEQUALITY AND SPONTANEOUS MAGNETIZATION IN La_2CuO_4

The Hamiltonian describing the spin interactions in the La_2CuO_4-type structures is

$$\hat{H} = \frac{1}{2} \sum_{\substack{p,\vec{n}_\alpha,\vec{m}_\beta \\ \alpha,\beta=a,b}} J(\vec{n}_\alpha - \vec{m}_\beta)\vec{S}^{(\alpha)}_{p,\vec{n}_\alpha}\vec{S}^{(\beta)}_{p,\vec{m}_\beta} + J^{(1)}_\perp \sum_{\substack{p,\vec{n}_\alpha,\vec{\delta}^{\alpha\beta}_\perp \\ \alpha,\beta=a,b;\ \alpha\neq\beta}} \vec{S}^{(\alpha)}_{p,\vec{n}_\alpha}\vec{S}^{(\beta)}_{(p,\vec{n}_\alpha)+\vec{\delta}^{\alpha\beta}_\perp} + J^{(2)}_\perp \sum_{\substack{p,\vec{n}_\alpha,\vec{\delta}^{\alpha\alpha}_\perp \\ \alpha=a,b}} \vec{S}^{(\alpha)}_{p,\vec{n}_\alpha}\vec{S}^{(\alpha)}_{(p,\vec{n}_\alpha)+\vec{\delta}^{\alpha\alpha}_\perp} - h\sum_{\substack{p,\vec{n}_\alpha \\ \alpha=a,b}} \hat{S}^{z(\alpha)}_{p,\vec{n}_\alpha} e^{-i\vec{Q}(p,\vec{n}_\alpha)}. \quad (1)$$

Here, p denotes the plane, $\alpha,\beta=a,b$ refer to the two sublattices, $\vec{n}_{\alpha/\beta},\vec{m}_{\alpha/\beta}$ specify the position of the spin within the plane, $\vec{\delta}^{\alpha\alpha/\alpha\beta}_\perp$ connects the two ferro/antiferromagnetically coupled spins in the neighboring planes, $h=g\mu_B H$, where H signifies the external magnetic field, $\vec{Q}$ is taken in such a way that $e^{-i\vec{Q}\cdot\vec{n}}=1$ when $\vec{n}$ connects sites in the same sublattice, and -1 when it connects sites in different sublattices.

In order to be more specific, we emphasize that in the orthorhombic phase $J^{(1)}_\perp \equiv J^{ab}_\perp \neq J^{(2)}_\perp \equiv J^{aa}_\perp$, whereas the symmetry of the tetragonal phase imposes $J^{ab}_\perp = J^{aa}_\perp = J_\perp$. It should be stressed that our model takes into account the experimental fact that the interactions between the nearest neighbors in the adjacent planes are antiferromagnetic [$J^{(i)}_\perp > 0,\ i=1,2$]. However, the ordering of spins is dictated predominantly by the much stronger nearest neighbor interaction in the plane. Since $J_\perp \ll J$ we take into account only the interaction between the two neighboring planes. On the other hand, we include all the interactions among the spins within the same plane. Some examples of those interactions are given in Fig. 1.

The initial point of our calculation is the Bogoliubov's inequality[9]

$$1/2\langle\{\hat{A},\hat{A}^\dagger\}\rangle\langle[[\hat{C},\hat{H}],\hat{C}^\dagger]\rangle \geqslant k_B T|\langle[\hat{C},\hat{A}]\rangle|^2. \quad (2)$$

Here, $[\cdots]$ denotes the commutator, $\{\cdots\}$ anticommutator, $\hat{H}$ is the Hamiltonian of the system, $\langle\cdots\rangle$ signifies the average over the canonical ensemble with the Hamiltonian H, and $\hat{A}$ and $\hat{C}$ are two arbitrary operators chosen such that given ensemble averages exist. It is the careful choice of these operators that yields MWT.

Our choice will be

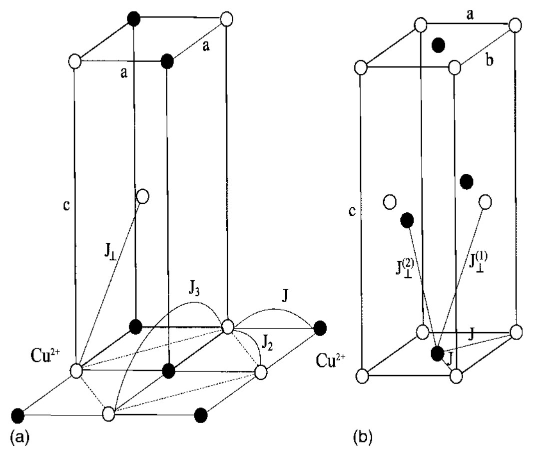

FIG. 1. Unit cell of the La_2CuO_4 in (a) tetragonal and (b) orthorhombic phase with exchange interactions labeled (Ref. 11). Only Cu^{2+} ions are shown. Two different orientations of spins are denoted by ○ and ●.

$$\hat C(\vec k) = \hat S^{+(a)}_{\vec k} + \hat S^{+(b)}_{\vec k}; \quad \hat A(\vec k) = \hat S^{-(a)}_{-\vec k} - \hat S^{-(b)}_{-\vec k}. \tag{3}$$

Introducing $\sigma = \langle \hat S^{z(a)}_{p,\vec n_a}\rangle = \langle -\hat S^{z(b)}_{p,\vec n_b}\rangle$, we arrive at

$$\langle[\hat C,\hat A]\rangle = 2N\sigma, \tag{4}$$

where N denotes the total number of magnetic ions. [Since relation (4) is valid at any $\vec k$, the $\vec k$ dependance in notation is henceforth neglected.]

The above expressions lead to the following form of the Bogoliubov's inequality:

$$\langle\{\hat A,\hat A^\dagger\}\rangle \geqslant \frac{8k_BTN^2\sigma^2}{\langle[[\hat C,\hat H],\hat C^\dagger]\rangle(\vec k)}. \tag{5}$$

A rather simple calculation gives the following expression for $\{\hat A,\hat A^\dagger\}$:

$$\{\hat A,\hat A^\dagger\} = \sum_{\substack{p,\vec n_\alpha,\vec m_\alpha\\ \alpha=a,b}} e^{-i\vec k(\vec n_\alpha - \vec m_\alpha)}\{\hat S^{-(\alpha)}_{\vec n_\alpha},\hat S^{+(\alpha)}_{\vec m_\alpha}\} - \sum_{\substack{p,\vec n_\alpha,\vec n_\beta\\ \alpha,\beta=a,b,\ \alpha\neq\beta}} e^{-i\vec k(\vec n_\alpha-\vec n_\beta)}\{\hat S^{-(\beta)}_{\vec n_\beta},\hat S^{+(\alpha)}_{\vec n_\alpha}\}. \tag{6}$$

Summing over $\vec k$, averaging and taking into account that $\vec n_a \neq \vec n_b$, yields the expression

$$\sum_{\vec k}\langle\{\hat A,\hat A^\dagger\}\rangle = \frac{N}{2}\sum_{\substack{p,\vec n_\alpha,\\ \alpha=a,b}}\langle\{\hat S^{-(\alpha)}_{\vec n_\alpha},\hat S^{+(\alpha)}_{\vec n_\alpha}\}\rangle = 2N\sum_{p,\vec n_\alpha}\langle S(S+1) - (\hat S^{z(\alpha)}_{\vec n_\alpha})^2\rangle \leqslant 2N^2S(S+1). \tag{7}$$

The above equality is standard property of angular moment operator [Eq. (3.15.b) in Ref. 10].

We confront the greatest complexity of the calculation during the evaluation of the average of the double commutator and its majorization. A rather lengthy algebraic procedure leads to

$$\begin{aligned}\langle[[\hat C,\hat H],\hat C^\dagger]\rangle = {} & \sum_{\substack{\vec\rho_{\alpha\beta}\\ \alpha,\beta=a,b}} J(\vec\rho_{\alpha\beta})(e^{-i\vec k(\vec\rho_{\alpha\beta})}-1) \\ & \times\sum_{p,\vec n_\alpha}\langle(2\hat S^{z(\alpha)}_{p,\vec n_\alpha}\hat S^{z(\beta)}_{(p,\vec n_\alpha)+\vec\rho_{\alpha\beta}} + \hat S^{-(\alpha)}_{p,\vec n_\alpha}\hat S^{+(\beta)}_{(p,\vec n_\alpha)+\vec\rho_{\alpha\beta}})\rangle \\ & + J_\perp^{(1)}\sum_{\substack{\vec\delta_\perp^{\alpha\beta}\\ \alpha,\beta=a,b,\ \alpha\neq\beta}}(e^{i\vec k\vec\delta_\perp^{\alpha\beta}}-1) \\ & \times\sum_{p,\vec n_\alpha}\langle(2\hat S^{z(\alpha)}_{p,\vec n_\alpha}\hat S^{z(\beta)}_{(p,\vec n_\alpha)+\vec\delta_\perp^{\alpha\beta}} + \hat S^{-(\alpha)}_{p,\vec n_\alpha}\hat S^{+(\beta)}_{(p,\vec n_\alpha)+\vec\delta_\perp^{\alpha\beta}})\rangle \\ & + J_\perp^{(2)}\sum_{\substack{\vec\delta_\perp^{\alpha\alpha}\\ \alpha=a,b}}(e^{i\vec k\vec\delta_\perp^{\alpha\alpha}}-1)\sum_{p,\vec n_\alpha}\langle(2\hat S^{z(\alpha)}_{p,\vec n_\alpha}\hat S^{z(\alpha)}_{(p,\vec n_\alpha)+\vec\delta_\perp^{\alpha\alpha}} \\ & + \hat S^{+(\alpha)}_{p,\vec n_\alpha}\hat S^{-(\alpha)}_{(p,\vec n_\alpha)+\vec\delta_\perp^{\alpha\alpha}})\rangle + 2h\left(\sum_{p,\vec n_a}\hat S^{z(a)}_{\vec n_a} - \sum_{p,\vec n_b}\hat S^{z(b)}_{\vec n_b}\right),\end{aligned} \tag{8}$$

where $\vec\rho_{\alpha\beta} = \vec n_\alpha - \vec n_\beta$.

We must perform the majorization of this expression very carefully for the following reason: the partial sums of spin correlation functions have to be majorized in different manner depending on whether the spins belong to the same or different sublattices. This is the essential difference comparing to the original MW approach. Let us look at the general expression for this partial sum

$$\begin{aligned}&\sum_{p,\vec n_\alpha}\langle(2\hat S^{z(\alpha)}_{p,\vec n_\alpha}\hat S^{+(\beta)}_{(p,\vec n_\alpha)+\vec\delta_\perp^{\alpha\beta}} + \hat S^{-(\alpha)}_{p,\vec n_\alpha}\hat S^{+(\beta)}_{(p,\vec n_\alpha)+\vec\delta_\perp^{\alpha\beta}})\rangle \\ &= \frac{8}{N^2}\sum_{p,\vec n_\alpha}\sum_{\vec k_1,\vec k_2}\left\langle\left(\hat S^{z(\alpha)}_{\vec k_1}\hat S^{z(\beta)}_{\vec k_2} + \tfrac14\{\hat S^{+(\alpha)}_{\vec k_1},\hat S^{-(\beta)}_{\vec k_2}\}\right)\right\rangle \\ &\quad\times e^{i(\vec k_1+\vec k_2)(p,\vec n_\alpha)+i\vec k_2\vec\delta_\perp^{\alpha\beta}} \\ &= \frac{4}{N}\sum_{\vec k}\left\langle\left(\hat S^{z(\alpha)}_{\vec k}\hat S^{z(\beta)}_{-\vec k} + \tfrac14\{\hat S^{+(\alpha)}_{\vec k},\hat S^{-(\beta)}_{-\vec k}\}\right)\right\rangle e^{-i\vec k\vec\delta_\perp^{\alpha\beta}}.\end{aligned} \tag{9}$$

If $\alpha=\beta$, following the reasoning of MW, we obtain

$$\begin{aligned}&\frac{4}{N}\sum_{\vec k}\left\langle\left(\hat S^{z(\alpha)}_{\vec k}\hat S^{z(\alpha)}_{-\vec k} + \tfrac14\{\hat S^{+(\alpha)}_{\vec k},\hat S^{-(\alpha)}_{-\vec k}\}\right)\right\rangle e^{-i\vec k\vec\delta_\perp^{\alpha\alpha}} \\ &\quad\leqslant \frac{4}{N}\sum_{\vec k}\left\langle\left(\hat S^{z(\alpha)}_{-\vec k}\hat S^{z(\alpha)}_{-\vec k} + \tfrac14\{\hat S^{+(\alpha)}_{\vec k},\hat S^{-(\alpha)}_{-\vec k}\}\right)\right\rangle \\ &\quad= \frac{4}{N}\sum_{p,\vec n_\alpha}\left\langle\left(\hat S^{z(\alpha)}_{p,\vec n_\alpha}\hat S^{z(\alpha)}_{p,\vec n_\alpha} + \tfrac14\{\hat S^{+(\alpha)}_{p,\vec n_\alpha},\hat S^{-(\alpha)}_{p,\vec n_\alpha}\}\right)\right\rangle\sum_{\vec k}e^{-i\vec k(\vec n_\alpha-\vec n_\alpha)} \\ &\quad= 2\sum_{p,\vec n_\alpha}\left\langle\left(\hat S^{z(\alpha)}_{p,\vec n_\alpha}\hat S^{z(\alpha)}_{p,\vec n_\alpha} + \tfrac14\{\hat S^{+(\alpha)}_{p,\vec n_\alpha},\hat S^{-(\alpha)}_{p,\vec n_\alpha}\}\right)\right\rangle.\end{aligned} \tag{10}$$

However, for $\alpha\neq\beta$, assuming that the last term in (9) is positive, we proceed in similar manner, yet in this case the sum over $\vec k$ vanishes, leading to the essential conclusion

$$\sum_{p,\vec{n}_a}\langle(2\hat{S}^{z(a)}_{p,\vec{n}_a}\hat{S}^{z(b)}_{(p,\vec{n}_a)+\vec{\delta}^{ab}_{\perp}}+\hat{S}^{-(a)}_{p,\vec{n}_a}\hat{S}^{+(b)}_{(p,\vec{n}_a)+\vec{\delta}^{ab}_{\perp}})\rangle \leqslant 0. \tag{11}$$

In order to demonstrate the plausibility of these results, let us first consider the case of the simple three-dimensional (3D) two-sublattice antiferromagnetic, in the nearest neighbor approximation. In that case,

$$\langle[[\hat{C},\hat{H}],\hat{C}^{\dagger}]\rangle=\sum_{\vec{\lambda}_{ab}}J(e^{-i\vec{k}\vec{\lambda}_{ab}}-1)\sum_{\vec{n}_a}\langle 2\hat{S}^{z(a)}_{p,\vec{n}_a}\hat{S}^{z(b)}_{(p,\vec{n}_a)+\vec{\lambda}_{ab}} + \hat{S}^{-(a)}_{p,\vec{n}_a}\hat{S}^{+(b)}_{(p,\vec{n}_a)+\vec{\lambda}_{ab}}\rangle. \tag{12}$$

It is known that this expression should be positive due to the properties of Bogoliubov's inner product, yet for $J>0$ this is fulfilled only if the sum of correlation functions is negative.

Let us now analyze the expression (8). The first term contains the interactions between the spins within the same plane. The leading interaction will be the one between the nearest neighbors, with negative partial sum of correlation functions [according to (11)]. Since the whole sum has to be positive, it can be majorized as the sum of absolute values (in MW manner).

However, for the second term, we shall not perform any majorization, but just regroup the terms:

$$\left\langle J^{(1)}_{\perp}\sum_{\substack{p,\vec{n}_{\alpha},\vec{\delta}^{\alpha\beta}_{\perp}\\ \alpha\neq\beta}}(e^{i\vec{k}\vec{\delta}^{\alpha\beta}_{\perp}}-1)(2\hat{S}^{z(\alpha)}_{p,\vec{n}_{\alpha}}\hat{S}^{z(\beta)}_{(p,\vec{n}_{\alpha})+\vec{\delta}^{\alpha\beta}_{\perp}} + \hat{S}^{-(\alpha)}_{p,\vec{n}_{\alpha}}\hat{S}^{+(\beta)}_{(p,\vec{n}_{\alpha})+\vec{\delta}^{\alpha\beta}_{\perp}})\right\rangle$$
$$=2J^{(1)}_{\perp}\sum_{\substack{\vec{\delta}^{\alpha\beta}_{\perp}\\ \alpha\neq\beta}}(1-e^{i\vec{k}\vec{\delta}^{\alpha\beta}_{\perp}})\left|\sum_{p,\vec{n}_{\alpha}}\left(\langle\hat{S}^{z(\alpha)}_{p,\vec{n}_{\alpha}}\hat{S}^{z(\beta)}_{(p,\vec{n}_{\alpha})+\vec{\delta}^{\alpha\beta}_{\perp}}\rangle + \tfrac{1}{4}\langle\{\hat{S}^{+(\beta)}_{(p,\vec{n}_{\alpha})+\vec{\delta}^{\alpha\beta}_{\perp}},\hat{S}^{-(\alpha)}_{p,\vec{n}_{\alpha}}\}\rangle\right)\right|, \tag{13}$$

where we have made use of (11). Also for the third term, we use the fact that these neighbors belong to the same sublattice, so the sum of correlation functions is positive. All these considerations can be summarized in

$$\begin{aligned}\langle[[\hat{C},\hat{H}],\hat{C}^{\dagger}]\rangle(\vec{k}) \leqslant{}& 2\sum_{\substack{\vec{\rho}_{\alpha\beta}\\ \alpha,\beta=a,b}}J(\vec{\rho}_{\alpha\beta})(1-e^{-i\vec{k}\vec{\rho}_{\alpha\beta}})\sum_{p,\vec{n}_{\alpha}}\left|\left(\langle\hat{S}^{z(\alpha)}_{p,\vec{n}_{\alpha}}\hat{S}^{z(\beta)}_{(p,\vec{n}_{\alpha})+\vec{\rho}_{\alpha\beta}}\rangle + \tfrac{1}{4}\langle\{\hat{S}^{+(\alpha)}_{p,\vec{n}_{\alpha}},\hat{S}^{-(\beta)}_{(p,\vec{n}_{\alpha})+\vec{\rho}_{\alpha\beta}}\}\rangle\right)\right| + 2J^{(1)}_{\perp}\sum_{\substack{\vec{\delta}^{\alpha\beta}_{\perp}\\ (\alpha\neq\beta)}}(1-e^{-i\vec{k}\vec{\delta}^{\alpha\beta}_{\perp}})\\ &\times\left|\sum_{p,\vec{n}_{\alpha}}\left(\langle\hat{S}^{z(\alpha)}_{p,\vec{n}_{\alpha}}\hat{S}^{z(\beta)}_{(p,\vec{n}_{\alpha})+\vec{\delta}^{\alpha\beta}_{\perp}}\rangle + \tfrac{1}{4}\langle\{\hat{S}^{+(\alpha)}_{p,\vec{n}_{\alpha}},\hat{S}^{-(\beta)}_{(p,\vec{n}_{\alpha})+\vec{\delta}^{\alpha\beta}_{\perp}}\}\rangle\right)\right|\\ &+2J^{(2)}_{\perp}\sum_{\vec{\delta}^{\alpha\alpha}_{\perp}}(e^{-i\vec{k}\vec{\delta}^{\alpha\alpha}_{\perp}}-1)\sum_{p,\vec{n}_{\alpha}}\left(\langle\hat{S}^{z(\alpha)}_{p,\vec{n}_{\alpha}}\hat{S}^{z(\alpha)}_{(p,\vec{n}_{\alpha})+\vec{\delta}^{\alpha\alpha}_{\perp}}\rangle + \tfrac{1}{4}\langle\{\hat{S}^{+(\alpha)}_{p,\vec{n}_{\alpha}},\hat{S}^{-(\alpha)}_{(p,\vec{n}_{\alpha})+\vec{\delta}^{\alpha\alpha}_{\perp}}\}\rangle\right)+2Nh\sigma.\end{aligned} \tag{14}$$

In order to perform the majorization to the sums appearing in the previous expression, we use the relation $\langle(\hat{S}^i_{p,\vec{n}_a}\pm\hat{S}^i_{p,\vec{m}_b})^2\rangle\geqslant 0$, $i=x,y,z$ and the fact that the two sublattices are equivalent $\langle(\hat{S}^i_{p,\vec{n}_a})^2\rangle=\langle(\hat{S}^i_{p,\vec{m}_b})^2\rangle$, which yields

$$|\langle\hat{S}^i_{p,\vec{n}_{\alpha}}\hat{S}^i_{p,\vec{m}_{\alpha/\beta}}\rangle|\leqslant\langle(\hat{S}^i_{p,\vec{n}_{\alpha}})^2\rangle. \tag{15}$$

Taking into account Eq. (15) and the fact that $\langle(\hat{S}^i_{p,\vec{n}_a})^2\rangle\leqslant S(S+1)$, we conclude that all the partial sums of the correlation functions in Eq. (14) are equal or less than $NS(S+1)$, whereby Eq. (14) becomes

$$\begin{aligned}\langle[[\hat{C},\hat{H}],\hat{C}^{\dagger}]\rangle(\vec{k})&\leqslant 2NS(S+1)\times\left[\sum_{\vec{\rho}_{\alpha\beta}}|J(\vec{\rho}_{\alpha\beta})|(1-e^{-i\vec{k}\vec{\rho}_{\alpha\beta}}) + J^{(1)}_{\perp}\sum_{\vec{\delta}^{\alpha\beta}_{\perp}}(1-e^{-i\vec{k}\vec{\delta}^{\alpha\beta}_{\perp}})+J^{(2)}_{\perp}\sum_{\vec{\delta}^{\alpha\alpha}_{\perp}}(e^{-i\vec{k}\vec{\delta}^{\alpha\alpha}_{\perp}}-1)\right]+2Nh\sigma\\ &=2NS(S+1)\left[\sum_{\vec{\rho}_{\alpha\beta}}|J(\vec{\rho}_{\alpha\beta})|(1-\cos\vec{k}_{\parallel}\vec{\rho}_{\alpha\beta})+J^{(1)}_{\perp}\sum_{\vec{\delta}^{\alpha\beta}_{\perp}}(1-\cos\vec{k}\vec{\delta}^{\alpha\beta}_{\perp})+J^{(2)}_{\perp}\sum_{\vec{\delta}^{\alpha\alpha}_{\perp}}(\cos\vec{k}\vec{\delta}^{\alpha\alpha}_{\perp}-1)\right]+2Nh\sigma.\end{aligned} \tag{16}$$

The next important question we confront is how to apply the majorization to this expression. According to Mermin and Wagner,[1] one should take $1-\cos x\leqslant\frac{1}{2}x^2$, which is proper since it is essential to look for the terms that make the integral in Eq. (12) in Ref. 1 diverge in the vicinity of $|\vec{k}|\approx 0$.

In our case, we have

$$1-\cos\vec{k}_{\parallel}\vec{\rho}_{\alpha\beta}\leqslant\tfrac{1}{2}k^2_{\parallel}\vec{\rho}^{\,2}_{\alpha\beta};\quad 1-\cos\vec{k}\vec{\delta}^{\alpha\beta}_{\perp}\leqslant\tfrac{1}{2}k^2(\vec{\delta}^{\alpha\beta}_{\perp})^2 \tag{17}$$

within the CuO_2 plane and between the two planes, respectively.

After this majorization, Eq. (16) takes the form

$$\begin{aligned}\langle[[\hat{C},\hat{H}],\hat{C}^{\dagger}]\rangle(\vec{k})\leqslant 2NS(S+1)\times&\left\{\left[\sum_{\vec{\rho}_{\alpha\beta}}|J(\vec{\rho}_{\alpha\beta})|\rho^2_{\alpha\beta}\right]k^2_{\parallel}/2+\left[J^{(1)}_{\perp}\sum_{\vec{\delta}^{\alpha\beta}_{\perp}}(\delta^{\alpha\beta}_{\perp})^2-J^{(2)}_{\perp}\sum_{\vec{\delta}^{\alpha\alpha}_{\perp}}(\delta^{\alpha\alpha}_{\perp})^2\right]k^2/2\right\}\\ &+2Nh\sigma,\end{aligned} \tag{18}$$

which is valid for the orthorhombic phase of La_2CuO_4.

In the *tetragonal* phase of the system, $J^{(1)}=J^{(2)}$ and $|\vec{\delta}^{ab}_{\perp}|=|\vec{\delta}^{aa}_{\perp}|$, so Eq. (15) is reduced to

$$\begin{aligned}\langle[[\hat{C},\hat{H}],\hat{C}^{\dagger}]\rangle(\vec{k})&\leqslant 2NS(S+1)\left[\sum_{\vec{\rho}_{\alpha\beta}}|J(\vec{\rho}_{\alpha\beta})|\rho^2_{\alpha\beta}\right]k^2_{\parallel}/2+2Nh\sigma\\ &=NS(S+1)\left[\sum_{\vec{\rho}}|J(\vec{\rho})|\rho^2\right]k^2_{\parallel}+2Nh\sigma\\ &=NS(S+1)Ak^2_{\parallel}+2Nh\sigma,\end{aligned} \tag{19}$$

where the quantity A is obviously given by $A=\Sigma_{\vec{\rho}}|J(\vec{\rho})|\rho^2$.

Summing Eq. (5) over $\vec{k}$ and making use of the Eqs. (7) and (19), and, we arrive at the following expression:

$$2N^2S(S+1) \geqslant 2k_BT4\sigma^2N^2\frac{1}{N}\sum_{\vec{k}}\frac{1}{AS(S+1)k_\parallel^2+2Nh\sigma}. \quad (20)$$

We now transform the sum into the integral and observe that the function under the integral does not depend on k_z. Therefore, after the integration over k_z, the integration over $\vec{k}$ reduces to two dimensions, where we obtain

$$\sigma^2 \leqslant \frac{S(S+1)}{4k_BT}\left\{\frac{a^2}{(2\pi)^2}\int_{I\,BZ} d^2\vec{k}\frac{1}{\alpha k_\parallel^2+2Nh\sigma}\right\}^{-1}, \quad (21)$$

where a denotes the lattice constant within the plane and $\alpha = AS(S+1)$.

If we (similar to MW procedure)[1] integrate only over a sphere of radius k_0 contained in the first Brillouin zone, then an elementary integration shows that the value of the bracketed factor is

$$\frac{a^2}{(2\pi)^2}\int_{I\,BZ} d^2\vec{k}\frac{1}{\alpha k_\parallel^2+2Nh\sigma} = \frac{a^2}{4\pi\alpha}\ln\left(1+\frac{\alpha k_0^2}{2Nh\sigma}\right), \quad (22)$$

and we obtain the following expression for the spontaneous magnetization in the tetragonal phase of the system:

$$\sigma^2 \leqslant \frac{S(S+1)}{k_BT}\frac{\pi\alpha}{a^2}\left\{\ln\left(1+\frac{\alpha k_0^2}{2Nh\sigma}\right)\right\}^{-1}. \quad (23)$$

In the limit $h \to 0$, $\sigma^2 \leqslant 0$, hence, we infer that $\sigma = 0$, i.e., the long-range order does not exist at any finite temperature $T \neq 0$.

Quite contrary, in the *orthorhombic* phase the second bracketed factor in Eq. (18) differs from zero, so Eq. (19) becomes

$$\langle[[\hat{C},\hat{H}],\hat{C}^\dagger]\rangle(\vec{k}) \leqslant NS(S+1)[Ak_\parallel^2 + Bk^2] + 2Nh\sigma, \quad (24)$$

where $B = J_\perp^{(1)}\sum_{\delta_\perp^{ab}}(\delta_\perp^{ab})^2 - |J_\perp^{(2)}|\sum_{\delta_\perp^{aa}}(\delta_\perp^{aa})^2$. The main difference with respect to the procedure performed for the tetragonal phase is that the integration cannot be reduced here to the two-dimensional (2D) case, which leads to the convergency of the integral analogous to the one in Eq. (21) and, hence, to the finite spontaneous magnetization, up to a certain temperature (Néel temperature).

III. CONCLUSION

In this paper we present results which show that the conclusions of Mermin and Wagner[1] concerning the nonexistence of the spontaneous magnetization in isotropic one-dimensional (1D) and 2D systems with finite range interactions can be also extended to some 3D isotropic systems.

Namely, we analyze the two phases (tetragonal and orthorhombic) of the spin model describing high-T_C superconductor parent compound La_2CuO_4 and, taking into account only the interaction between the two neighboring planes, we infer that in the tetragonal phase the spontaneous magnetization at any finite temperature equals zero, contrary to the orthorhombic phase in which long-range order exists up to a certain temperature (Néel temperature), which agrees with the experiment. These results are obtained exactly, by making use of Bogoliubov's inequality.

It is important to emphasize that these results are strictly valid only in the case of this specific spin model where only the interaction of nearest neighbors in the adjacent planes is taken into account. This is justified by the experimental results according to which the interaction of those first neighbors is several orders of magnitude (10^{-5}) times smaller than the in-plane interaction of the nearest neighbors. Formally, the interaction of the next neighbors would definitely change the result.

In the case of $YBa_2Cu_3O_6$,[11] there appears a bilayer motive, so that in the direction orthogonal to the bilayer there occur two types of interaction: intrabilayer and interbilayer. However, the nearest neighbor interaction occurs always between antiferromagnetically ordered spins, contrary to the lanthanide case, where the competition between ferro- and antiferromagnetically ordered spins leads to the two dimensionality of the integral (21). Consequently, in the case of the $YBa_2Cu_3O_6$-type compound spin model, the integration which would follow from the equation analogous to (16), would possess the three-dimensional character, yielding the long-range order up to the Néel temperature.

The analysis presented in this paper suggests that the domain of the applicability of Bogoliubov's inequality in studying the presence of the long-range order in various groups of systems seems to be very wide. All the possibilities of usage of this rigorous relation have not yet been exhausted and are about to be examined.

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