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LETTER TO THE EDITOR

Spin-wave theory and Marshall's theorems

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Abstract. The spin-wave ground state $|\Psi_{SW}\rangle$ of the spin-1/2 Heisenberg antiferromagnet on the square lattice is analysed in relation to Marshall's theorems. It is shown that $|\Psi_{SW}\rangle$ obeys the Marshall sign rule and is an eigenstate of S^z to the eigenvalue $M = 0$, but not an eigenstate of $\boldsymbol{S}^2$.

In studies of complicated models like the Heisenberg antiferromagnet (HAF) it is often very helpful to have a few exact theorems at one's disposal, which may serve as guidelines to construct reasonable approximate solutions. For the eigenstates of the HAF on a *finite* bipartite lattice, described by the usual Hamiltonian

$$\mathcal{H} = J \sum_{\langle ij\rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j \tag{1}$$

with $J > 0$, two such theorems have been formulated by Marshall [1] which have later been extended by Lieb and Mattis [2]. In his formulation of the theorems, Marshall utilizes the fact that $\boldsymbol{S}^2$ and S^z, the square of the total spin $\boldsymbol{S} = \sum_i \boldsymbol{S}_i$ and its z component, with respective eigenvalues $S(S+1)$ and M, commute with each other and with $\mathcal{H}$. He then proceeds to construct common eigenvectors $|\Psi^M\rangle$ of $\mathcal{H}$ and S^z in terms of the basis vectors $|\Phi_\alpha^M\rangle$, where each $|\Phi_\alpha^M\rangle$ describes a spin configuration on the lattice belonging to the eigenvalue M. The first of the Marshall theorems restricts the form of the coefficients ψ_α^M in the expansion

$$|\Psi_0^M\rangle = \sum_\alpha \psi_\alpha^M |\Phi_\alpha^M\rangle \tag{2a}$$

with $|\Psi_0^M\rangle$ denoting the state of lowest energy within the given M sector. In the simplest and most important case of atomic spins $S_i = 1/2$, the coefficients must obey the *Marshall sign criterion*

$$\psi_\alpha^M = (-1)^{A_\alpha} \phi_\alpha^M \tag{2b}$$

with positive definite ϕ_α^M and the phases being defined by the number A_α of up-spins on the A sublattice. The second Marshall theorem states that the absolute ground state $|\Psi_0\rangle$ of $\mathcal{H}$ is a *singlet of the total spin*, i.e.,

$$\boldsymbol{S}^2|\Psi_0\rangle = 0. \tag{3}$$

For a proof of these theorems and their generalization to atomic spins $S_i > 1/2$ the reader is referred to the original articles [1,2] and to the lucid discussion by Auerbach [3].

Because of the complicated nature of the Hamiltonian the exact ground state $|\Psi_0\rangle$ is, in general, not available and we are forced to resort to a suitable approximate treatment. The simplest and most popular way of dealing with the HAF is the linear spin-wave (SW) approach [4] which yields an approximate ground state $|\Psi_{SW}\rangle$ of $\mathcal{H}$. The question we shall mainly be concerned with in the present work is to what extent $|\Psi_{SW}\rangle$ satisfies the Marshall theorems.

Interest in this problem arose in connection with the $t-J$ model describing the hopping of a hole in an otherwise perfect HAF. In the traditional and widely accepted picture the hole is seen as being dressed by a cloud of virtual magnons which, together with the hole, form a coherently moving quasiparticle ('spin polaron'), and in its analytic description the SW approach is an important ingredient [5]. This picture has been questioned in recent work [6], where the authors argue that the moving hole picks up a sequence of phases originating from the Marshall signs which are scrambled by the hopping of the hole. Moreover, they claim that this 'phase string' is non-repairable at low energy and leads to a vanishing spectral weight, i.e., to the failure of the quasiparticle picture. We shall not touch upon these conflicting views here, rather we will restrict ourselves to a re-examination of the SW approach in the light of Marshall's theorems. In view of the preceding remarks the question of particular interest is, whether the sign rule (2*b*) is properly incorporated in $|\Psi_{SW}\rangle$ or not. We shall return to this problem after a short summary of SW theory.

Our SW approach is based on a projected version of the Dyson–Maleev representation [7], where the spin operators $S_i^{\pm} = S_i^x \pm i S_i^y$ and S_i^z are expressed in terms of two sets of boson operators (a_i, b_i), one set for each sublattice (A, B) of the underlying square lattice, which is chosen here because of its relevance to the $t-J$ model. For spins $S_i = 1/2$ the spin operators take the general form [7]

$$S_i^{\mu} = P M_i^{\mu} \quad (\mu = +, -, z) \tag{4}$$

where P is a projection operator projecting onto the physical subspace, while the M_i^{μ} are defined by the following expressions:

$$M_i^+ = a_i^\dagger \qquad M_i^- = (1 - a_i^\dagger a_i)a_i \qquad M_i^z = a_i^\dagger a_i - 1/2 \qquad (i \in A) \tag{5a}$$

$$M_i^+ = (1 - b_i^\dagger b_i)b_i \qquad M_i^- = b_i^\dagger \qquad M_i^z = 1/2 - b_i^\dagger b_i \qquad (i \in B). \tag{5b}$$

The operators defined by (4) and (5) form a representation of the original spin-1/2 operators, since they satisfy the spin commutation relations and act on the same Hilbert space. The latter property follows from the presence of the projection operator whose explicit form is derived in [7]. Upon substitution of (4) and (5) into (1) the Hamiltonian takes the form

$$\mathcal{H} = PH \tag{6a}$$

where

$$H = -NJ/2 + (J/2)\sum_{\langle ij\rangle}(a_i^\dagger b_j^\dagger + a_i^\dagger a_i + b_j^\dagger b_j + a_i b_j) + H_4 + H_6 \tag{6b}$$

and H_4 and H_6 contain products of four and six boson operators, respectively. By substituting (6*a*) into the commutator expression $[\mathcal{H}, P] = 0$, whose validity is shown in [7], we recover Dyson's [8] relation $PH = PHP$, which leads to a useful theorem relating the eigenvalues and eigenstates of H to those of the complete Hamiltonian $\mathcal{H}$. The theorem states that if $|\Phi\rangle$ is an eigenvector of H belonging to some eigenvalue E, then

$$|\Psi\rangle = P|\Phi\rangle \tag{7}$$

is an eigenvector of $\mathcal{H}$ belonging to the *same* eigenvalue E, provided $|\Psi\rangle \neq 0$. The proof is very simple and given in [7]. Thus, to obtain the eigenvalues and eigenstates of $\mathcal{H}$, it would suffice to solve the eigenvalue problem of the much simpler Hamiltonian H. Unfortunately, however, even the latter Hamiltonian cannot be diagonalized exactly and is usually treated in the SW approximation, where only the bilinear part of H is retained, whereas H_4 and H_6 are neglected. It should be mentioned here that the SW approximation leads to a violation of the above theorem, whose validity rests on the full Hamiltonian H rather than on its bilinear part alone. However, this violation does not seem to be very serious in two and higher dimensions, since various alternative treatments, analytical as well as numerical, are all in good quantitative agreement with the results of SW theory [4].

The treatment of the bilinear part of (6b) proceeds in the usual way, i.e., the Wannier operators a_i, b_j are Fourier-transformed and then subjected to the Bogoliubov transformation

$$U = \exp\left[\sum\nolimits_{\boldsymbol{q}} \theta_{\boldsymbol{q}} (a_{\boldsymbol{q}}^\dagger b_{-\boldsymbol{q}}^\dagger - \mathrm{H.c.})\right] \tag{8}$$

where here and in the following all wave-vector summations are restricted to the magnetic Brillouin zone (BZ), unless stated otherwise. The real parameter $\theta_{\boldsymbol{q}} (= \theta_{-\boldsymbol{q}})$ is determined from the requirement that $U^\dagger H U$ assume diagonal form. This leads to the condition $\tanh 2\theta_{\boldsymbol{q}} = -\gamma_{\boldsymbol{q}}$, where $\gamma_{\boldsymbol{q}} = (\cos q_x + \cos q_y)/2$ is the structure factor of the square lattice. Thus, in the SW approximation the transformed H becomes

$$U^\dagger H U \approx E_0 + 2J \sum_{\boldsymbol{q}} \omega_{\boldsymbol{q}} (a_{\boldsymbol{q}}^\dagger a_{\boldsymbol{q}} + b_{\boldsymbol{q}}^\dagger b_{\boldsymbol{q}}) \tag{9}$$

where $\omega_{\boldsymbol{q}} = (1 - \gamma_{\boldsymbol{q}}^2)^{1/2}$ and $E_0/N \approx -0.658J$ is the well known SW result [4,7] for the ground-state energy per spin of the square-lattice HAF. Equation (9) shows that the SW ground state of H is $|\Phi_0\rangle = U|0\rangle$, where the boson vacuum $|0\rangle$ corresponds to the Néel state with all spins down on A and all spins up on B. If this is inserted into (7) we find that $|\Psi_{SW}\rangle$, the desired ground state of $\mathcal{H}$ in the SW approximation, is of the form

$$|\Psi_{SW}\rangle = P|\Phi_0\rangle = PU|0\rangle. \tag{10}$$

Subsequently this expression will be further analysed in relation to the Marshall theorems.

The analysis of the SW ground state (10) requires some formal manipulations of the Bogoliubov transformation (8). Following Kirzhnits [9] one finds that $|\Phi_0\rangle$, the unprojected ground state, may be written in the alternative form

$$|\Phi_0\rangle = \mathcal{N} \exp\left(\sum\nolimits_{\boldsymbol{q}} \tanh\theta_{\boldsymbol{q}} a_{\boldsymbol{q}}^\dagger b_{-\boldsymbol{q}}^\dagger\right)|0\rangle \tag{11}$$

where

$$\tanh\theta_{\boldsymbol{q}} = -(1 - \omega_{\boldsymbol{q}})/\gamma_{\boldsymbol{q}} \tag{12}$$

and $\mathcal{N}$ is a normalization factor, whose explicit form is irrelevant to the present discussion. As the next step, the operators in the exponent of (11) are re-expressed in terms of the Wannier operators a_i and b_j. Making use of (12),

$$|\Phi_0\rangle = \mathcal{N} \exp\left(-\sum_{i\in A}\sum_{j\in B} u_{ij} a_i^\dagger b_j^\dagger\right)|0\rangle \tag{13}$$

where (setting $\boldsymbol{R}_{ij} = \boldsymbol{R}_i - \boldsymbol{R}_j$)

$$u_{ij} = \frac{2}{N}\sum_{\boldsymbol{q}} \frac{1 - \omega_{\boldsymbol{q}}}{\gamma_{\boldsymbol{q}}} \cos(\boldsymbol{q}\cdot\boldsymbol{R}_{ij}). \tag{14}$$

To establish the connection with Marshall's theorems, we still need to bring $|\Psi_{SW}\rangle$ into the form of equation (2a). This is readily achieved by means of the series expansion of the exponential in (13) and subsequent multiplication of the whole series by the projection operator. We thus arrive at the final expression

$$|\Psi_{SW}\rangle = \mathcal{N}\sum_{n=0}^{\infty} (-1)^n |\chi_n\rangle \tag{15a}$$

where

$$|\chi_n\rangle = \frac{1}{n!}{\sum_{i_1\ldots i_n}}'{\sum_{j_1\ldots j_n}}' u_{i_1 j_1}\ldots u_{i_n j_n} a^\dagger_{i_1}\ldots a^\dagger_{i_n} b^\dagger_{j_1}\ldots b^\dagger_{j_n}|0\rangle \tag{15b}$$

with $|\chi_0\rangle \equiv |0\rangle$. Here the primes on the summation signs indicate that all $i_\nu \in A$ and all $j_\mu \in B$ must be different. The effect of P thus manifests itself merely in the restricted summations, whereby all unphysical configurations with more than one boson (spin deviation) per site are excluded. Each basis state in (15b) corresponds to a spin configuration $|\Phi_\alpha^{M=0}\rangle$ with n up-spins on sublattice A and the same number of down-spins on sublattice B. Hence, by denoting the summations in (15a, b) collectively as a single summmation over configurations α, $|\Psi_{SW}\rangle$ is expressed in the form of equation (2a) with $M = 0$. This establishes the desired connection between the expansions (2a) and (15) and enables us to answer the question as to the extent the SW ground state satisfies the Marshall theorems. The answer is given by the following:

Theorem: The spin-wave ground state $|\Psi_{SW}\rangle$ defined by equation (10) satisfies the Marshall sign criterion (2b) and is an eigenstate of S^z to the eigenvalue $M = 0$, but is *not* an eigenstate of $\boldsymbol{S}^2$.

Proof: To prove that the coefficients in (15) satisfy the Marshall sign criterion (2b), we start with the observation that the sign factors in (15a) and (2b) may be identified, since they are both determined by the number of up-spins on sublattice A. Thus it suffices to show that all u_{ij} in (15b) are positive definite. To prove this we use the power-series expansion of $\omega_{\boldsymbol{q}}$ and insert it into equation (14). The coefficient u_{ij} is then expressed as

$$u_{ij} = \sum_{n=1}^{\infty} \frac{4^{-n}}{2n-1}\binom{2n}{n} F_{ij}^{(2n-1)} \tag{16}$$

where

$$F_{ij}^{(2n-1)} = \frac{1}{N}\sum_{\boldsymbol{q}} \gamma_{\boldsymbol{q}}^{(2n-1)} \cos(\boldsymbol{q}\cdot\boldsymbol{R}_{ij}) \tag{17}$$

and the summation in (17) runs over the entire BZ. As the next step we use the binomial expansion of $\gamma_{\boldsymbol{q}}^{(2n-1)}$ which, after insertion into (17), leads to the expression

$$F_{ij}^{(2n-1)} = \frac{2}{4^n}\sum_{m=0}^{2n-1}\binom{2n-1}{m} I_{2n-m-1}(|X_{ij}|) I_m(|Y_{ij}|) \tag{18}$$

where X_{ij} and Y_{ij} are the components of $\boldsymbol{R}_{ij}$ and

$$I_m(r) = \frac{1}{\pi}\int_0^{\pi} dq\,(\cos q)^m \cos(rq). \tag{19}$$

This integral is tabulated [10] and one has

$$I_m(r) = 2^{-m}\binom{m}{k} \quad \text{for } m \geqslant r \text{ and } m - r = 2k \tag{20}$$

where $k = 0, 1, 2, \ldots$; in all other cases the integral vanishes. Upon substitution of this into (18) one finds that $F_{ij}^{(2n-1)} > 0$ for $2n - 1 \geqslant |X_{ij}| + |Y_{ij}|$ and equal to zero otherwise. Hence, $u_{ij} > 0$ because of (16), which proves the first part of our theorem.

To prove the remaining claims of the theorem, we first need to express S^z and $\boldsymbol{S}^2$ in terms of the boson operators a_i and b_j. Using relations (4) and (5) one readily finds that

$S^z = PM^z$, where $M^z = \sum_i a_i^\dagger a_i - \sum_j b_j^\dagger b_j$. By applying this to the SW ground state, equations (15), we find that

$$S^z|\Psi_{SW}\rangle = 0 \tag{21}$$

an obvious result that has already been used in the discussion preceding the theorem. To obtain $\boldsymbol{S}^2|\Psi_{SW}\rangle$ one proceeds in the same fashion. A somewhat lengthy but straightforward calculation gives the result

$$\boldsymbol{S}^2|\Psi_{SW}\rangle = -2\mathcal{N}\sum_{n=0}^{\infty}(-1)^n n|\chi_n\rangle \tag{22}$$

which clearly shows that $|\Psi_{SW}\rangle$ is not an eigenstate of $\boldsymbol{S}^2$. Equations (21) and (22) conclude the proof of our theorem.

The failure of $|\Psi_{SW}\rangle$ to satisfy the requirement (3) does not come as a surprise, since it is known that in SW theory the symmetry is broken from the outset. This is *not* in conflict with Marshall's second theorem, as a closer look reveals, since equation (3) holds on a *finite* lattice, whereas $|\Psi_{SW}\rangle$ is designed to describe the system in the *thermodynamic limit* where spontaneous symmetry breaking occurs. The way symmetry is broken in the HAF on the square lattice has been described in an illuminating paper by Horsch and von der Linden [11]. Using numerical techniques and analytic arguments the authors show that for an increasing number N of sites an excited triplet state comes down and becomes degenerate with the singlet ground state in the thermodynamic limit. This triplet state leads to spontaneous symmetry breaking at $T = 0$ K [12].

In summary, we have proved that the SW ground state of the HAF obeys the Marshall sign criterion, the sign factor being properly included in the Bogoliubov transformation. Hence, SW theory is not to be blamed for issues related to a possible failure of the quasi-particle description of holes in the $t - J$ model [6]. Moreover, we have shown that the SW ground state is an eigenstate of S^z to the eigenvalue $M = 0$, but is not an eigenstate of $\boldsymbol{S}^2$.

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