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Spin-Wave Results for the Staggered Magnetization of Triangular Heisenberg Antiferromagnet

Satoru J. MIYAKE

Department of Physics, Tokyo Institute of Technology, Oh-okayama, Meguro-ku, Tokyo 152

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The staggered magnetization of the Heisenberg antiferromagnet on triangular lattice is calculated by means of the usual spin-wave theory. The magnetization is derived from the ground-state energy as its derivative with respect to the staggered field, and given in a form of $1/S$ expansion, S being the magnitude of spins. The second-lowest correction, a term of $O(1/S)$, consists of two contributions; one from the first-order effect of four-boson terms in the Hamiltonian, and another from the second-order perturbation due to a three-boson term. Each contribution diverges when the exchange interaction is isotropic, but the divergent parts of the two contributions are found to cancel, leaving a finite result for the staggered magnetization to this order. Numerical result for the staggered magnetization is $S-0.2613+0.0055/S$.

[antiferromagnet, Heisenberg spin, triangular lattice, staggered magnetization, sublattice magnetization, spin wave, theory]

§1. Introduction

The ground state of the Heisenberg antiferromagnet on a triangular lattice has attracted much interest since Anderson's proposal of a resonance-valence-bond (RVB) state for this model.[1] Much work has been done to estimate the ground-state energy and to clarify whether the Néel-type long-range order exists or not in the ground state.[2-17] Although the energy seems favorable for the Néel-type state compared with RVB state, existence or non-existence of the Néel-type order is not clear.

Among various methods of study, the spin-wave theory has been used by many investigators.[4-8] In its conventional form, it starts from the assumption that the Néel-type order exists. Hence the theory looks useless to tell whether the order exists or not. But it tells something by testing self-consistency of the assumption. For example, the spin-wave theory gives a divergent staggered magnetization for a linear chain, suggesting that the existence of the Néel-type order is inconsistent and the order should vanish in this model. The absence of the order is in accord with the exact solution of the model.

Recently Tamaribuchi and Ishikawa[8] applied the spin-wave theory to the antiferromagnet on a triangular lattice using the Dyson-Maleev transformation. They calculated the sublattice magnetization up to the order of $1/S$, S being the magnitude of spins. To this order, there are two kinds of contribution. The one, which they calculated explicitly, was found divergent. They made a rough estimate of the other and concluded that the divergence was not cancelled. The estimate, however, is not quite convincing.

In a previous paper,[6] the present author calculated the ground-state energy of antiferromagnets with anisotropic exchange interaction, using the spin-wave theory. For the triangular lattice, a certain kind of singular behavior as a function of an anisotropy parameter, is observed at the isotropic point in each of two $O(S^0)$ terms. But the singularity is cancelled when the two terms are added. There is a close correspondence between the contribution to energy and that to sublattice magnetization. The singularity in energy corresponds to the divergence of sublattice magnetization mentioned above. Hence, it is natural to expect cancellation of divergence in the sublattice magnetization.

In the present paper, the ground-state

energy of anisotropic antiferromagnets on triangular lattice is calculated including a staggered magnetic field in the Hamiltonian. The staggered magnetization is obtained from the behavior of energy in the limit of zero staggered field.

§2. Energy and Staggered Magnetization

An anisotropic Heisenberg model considered in the present paper, is represented by the Hamiltonian

$$H=\sum_{\langle ij\rangle}[S_i^x S_j^x+S_i^y S_j^y+\varDelta S_i^z S_j^z],\quad (1\geqq\varDelta\geqq 0),\tag{1}$$

where S_i represents a spin located at site i, and the sum extends over all nearest neighbor pairs $\langle ij\rangle$. We have taken the exchange energy in the easy plane, which is assumed positive, as a unit of energy.

For a triangular lattice, the classical ground state takes a well-known 120° structure; the lattice is divided into three sublattices where the direction of spins on one sublattice differs by 120° from that on other sublattices. We add a staggered field term to the Hamiltonian above. Choosing the direction of classical orientation as a new S^z-axis for each spin and the direction of anisotropic exchange as a new S^y-axis, we have

$$\begin{aligned}H=-\sum_{\langle ij\rangle}\Big[&cS_i^z S_j^z+\frac{1}{4}(c+\varDelta)(S_i^+ S_j^+ +S_i^- S_j^-)+\frac{1}{4}(c-\varDelta)(S_i^+ S_j^- +S_i^- S_j^+)\\&-\sin(\phi_i-\phi_j)(S_i^x S_j^z-S_i^z S_j^x)\Big]-\sum_i S_i^z B.\end{aligned}\tag{2}$$

In the above, $c=|\cos(120°)|=1/2$, $S^{\pm}=S^x\pm iS^y$ and ϕ_i is the classical direction of the spin at site i referred to a certain fixed direction in the easy plane. The last term represents the effect of staggered field B. In the following, we calculate the ground-state energy as a function of B, the derivative of which gives the staggered magnetization in the limit $B\to 0$.

We introduce the Holstein-Primakoff transformation[18] of spin operators to boson operators b and $b^\dagger$ as

$$S^z=S-b^\dagger b,\tag{3a}$$

$$S^+=(2S-b^\dagger b)^{1/2}b,\tag{3b}$$

and S^- is given as the Hermite conjugate of S^+. We note that for the purpose of calculating the energy to the order of S^0, the Dyson-Maleev transformation[19-21] gives the same final result. Substituting eqs. (3a) and (3b) into eq. (2), and expanding eq. (2) in $1/S$, we obtain

$$H=-\frac{1}{2}NzS^2c(1+2h)+S[H_2+H_3+H_4+\cdots],\tag{4a}$$

$$H_2=c\sum_{\langle ij\rangle}\left[(1+h)(b_i^\dagger b_i+b_j^\dagger b_j)-\frac{1}{2}(1+\delta)(b_i^\dagger b_j^\dagger+b_i b_j)-\frac{1}{2}(1-\delta)(b_i^\dagger b_j+b_i^\dagger b_j)\right],\tag{4b}$$

$$H_3=(2S)^{-1/2}\sum_{\langle ij\rangle}(b_i^\dagger+b_i)\sin(\phi_i-\phi_j)\,n_j,\tag{4c}$$

$$\begin{aligned}H_4=\frac{c}{S}\sum_{\langle ij\rangle}\Big[&n_i n_j-\frac{1+\delta}{8}\{(n_i+n_j)b_i b_j+b_i^\dagger b_j^\dagger(n_i+n_j)\}\\&-\frac{1-\delta}{8}\{b_j^\dagger(n_i+n_j)b_i+b_i^\dagger(n_i+n_j)b_j\}\Big],\end{aligned}\tag{4d}$$

$$h=B/(zcS),\tag{4e}$$

$$\delta=\varDelta/c,\tag{4f}$$

where N is the number of lattice points, and z the number of the nearest neighbors.

The effect of kinematical interaction was examined in the previous paper.[6] Its contribution to the energy was shown to be of the form $\exp(-aS)$ $(a>0)$; it does not affect the asymptotic expansion of the energy in $1/S$. Hence, we have neglected the kinematical interaction.

The two-phonon part, H_2, is diagonalized by Fourier-transforming b_i's into b_k's, and then by applying the Bogoliubov transformation upon b_k and $b_k^\dagger$:

$$b_i=N^{-1/2}\sum_k b_k \exp(i\boldsymbol{k}\boldsymbol{r}_i), \tag{5a}$$

$$b_k=\alpha_k \cosh\theta_k+\alpha^\dagger_{-k}\sinh\theta_k, \tag{5b}$$

$$\tanh(2\theta_k)=\tanh(2\theta_{-k})=\frac{(1+\delta)\gamma_k}{2(1+h)-(1-\delta)\gamma_k}, \tag{5c}$$

$$\gamma_k=z^{-1}\sum_n \exp(i\boldsymbol{k}\boldsymbol{d}_n), \tag{5d}$$

where the $\boldsymbol{k}$-summation extends over the first Brillouin zone, and $\boldsymbol{d}_n$ represents the relative position of the nearest neighbors.

In this way we have

$$H_2=-\frac{1}{2}zc\sum_k[1-\nu_k]+zc\sum_k \nu_k\alpha_k^\dagger\alpha_k. \tag{6a}$$

$$\nu_k=[(1+h-\gamma_k)(1+h+\delta\gamma_k)]^{1/2}. \tag{6b}$$

The ground state is the vacuum for α_k's and its energy is given by the first term of eq. (6a).

In order to obtain the correction to the ground-state energy in ascending powers of $1/S$, we note that the order of H_3 and H_4 are, respectively, higher by $1/\sqrt{S}$ and $1/S$ than that of H_2, and that the expectation value of H_3 is zero in the ground state. Then the correction of order $1/S$ is given by two terms: the expectation value of H_4 and the second-order perturbation arising from H_3.

By virtue of Wick's theorem and by rewriting b_i and $b_i^\dagger$ in terms of α_k and $\alpha_k^\dagger$, we can easily evaluate the expectation value of H_4 as follows.

$$\langle H_4\rangle=-\frac{1}{2}NzcS^{-1}\left[u_0^2+u_1^2+v_1^2-(1+\delta)\left(u_0v_1+\frac{1}{2}u_1v_0\right)-(1-\delta)\left(u_0u_1+\frac{1}{2}v_0v_1\right)\right], \tag{7a}$$

$$u_0=\langle b_i^\dagger b_i\rangle=N^{-1}\sum_k\sinh^2\theta_k=\frac{1}{4}(A_1+A_2-2), \tag{7b}$$

$$u_1=\langle b_i^\dagger b_j\rangle=\langle b_ib_j^\dagger\rangle=N^{-1}\sum_k\gamma_k\sinh^2\theta_k=\frac{1}{4}(B_1+B_2), \tag{7c}$$

$$v_0=\langle b_ib_i\rangle=\langle b_i^\dagger b_i^\dagger\rangle=N^{-1}\sum_k\sinh\theta_k\cosh\theta_k=\frac{1}{4}(A_1-A_2), \tag{7d}$$

$$v_1=\langle b_ib_j\rangle=\langle b_i^\dagger b_j^\dagger\rangle=N^{-1}\sum_k\gamma_k\sinh\theta_k\cosh\theta_k=\frac{1}{4}(B_1-B_2), \tag{7e}$$

where j is one of i's nearest neighbors, and we have put

$$A_1\equiv N^{-1}\sum_k\exp(2\theta_k)=N^{-1}\sum_k[(1+h+\delta\gamma_k)/(1+h-\gamma_k)]^{1/2}, \tag{8a}$$

$$A_2\equiv N^{-1}\sum_k\exp(-2\theta_k)=N^{-1}\sum_k[(1+h-\gamma_k)/(1+h+\delta\gamma_k)]^{1/2}, \tag{8b}$$

$$B_1\equiv N^{-1}\sum_k\gamma_k\exp(2\theta_k), \tag{8c}$$

$$B_2\equiv N^{-1}\sum_k\gamma_k\exp(-2\theta_k), \tag{8d}$$

$$J_1\equiv N^{-1}\sum_k[(1+h-\gamma_k)(1+h+\delta\gamma_k)]^{1/2}=(1+h)A_1-B_1=(1+h)A_2+\delta B_2. \tag{8e}$$

Using these relations, we obtain

$$\langle H_4\rangle = -\{Nzc/(8S)\}\left[\left\{1-J_1+\frac{1}{2}h(A_1+A_2)\right\}^2+\frac{1}{2}(1-\delta^2)B_2^2 + h(1+h)\left\{\frac{1}{2}(A_1-A_2)\right\}^2\right], \tag{9a}$$

$$\lim_{h\to 0}\frac{\mathrm{d}\langle H_4\rangle}{\mathrm{d}h} = -\frac{Nzc}{8S}\lim_{h\to 0}\left[(1-\delta^2)B_2\frac{\mathrm{d}B_2}{\mathrm{d}h}+\left\{\frac{1}{2}(A_1-A_2)\right\}^2\right]. \tag{9b}$$

As pointed out by Tamaribuchi and Ishikawa,[8] when $\delta=2(\Delta=1)$ $\mathrm{d}B_2/\mathrm{d}h$ diverges as $h^{-1/2}$ in the limit $h\to 0$. This can be easily seen from the expressions for A_2 and B_2, eqs. (8b) and (8d). They contain a factor $(1+h+\delta\gamma_k)^{-1/2}$ which is divergent if $h=0$ and $\delta=2$ at $\boldsymbol{k}=\boldsymbol{Q}\equiv\frac{1}{3}(\boldsymbol{K}_1+\boldsymbol{K}_2)$. $\boldsymbol{K}_1$ and $\boldsymbol{K}_2$ are primitive vectors of the reciprocal lattice which are chosen to make an angle of 60° each other. At $\boldsymbol{k}=\boldsymbol{Q}$, γ_k takes its minimum value $-\frac{1}{2}$, and the integral from the neighborhood of the point is proportional to $(1-\Delta+h)^{1/2}$. Hence, it behaves as $(1-\Delta)^{1/2}$ when $h=0$, and as $h^{1/2}$ when $\Delta=1$. The former behavior is the singularity mentioned in Introduction. We note that a factor $(1+h-\gamma_k)^{-1/2}$, which is singular at $\boldsymbol{k}=0$, also gives $h^{1/2}$ term to A_1 and B_1 on integration in $\boldsymbol{k}$-space. A_1 and B_1 are, however, multiplied by h in eq. (9a) and do not give any $h^{1/2}$ term to $\langle H_4\rangle$.

Calculation of the second-order perturbation arising from the three-boson term, H_3, can be done in exactly the same way as in the previous paper.[6] Referring details of the calculation to ref. 6, we write down the final result for the ground-state energy, E_0, up to the order of $(1/S)^0$.

$$E_0 = -\frac{1}{2}NzcS\left[S(1+2h)+(1+h-J_1)+\frac{1}{4}(I_1+I_2)/S\right], \tag{10a}$$

$$I_1 = \left\{1-J_1+\frac{1}{2}h(A_1+A_2)\right\}^2+\frac{1}{2}(1-\delta^2)B_2^2+\frac{1}{4}h(1+h)(A_1-A_2)^2, \tag{10b}$$

$$I_2 = \frac{2}{3}(f/c)^2N^{-2}\sum_k\sum_q F(\boldsymbol{k},\boldsymbol{q})^2/(\nu_k+\nu_q+\nu_{k+q}), \tag{10c}$$

$$F(\boldsymbol{k},\boldsymbol{q}) \equiv \beta(\boldsymbol{k})\exp(\theta_k)\sinh(\theta_q+\theta_{k+q})+\beta(\boldsymbol{q})\exp(\theta_q)\sinh(\theta_k+\theta_{k+q}) - \beta(\boldsymbol{k}+\boldsymbol{q})\exp(\theta_{k+q})\sinh(\theta_k+\theta_q), \tag{10d}$$

$$\beta(\boldsymbol{k}) \equiv z^{-1}\sum_i \mathrm{sgn}\,[\sin(\phi_i-\phi_j)]\sin[\boldsymbol{k}(\boldsymbol{r}_i-\boldsymbol{r}_j)], \tag{10e}$$

$$f \equiv |\sin(\phi_i-\phi_j)|. \tag{10f}$$

In the above, I_2 is the contribution from the second-order perturbation of H_3, while I_1 comes from $\langle H_4\rangle$. We can see that there is also a singular term proportional to $(1-\Delta+h)^{1/2}$ in I_2, since the summand contains the factor $(1+h+\delta\gamma_k)^{-1/2}$. We can extract terms proportional to $(1-\Delta+h)^{1/2}$ from I_1 and I_2, whose multiplying constants will be denoted by D_1 and D_2, respectively. Details of the calculation are presented in Appendix. Results are as follows:

$$I_n(\Delta,h) = I_n(1,0)+D_n(1-\Delta+h)^{1/2}, \quad (n=1,2) \tag{11a}$$

$$D_1 = -[9/(\sqrt{2}\,\pi)]B_2(\Delta=1,h=0), \tag{11b}$$

$$D_2 = -[9/(\sqrt{2}\,\pi)]N^{-1}\sum_q g(\boldsymbol{q})^2/(\nu_q+\nu_{Q+q}). \tag{11c}$$

$$g(\boldsymbol{q}) = \beta(\boldsymbol{q})\exp(\theta_q-\theta_{Q+q})-\beta(\boldsymbol{Q}+\boldsymbol{q})\exp(\theta_{Q+q}-\theta_q). \tag{11d}$$

By numerical integration, the two constants are seen to cancel within the precision of numerical calculation ($\approx 10^{-9}$), i.e.,

$$D_1 = -0.9089361880\cdots, \tag{12a}$$

$$|(D_1+D_2)/D_1| < 2\times 10^{-10}. \tag{12b}$$

Thus it would be safe to say that the two singularities cancel that come from I_1 and I_2. As a result, the staggered magnetization, which is equal to the derivative of the energy with respect to the staggered field, is finite to the order calculated above even if the exchange is isotropic. We obtain

$$\begin{aligned}\langle S_i^z\rangle &= -\frac{1}{N}\lim_{B\to 0}\frac{\mathrm{d}E_0}{\mathrm{d}B} = -\frac{1}{NzcS}\lim_{h\to 0}\frac{\mathrm{d}E_0}{\mathrm{d}h}\\ &= S-\frac{1}{4}(A_1+A_2-2)+(8S)^{-1}\lim_{h\to 0}[\mathrm{d}(I_1+I_2)/\mathrm{d}h].\end{aligned} \tag{13}$$

The second term, which is equal to $-\langle b_i^\dagger b_i\rangle$, is well-known and its numerical value for the isotropic case ($=-0.2613\cdots$) is already reported.[7] In order to evaluate the third term, I_1+I_2 is numerically calculated for several values of h and then extrapolated to $h=0$. Expressing I_1+I_2 as a polynomial of $h^{1/2}$, we can check that the coefficient of $h^{1/2}$ is very small, and estimate the derivative from the coefficient of h. In this way, we obtain

$$\lim_{h\to 0}[\mathrm{d}(I_1+I_2)/\mathrm{d}h]=0.044\pm 0.001. \tag{14}$$

Hence the numerical result for the asymptotic expansion of the staggered magnetization in $1/S$ is recapitulated for the isotropic case as

$$\langle S_i^z\rangle = S-0.2613+0.0055/S. \tag{15}$$

§3. Summary and Discussion

The ground-state energy of antiferromagnet on a triangular lattice is calculated in the presence of staggered magnetic field. The energy is obtained in an asymptotic expansion in $1/S$ up to the order of $(1/S)^0$. The staggered magnetization is derived from the energy by differentiating it with respect to the field. Each term in the expansion of the energy in $1/S$ gives its corresponding term for the staggered magnetization. Hence, the magnetization is also expressed in a form of expansion in $1/S$: the leading term S, and the corrections of order $(1/S)^0$ and $1/S$. The correction of order $1/S$ consists of two terms; one from the four-boson interaction, and another from the second-order perturbation of the three-boson interaction peculiar to the triangular antiferromagnet.

The expression for the magnetization is found convergent to the order calculatetd here. This result contradicts Tamaribuchi and Ishikawa's conclusion that the magnetization is divergent.[8] Their conclusion was derived from the observation that each of two terms of order $1/S$ is divergent but the divergences differ in degree and fail to cancel. The investigation in the present paper shows that their estimate for the second term is too crude. Actually, when expressed as integrals in the wave number space, the two divergences come from factors of the same form and their degrees of divergence are the same. Moreover, the two coefficients of divergences turn out to cancel. This fact is anticipated from the behavior of the energy reported in a previous paper by the present author.[6] There, the expectation value of the four-boson interaction and the second-order perturbation of the three-boson interaction contribute to the term of $O(S^0)$. Both of them behave as $(1-\Delta)^{1/2}$ near the isotropic point ($\Delta=1$). But the numerical result appears to be regular at $\Delta=1$ when the two terms are added. In the present paper, the singularity in the presence of staggered field is found to be proportional to $(1-\Delta+h)^{1/2}$, whose coefficient is closely examined and shown to cancel to the precision of one part in 10^9. Hence, the cancellation of the singularities in the energy is confirmed, along with the cancellation of the divergences in the staggered magnetization.

Because of the cancellation of divergences, the staggered magnetization remains finite. Its numerical value is evaluated by calculating the energy as a function of staggered field. It is found that the correction of $O(1/S)$ is quite small. This result resembles that of the energy. When the exchange is isotropic, the energy is given as $-\frac{1}{2}NzcS(S+0.2184+0.0053/S)$. The second correction is very small compared with the first correction.

Appendix

The singular behavior of I_1 and I_2, eqs. (10b) and (10c), comes from the singularity of $(1+h+\delta\gamma_k)^{-1/2}$ at $\boldsymbol{k}=\boldsymbol{Q}=\frac{1}{3}(\boldsymbol{K}_1+\boldsymbol{K}_2)$, $\boldsymbol{K}_1$ and $\boldsymbol{K}_2$ being primitive vectors of the reciprocal lattice. The factor is contained in the summand of the expressions for A_2, B_2 and I_2. If we put $\boldsymbol{k}=\boldsymbol{Q}+\boldsymbol{\kappa}$ and set the lattice constant to unity, the singular factor becomes $(1+h-\varDelta-\frac{1}{4}\varDelta\boldsymbol{\kappa}^2)^{-1/2}$ for $\kappa\ll 1$.

Using the relation

$$\lim_{s\to 0}\,[\{(s^2+\boldsymbol{\kappa}^2)^{-1/2}-\kappa^{-1}\}/s]=-2\pi\delta^{(2)}(\boldsymbol{\kappa}), \tag{A·1}$$

where $\delta^{(2)}(\boldsymbol{\kappa})$ is a two-dimensional delta function, we can determine multiplying constants of $(1+h-\varDelta)^{1/2}$. They are calculated from the value at $\boldsymbol{k}=\boldsymbol{Q}$ of regular factors other than the singular factor $(1+h+\delta\gamma_k)^{-1/2}$. Results are as follows:

$$B_2(\varDelta, h)\approx B_2(1, 0)+[3/(\sqrt{2}\,\pi)](1+h-\varDelta)^{1/2}, \tag{A·2}$$

$$I_1(\varDelta, h)\approx I_1(1, 0)+D_1(1+h-\varDelta)^{1/2}, \tag{A·3}$$

$$D_1=-[9/(\sqrt{2}\,\pi)]\,B_2(1, 0). \tag{A·4}$$

$$I_2(\varDelta, h)\approx I_2(1, 0)+D_2(1+h-\varDelta)^{1/2}, \tag{A·5}$$

$$D_2=-[9/(\sqrt{2}\,\pi)]\sum_{q} g(\boldsymbol{q})^2/(\nu_q+\nu_{Q+q}), \tag{A·6}$$

$$g(\boldsymbol{q})=\beta(\boldsymbol{q})\exp(\theta_q-\theta_{Q+q})-\beta(\boldsymbol{Q}+\boldsymbol{q})\exp(\theta_{Q+q}-\theta_q). \tag{A·7}$$

In evaluating (A·2), we took into account the singularity of the summand at $\boldsymbol{k}=2\boldsymbol{Q}$ besides $\boldsymbol{Q}$. For I_2, singularities at $\boldsymbol{q}=\boldsymbol{Q}$, $2\boldsymbol{Q}$ and at $\boldsymbol{k}+\boldsymbol{q}=\boldsymbol{Q}$, $2\boldsymbol{Q}$ also contribute to (A·6) besides those at $\boldsymbol{k}=\boldsymbol{Q}$ and $2\boldsymbol{Q}$.

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