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The Quantum Ground State of a Heisenberg Ferromagnet with an "Easy-Plane" Type Anisotropy

A. A. Zvyagin[1] **and V. M. Tsukernik**[1]

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For the Heisenberg ferromagnet with the "easy-plane" type anisotropy the ground state energy and the magnetization are found with the help of perturbation theory supposing that the anisotropy energy is less than the exchange one. The study is carried out exactly without using any spin operators representation. Therefore, it is valid for a spin of any magnitude.

KEY WORDS: Uniaxial ferromagnet; ground state; susceptibility; critical words.

In a uniaxial ferromagnet with an "easy-plane" type anisotropy, situated in the longitudinal constant magnetic field, the projection of the total spin of the system along the chosen axis is conserved. That is why the stationary states can be classified by the magnitude of that projection. If the field is sufficiently high one, the ground state corresponds to the maximum projection of the total spin, and, therefore, to the maximum projections of each spin separately. In that case, the ground state can be found exactly.

If the field is less than the critical one defined by the anisotropy constant it is not so far possible to find an exact solution. However, if one can consider that the magnetic anisotropy energy in the typical ferromagnets is less than the exchange one, we can make use of perturbation theory.

In the present paper the ground state energy and the magnetization are calculated in the interval of fields less than the critical one without using any approximate representation of spin operators. The analogous system was considered in paper Ref. 1 using the Holstein–Primakoff representation. It turns out that the magnetization, as it must be, is the continuous one with the

[1] Institute for Low Temperature Physics and Engineering, UkrSSR Academy of Sciences, Kharkov, USSR.

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field critical value and that the magnetic susceptibility has a discontinuity. The results obtained in this paper concern the one-dimensional system as far as, first, in this case the calculations may be obviously brought to an end; second, the discontinuities of the magnetic characters are displayed most strongly there.

If the field is higher than the critical one, the ground state energy, calculated exactly, and the semiclassical one, which is found using the Holstein–Primakoff representation[2] coincide. In the interval of fields, less than the critical one, such coincidence, generally speaking, is not expected. It is found, still, that if a separate atom's spin $S \gg 1$, the quantum results turn into the semiclassical ones.

1. The Hamiltonian of the considered system has a form

$$\mathscr{H} = -2\mathscr{J} \sum_m \mathbf{S}_m \mathbf{S}_{m+1} + \frac{\beta}{2} \sum_m (S_m^z)^2 - 2\mu H \sum_m S_m^z \tag{1}$$

where $\mathbf{S}_m$ is the operator for the spin ($S \geqslant 1$) at the mth site, $\mathscr{J} > 0$ is the exchange integral for the nearest neighbors, β is the magnetic anisotropy constant (the positivity of β corresponds to the easy-plane case), μ is the magneton, and H is the external constant magnetic field.

As an unperturbed Hamiltonian $\mathscr{H}_0$ we choose the diagonal part of Hamiltonian (1) in the representation of the eigenfunctions of the exchange interaction treated to the definite magnitude of the total spin projection. The nondiagonal part in this representation is the perturbation V the contribution to which is given only by the energy of the anisotropy. Such choice of the unperturbed Hamiltonian permits us to consider the field of any strength.

The vector of the unperturbed ground state is the vector

$$|\psi_0\rangle = C(S^-)^n |0\rangle \tag{2}$$

Here, $S^- = S^x - iS^y$ is the cyclical total spin projection, $|0\rangle$ is the vector of the "ferromagnetic" state with the maximum magnitude of S^Z, equal to NS (N is the number of points), C is the normalization multiplier, and $n \geqslant 0$ is the integer number governing the magnitude of the total spin Z projection σ_n in the state $|\psi_0\rangle$:

$$\sigma_n = NS - n$$

Taking into consideration the perturbation, the ground state energy is determined as

$$E_0 = E_0^{(0)} + E_0^{(2)} + \cdots$$

Owing to such choice of perturbation, the correction $E_0^{(1)}$ is equal to zero, and the unperturbed energy is

$$E_0^{(0)} \equiv \langle\psi_0|\mathscr{H}_0|\psi_0\rangle = -2JS^2N - 2\mu HNS + \frac{\beta}{2}NS^2$$
$$-\frac{\beta}{2}\cdot\frac{(2S-1)}{(2NS-1)}\times\left[NS - \frac{2\mu H(2NS-1)}{\beta(2S-1)}\right]^2$$
$$+\frac{\beta(2S-1)}{2(2NS-1)}\left\{n - \left[NS - \frac{2\mu H(2NS-1)}{\beta(2S-1)}\right]\right\}^2 \quad (3)$$

The index n is chosen by the condition of the last term minimum in (3). Considering the integerness of n and neglecting here and further on the terms of the order of $(NS)^{-1}$, we have $n = n_0$ or $n = n_0 + 1$

$$n_0 = \left[NS\left(1 - \frac{4\mu H}{\beta(2S-1)}\right)\right] \quad (4)$$

depending on the magnetic field strength [square brackets in (4) mean the integral part]. As a result the last term in (3) becomes of the order of $(2NS)^{-1}$ and may be neglected. Note that in the zero-order approximation, the relative addition (proportional to β) as well as the value of n_0 has no exchange constant. Then the form of the wave function in the ground state is dictated precisely by the exchange interaction.

2. The dependence on the exchange constant appears in the next, second approximation of perturbation theory:

$$E_0^{(2)} = \sum_{j\neq 0}\frac{|\langle\psi_j|V|\psi_0\rangle|^2}{E_0^{(0)} - E_j^{(0)}} \quad (5)$$

Let us treat vector $|\psi_0\rangle$ with operator V to find the nonzero matrix elements which gives

$$V|\psi_0\rangle = \frac{\beta}{2}\frac{n(n-1)}{\langle 0|(S^+)^n(S^-)^n|0\rangle^{1/2}}(S^-)^{n-2}\sum_m (S_m^-)^2|0\rangle$$

One can see that vector $V|\psi_0\rangle$ is the linear combination of vectors, corresponding to the two-magnon excitations with the $(n-2)$ multiple "turned" total spin. The states of $j \neq 2$ magnons with the $(n-j)$ multiple "turned" spin have different energy, and, therefore, are orthogonal to $V|\psi_0\rangle$. On the other hand, the two-magnon states with the other multiplicity of total spin "turning," though having the same energy, differ by the value of σ_n, and are also orthogonal to $V|\psi_0\rangle$. As one can see from the form of the series of $V|\psi_0\rangle$, only two-magnon states with the zero total quasimomentum are making the contribution to energy. It is well known[3] that there are no bound states if the total quasimomentum is zero without the nondiagonal part of the anisotropy energy contribution.[2]

The wave function describing the continuous spectrum states is defined by the equation

$$|\psi_2\rangle = \sum_{l \leqslant m} A_{l,m} S_l^- S_m^- (S^-)^{n-2} |0\rangle \tag{6}$$

where the coefficients $A_{l,m}$, representing the wave function in the lattice site representation, satisfy the set of equations which follows from the Schrödinger equation with the unperturbed system Hamiltonian[4]:

$$\begin{aligned}
&-2\mathscr{J}S(A_{l-1,m} + A_{l+1,m} + A_{l,m-1} + A_{l,m+1}) \\
&\qquad + [8\mathscr{J}S - \beta(2S-1) + 4\mu H]\, A_{l,m} = \varepsilon A_{l,m}, \qquad l < m-1 \\
&-2\mathscr{J}S(A_{m-2,m} + A_{m-1,m+1}) - 2\mathscr{J}(2S-1)(A_{m-1,m-1} + A_{m,m}) \\
&\qquad + [2\mathscr{J}(4S-1) - (2S-1)\beta + 4\mu H]\, A_{m-1,m} = \varepsilon A_{m-1,m} \\
&-2\mathscr{J}S(A_{m-1,m} + A_{m,m+1}) + [8\mathscr{J}S - (2S-1)\beta + 4\mu H]\, A_{m,m} = \varepsilon A_{m,m}
\end{aligned}$$

Solving this set we find

$$\begin{aligned}
|\langle\psi_2| V |\psi_0\rangle|^2 &= \Delta^2 \frac{S^2 \sin^2 \kappa}{|(2S - e^{i\kappa}) \cos \kappa - (2S-1)\, e^{i\kappa}|^2}\, \delta_{K,0} \\
\Delta &= \frac{\beta}{2}(2S-1)\frac{n}{NS}\left(2 - \frac{n}{NS}\right)
\end{aligned} \tag{7}$$

where K is the summary quasimomentum and κ is the quasimomentum of the magnetons relative motion.

The energy $E_2^{(0)}$ in the denominator of Eq. (5) is found as a diagonal matrix element

$$E_2^{(0)} = \langle\psi_2|\mathscr{H}_0|\psi_2\rangle$$

During its calculation one must take into account that the operator of the exchange energy commutates with $(S^-)^n$ and $|\psi_2\rangle$ is the eigenvector of the Zeeman energy

$$-2\mu H \sum_m S_m^z |\psi_2\rangle = -(NS - n)\, 2\mu H\, |\psi_2\rangle$$

[2] We note that in the case of "easy-plane" type of anisotropy if $\beta \ll \mathscr{J}$, there are no bound two-magneton states either.

When calculating the diagonal matrix element of the magnetic anisotropy energy, one has to deal with the operator S^+S^- acting on the vector $|2\rangle$, which coincides with $|\psi_2\rangle$ as $n=2$. As far at $S^+S^-=\hat{S}^2-S_Z^2+S_Z$, the result is determined by treating $|2\rangle$ with the square total spin operator. One can make sure that

$$\hat{S}^2|2\rangle=\begin{cases}(NS-2)(NS-1)|2\rangle & \text{at} \quad K\neq\pm2\kappa\\ (NS-1)\cdot NS|2\rangle & \text{at} \quad K=2\kappa \text{ or } K=-2\kappa\\ NS(NS+1)|2\rangle & \text{at} \quad K=\kappa=0\end{cases}$$

In our case $K\neq 2\kappa$ ($K=0$ but $\kappa\neq 0$) that corresponds to the total spin equal to $NS-2$. Therefore, the following recurrent correlation takes place[3]:

$$(S^+)^\rho(S^-)^\rho|2\rangle=\rho[2NS-(\rho+3)](S^+)^{\rho-1}(S^-)^{\rho-1}|2\rangle$$

using which we find

$$E_2^{(0)}-E_0^{(0)}=8\mathcal{J}S\left(1-\cos\frac{K}{2}\cdot\cos\kappa\right)+\Delta \tag{8}$$

It is seen that the two-magnon state energy, existing with the $(n-2)$ multiple "turned" total spin, is separated from the energy of corresponding ground state by the gap depending on the magnetic field strength. With the critical magnitudes of the field determined from Eq. (4) by the conditions $n_0=0$ or $n_0=2NS$ this gap vanishes which as shown below causes the appearance of the magnetic susceptibility discontinuity. With the aid of (7) and (8) we obtain an expression for the second-order correction to the ground state energy

$$E_0^{(2)}=-\frac{N}{4\pi}\Delta^2S^2\int_{-\pi}^{\pi}\frac{\sin^2\kappa}{|(2S-e^{i\kappa})\cos\kappa-(2S-1)e^{i\kappa}|^2}\cdot\frac{d\kappa}{8\mathcal{J}S(1-\cos\kappa)+\Delta} \tag{9}$$

Calculating the integral by residue theory and taking into account the smallness of the ratio $\Delta/\mathcal{J}S$, we find

$$E_0^{(2)}=-\frac{N\Delta^2}{32\mathcal{J}S}\left[\frac{6S-1}{(2S-1)8S}-\left(\frac{\mathcal{J}S}{\Delta}\right)^{1/2}\right] \tag{10}$$

[3] Such correlation can be used to find the matrix element $\langle\psi_2|V|\psi_0\rangle$.

From Eqs. (3) and (10) one can obtain the magnetic momentum and the magnetic susceptibility at zero temperature

$$\Delta M = -\frac{N}{32\mathcal{J}S} \cdot \frac{(4\mu)^2 H}{\beta(2S-1)} \left[\frac{(6S-1)\Delta}{(2S-1)\,4S} + \frac{3}{2}(\mathcal{J}S\Delta)^{1/2}\right]$$

It is easy to see that at $H=0$ the magnetic momentum vanishes linearly with the field, and the susceptibility tends to the finite limit. When the field approaches its critical strength the addition containing the exchange constant tends to zero as $\sqrt{\Delta}$ and the magnetic momentum defined by the unperturbed ground state energy becomes nominal and equal to $2\mu NS$. As to the susceptibility, it has the form of

$$\Delta\chi|_{H\to H_{\rm cr}} = -\frac{N}{32\mathcal{J}S}(4\mu)^2 \cdot \frac{3}{4}(\mathcal{J}S)^{1/2} \cdot \frac{1}{[(1/2)\,\beta(2S-1)(1-H^2/H_{\rm cr}^2)]^{1/2}}$$

3. Let us compare the obtained results with the semiclassical consideration date, based on the Holstein–Primakoff representation for the spin operators.

That representation is used in the coordinate system turned about the initial one in which the Hamiltonian is defined by Eq. (1). The axes of the new system can be selected in such a way that the classical spin system energy with the same Hamiltonian should be the minimum one. Retaining, as usually, only the term squared in the Bose operators and diagonalizing the Hamiltonian with the aid of the Fourier transformation and the Bogolyubov linear uv transformation, we shall obtain

$$\mathcal{H} = E_0^{\rm cl} + \frac{1}{2}\sum_K (\varepsilon_K - A_K) + \sum_K \varepsilon_K b_K^+ b_K \tag{11}$$

where $E_0^{\rm cl}$ is the classical energy of the equilibrium spin configuration

$$A_K = 4\mathcal{J}S(1-\cos K) + B, \qquad \varepsilon_K = (A_K^2 - B^2)^{1/2}$$

$$B = \frac{\beta S}{2}\left[1 - \frac{(4\mu H)^2}{\beta^2(2S-1)^2}\right]$$

The second term in (11) is the quantum correction to the energy $E_0^{\rm cl}$. Hence the first two terms are the ground state energy of the system in a semiclassical approximation.

Using as above the smallness of the relative interaction in comparison to the exchange one, we shall expand the magnon energy ε_K by a small ratio B/A_K

$$\varepsilon_K \simeq A_K - \frac{1}{2}\frac{B^2}{A_K}$$

The condition of smallness is broken at K small enough $[K \sim (B/\mathcal{J}S)^{1/2}]$. However, the region of the small K is insignificant when calculating the macroscopic values. As a result, for the semiclassical correction to the ground state energy we obtain

$$E_0^{(2)\mathrm{cl}} = -\frac{B^2}{4} \cdot \frac{N}{2\pi} \int_{-\pi}^{\pi} \frac{dK}{4\mathcal{J}S(1-\cos K) + B} \simeq -\frac{NB^{3/2}}{8(2\mathcal{J}S)^{1/2}} \qquad (12)$$

Comparing (10) and (12) we see that the quantum correction (10) in addition to its nonanalytical dependence on Δ, contains a regular part, proportional to Δ^2. Accordingly, the magnetic susceptibility contains an H-independent addend. As to the singular parts of (10) and (12), they give the same field dependence, when substituting $2S-1$ with $2S$. In such a way, the main difference between the exact quantum result and the semiclassical one consists in the presence of the regular part which is essential far from the critical field strength. If $S \gg 1$ Eqs. (10) and (12) coincide. The next corrections of perturbation theory give the higher-order additions by the small ratio $\Delta/\mathcal{J}S$ than (10).

The considered one-dimensional system differs essentially from the three-dimensional one because the magneton density of states in the case of one dimension has a square root discontinuity causing to the integral divergence in (9) at $\Delta = 0$. In the three-dimensional case the integral at $\Delta = 0$ exists, so there are no singular terms in the correction $E_2^{(0)}$ and the corresponding integral can be calculated at $\Delta = 0$. As a result, the ground state energy has the following magnetic field dependence

$$\frac{E_0}{N} = -2z\mathcal{J}S^2 + \frac{\beta S}{4} - \frac{(2\mu H)^2 S}{\beta(2S-1)} + A\frac{\beta^2}{\mathcal{J}}\left[1 - \frac{(4\mu H)^2}{\beta^2(2S-1)^2}\right]$$

where z is the nearest-neighbors number and the multiplier A depends on S and is determined by the integral containing the wave function of two-magneton states. In the three-dimensional case, the explicit expression of that function is so far absent.

The susceptibility at the critical point of such system is finite and has a finite leap.

REFERENCES

1. A. V. Chubukov, *Zh. Eksp. Teor. Fiz.* **85** No. 4 (10):1319–1334 (1983) (in Russian).
2. A. I. Akhiezer, V. G. Bar'yakhtar, and S. V. Pebtminskii, *Spinovye volny (Spin Waves)* (Nauka, Moscow, 1967) (English translation, Wiley, New York, 1968).
3. H. Bethe, *Z. Phys.* **71**:205–226 (1931).
4. L. D. Filatova and V. M. Tsukernik, *Fiz. Nizk. Temp.* 7(11):1423–1429 (1981) [*Sov. J. Low Temp. Phys.* 7(11):689–692 (1981)].