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INFLUENCE OF UNIAXIAL AND BIAXIAL ANISOTROPY ON THE SPECTRUM IN SYSTEMS WITH BIQUADRATIC EXCHANGE

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Влияние одно- и двухосного кристаллического поля на спектр в системах с биквадратным обменом

Рассмотрены элементарные возбуждения в системах с биквадратным обменом, одно- и двухосной анизотропией.

Препринт Объединенного института ядерных исследований.
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Westwański B.

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Influence of Uniaxial and Biaxial Anisotropy on the Spectrum in Systems with Biquadratic Exchange

The spectrum of elementary excitations in systems with Heisenberg and biquadratic pair interactions, uniaxial and biaxial crystal fields and in an external magnetic field consists of 2S branches connected with changing the quantum magnetic number, S^z, by one, and $2S-1$ branches corresponding to $|\Delta S^z| = 2$. By applying the diagrammatic technique, the expressions for spectrum for $S=1$ are obtained.

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Dubna, 1974

The Heisenberg and biquadratic exchange pair interactions with an external magnetic field h, uniaxial D and biaxial E crystal fields are of special interest [1-4]

$$\mathcal{H} = \sum_i [-h S_i^z - D (S_i^z)^2 - \frac{1}{2} E ((S_i^-)^2 + (S_i^+)^2)] - \tag{1}$$

$$- \frac{1}{2} \sum_{i \neq j} [J_{ij} \vec{S}_i \vec{S}_j + K_{ij} (\vec{S}_i \vec{S}_j)^2],$$

This Hamiltonian has the following properties [3] (here we assume $S=1$): only thermodynamical averages

$$\langle S^z \rangle = m_z , \quad \langle (S^-)^2 + (S^+)^2 \rangle = q_2 , \quad \langle (S^z)^2 \rangle - \frac{2}{3} = q_0 \tag{2}$$

are different from zero. Therefore we select from (1) a self-consistent field (in contrast to [3], where molecular field was considered) as a function of order parameters (2) and include it into the zeroth-order Hamiltonian [4]

$$\mathcal{H}_0 = \sum_i \mathcal{H}_{0i} ; \quad \mathcal{H}_{0i} = -\bar{h} S_i^z - \bar{D} (S_i^z)^2 - \frac{1}{2} \bar{E} ((S_i^-)^2 + (S_i^+)^2) ;$$

$$\bar{h} = h + \alpha I m_z , \quad \bar{D} = D + 3 I q_0 , \quad \bar{E} = E + \frac{1}{2} I q_2 , \quad I = \frac{1}{2} \sum_i K_{ij} ,$$

$$(\alpha + 1) I = \sum_i J_{ij} . \tag{3}$$

Then the Hamiltonian (1) takes the form

$$\mathcal{H} = \mathcal{H}_0 + C + \mathcal{H}' , \tag{4}$$

where constant, C , and interaction, $\mathcal{H}'$, are given in /3–4/ . Under the unitary transformation, $U = \Pi U_i$, with U_i presented in /3/, the Hamiltonian (4) becomes as follows

$$H = C + H_0 + V\,;\; H_0 = \sum_i H_{0i}\,;\; H_{0i} = -\Delta Q^{13}_i - \bar{D} Q^{\overline{13}}_i;$$

$$\Delta^2 = \bar{h}^2 + \bar{E}^2,\; V = U^+\mathcal{H}'U = -\frac{1}{2}\sum_{i\neq j,\gamma\delta,\mu\nu} V^{+\,-}_{\gamma\delta,\mu\nu}(i,j)\, I^{\mu\nu}_i \overset{+}{I}{}^{\gamma\delta}_j, \quad (5)$$

where indices $\gamma\delta$ and $\mu\nu$ run over the set $\{12, 23, \overset{+}{1}2, 2\overset{+}{3}, 13, 1\overset{+}{3}, 1, 2\}$, $I^1 = \hat{Q}^{13}$, $I^2 = \hat{Q}^{\overline{13}}$, $I^{13} = \hat{S}^{13}$, $(\hat{A} = A - \langle A \rangle)$ $I^{\mu\nu} = S^{\mu\nu}$ $(\mu\nu = 12, 23)$ and Q^{13}, $Q^{\overline{13}}$, S^{13}, S^{12}, S^{23} are the spin one operators S^z, $(S^z)^2$, $(S^-)^2$, S^-S^z, $-S^zS^-$, respectively, in the new representation. The Fourier transform of the symmetric interaction (in /3/ this interaction contains the operators $\hat{A} = A - \langle A \rangle_0$, and is presented in nonsymmetric form) matrix $V^{+\,-}(\vec{k})$ (5) has the form of the simple product of two 4x4 matrices. Elements of the first of them, $V^{+}_{\gamma\delta,}{}^{-}_{\mu\nu}(\vec{k})$, connect the operators changing the magnetic quantum number, S^z, by unity and those of the second matrix connect the operators, changing the magnetic quantum number, S^z, by two, and diagonal operators /4/.

According to (5) we define the Green functions as follows

$$G^{-\;+}_{\mu\nu,\,\gamma\delta}(\tau - \tau', i - j) = \langle T I^{\mu\nu}_i(\tau)\, \overset{+}{I}{}^{\gamma\delta}_j(\tau') \rangle \quad (6)$$

The 8x8 matrix Green function $G^{-\,+}(\vec{k}, i\omega_n)$ with components (6) has the simple product structure analogous to described above interaction matrix $V^{+\,-}(\vec{k})$. The spectrum of elementary excitations is given by the poles of the analytic continuation , $i\omega_n \to \omega$, of the Green functions (6) and is obtained from the condition /3–5/

$$\det[1 - \Sigma^{-\,+}(\vec{k}, i\omega_n)\, V^{+\,-}(\vec{k})] = 0, \quad (7)$$

where $\Sigma^{-\,+}$ is irreducible polarization part of $G^{-\,+}$. In the zeroth-order approximation of the selfconsistent field method non-zero elements of the matrix $\Sigma^{-\,+}$ are given in /4/. Due to (7) and relations (9-10), (22-23) in /4/ the

first Green function subsystem (constructed from operators with $|\Delta S^z| = 1$) gives two branches of spin waves

$$\omega^2_{1,2}(\vec{k}) = \{\epsilon^2_1(\vec{k}) + \epsilon^2_2(\vec{k}) - [b(J_{\vec{k}} - K_{\vec{k}})\bar{E}/\Delta]^2 \pm \delta_{\vec{k}}\}/2:$$

$$\epsilon_{1,2}(\vec{k}) = \Delta - bJ_{\vec{k}}/2 \pm \gamma_{\vec{k}}\;;\; \gamma^2_{\vec{k}} = \bar{D}^2 + (bJ_{\vec{k}}/2)^2 -$$

$$- \bar{D}J_{\vec{k}}\lambda - (J_{\vec{k}} - K_{\vec{k}}/2)K_{\vec{k}}(b^2 - \lambda^2)/2; \quad (8).$$

$$\delta^2_{\vec{k}} = [\epsilon^2_1(\vec{k}) - \epsilon^2_2(\vec{k})]^2 - 2[b(J_{\vec{k}} - K_{\vec{k}})\bar{E}/\Delta]^2 \times$$

$$\times [\epsilon^2_1(\vec{k}) + \epsilon^2_2(\vec{k}) - 2(\Delta\lambda/b - \bar{D})^2] + [b(J_{\vec{k}} - K_{\vec{k}})\bar{E}/\Delta]^4 .$$

The second Green function subsystem (constructed from the operators with $|\Delta S^z| = 2$ and diagonal ones) gives one more branch of elementary excitations

$$\omega^2_3(\vec{k}) = 4\Delta\{\Delta - b[(1 + K_{\vec{k}}/2\Delta')(J_{\vec{k}} - K_{\vec{k}})(\bar{E}/\Delta)^2 +$$

$$+ K_{\vec{k}}(1 + K_{\vec{k}}/4\Delta')]\}\,;\; b = \langle Q^{13} \rangle_0,\; \lambda = 3\langle Q^{\overline{13}} \rangle_0 - 2,\; \Delta' = -\Delta/b, \quad (9)$$

The averages $\langle Q^{\mu\nu} \rangle_0$ over the zeroth-order Hamiltonian H_0 (5) are functions of the order parameters (2) and are given in /3–4/. The selfconsistent equations for these parameters have the form

$$m_z = \langle Q^{13} \rangle \bar{h}/\Delta - \langle S^{13} + \overset{+}{S}{}^{13} \rangle \bar{E}/2\Delta,\; q_0 = \langle Q^{\overline{13}} \rangle - \frac{2}{3},$$

$$q_2 = \langle Q^{13} \rangle 2\bar{E}/\Delta + \langle S^{13} + \overset{+}{S}{}^{13} \rangle \bar{h}/\Delta , \quad (10)$$

where $\langle Q^{13} \rangle$, $\langle S^{13} + \overset{+}{S}{}^{13} \rangle$, $\langle Q^{\overline{13}} \rangle$ are to be calculated using the diagrammatic technique /3,5/. In the zeroth-order approximation of the selfconsistent field method $\langle S^{13} + \overset{+}{S}{}^{13} \rangle_0 = 0$ and from (10) we get

$$m_z = b\bar{h}/\Delta,\quad q_2 = 2b\bar{E}/\Delta\; (\bar{h} q_2 = 2\bar{E} m_z),\; q_0 = \lambda/3 . \quad (11)$$

The solutions of the equations (11) together with the expressions (8-9) give the spectrum for $T \neq 0$ in the above approximation.

When $E \to 0$ the expressions for spectrum (8-9) take the form of those in /6/. In the limit $E \to 0$, $D \to 0$ the equations similar to (11) are given also in /2/ and are solved for $h = D = E = 0$; from these solutions /2/ for $T = 0$ it follows that the branch $\omega_1(\vec{k})$ is acoustic /6,7/ and $\omega_3(\vec{k})$ is also acoustic, if $J_{ij} = K_{ij}$. This result is due to the fact, that the total dipolar moment commutes with isotropic part of Hamiltonian (1) and the total quadrupolar moment has the same propetry, when $J_{ij} = K_{ij}$.

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