IMPURITY IN AN ANTIFERROMAGNETIC SUBSTANCE WITH ANISOTROPY OF THE EASY PLANE TYPE

V. A. KOLGANOV

Moscow Physico-technical Institute

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The dependence of the energy of an impurity virtual level in an antiferromagnetic with anisotropy of the easy plane type on the magnitude and orientation of the magnetic field is investigated. The investigation is performed for cases when damping is weak. Dzyaloshinskiĭ interaction is taken into account. The temperature dependence of the spin-system parameters is calculated in the molecular field approximation. The calculations are extended to a complex consisting of two impurity atoms and a linear defect.

1. Investigations of the impurity problem began with the theoretical papers of I. M. Lifshitz[1]. The singularities in the results of a number of recent experiments on magnetically ordered crystals[2-4] are due to the presence of impurities in the crystals. Numerous later theoretical investigations of the impurity problem[5-10] are based on the Green's-function method, which was first used by Wolfram and Callaway[5] to determine impurity spin states. This method calls for writing down the equation of motion for the Green's function in the node representation, reduction of these equations to the Dyson form by separating the perturbation, and representing the solution explicitly in terms of Green's functions, determined by numerical integration, of the unperturbed system and of the perturbation. It is customary to change over here from arbitrary spin operators to Bose operators[6-9], a changeover shown by Oguchi and Ono[10] to be incorrect when a system of localized magnons is considered. Nonetheless, numerical calculations of the spectrum, performed in this manner for $T = 0$ and $S \gg 1$, do not reflect the fact that the solution is incorrect, and are worthy of attention.

Investigations of ferromagnetic (FM) and antiferromagnetic (AFM) impurities in antiferromagnets, with allowance for single-ion anisotropy in the absence of a magnetic field H, were performed by Lovesey[9]. His numerical calculations of the spectrum can serve as a basis for the investigation of the case of arbitrary magnetic fields.

We consider in this paper single- and two-atom substitution impurities and a linear impurity defect. The purpose of the paper is to determine the energy of the local and quasilocal spin oscillations realized on the impurity atoms (the so-called s_0 oscillations) in the case when the influence of the impurity spin on the nearest non-impurity environment can be neglected, a case ensured by the condition

$$|J'|S_0 \ll (z-1)|J|S, \qquad (1)$$

where the exchange integral J corresponds to an interaction of the matrix spins with one another, J' corresponds to the interaction of the matrix spin with the impurity spin S_0, and z is the number of nearest neighbors.

An analysis of the numerical results obtained by Izyumov and Medvedev[6,11] for a point-like impurity in a ferromagnet at arbitrary H and by Lovesey[9] for a point-like impurity in an antiferromagnet in the case $H = 0$ shows that to calculate the energy of the s_0 oscillations under condition (1) the impurity defects can be regarded as an isolated system situated in a certain effective field H_{eff}, determined by the interaction of the impurity spins with the nearest impurity surrounding and the external magnetic field H. In the simplest case of a point-like defect, in the absence of single-ion anisotropy, the energy of the s_0 oscillations, or in other words the energy of a virtual impurity level of the s_0 type, has the following form:

$$\varepsilon_0 \approx \mu_B g_0 H_{eff}, \qquad (2)$$

where μ_B is the Bohr magneton and g_0 the g-factor of the impurity.

2. We consider first an antiferromagnet with a body-centered cubic structure and with a point-like AFM ($J' < 0$) substitution impurity at the site with $\mathbf{R} = 0$ (Fig. 1). We seek the ground state of the spin system in the case S, $S_0 \gg 1$ by using the two-sublattice model of an antiferromagnet with exchange interaction between the nearest neighbors.

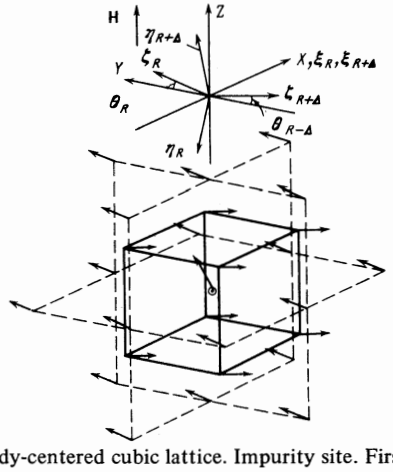

FIG. 1. Body-centered cubic lattice. Impurity site. First and second coordination spheres. Coordinate system.

The Hamiltonian of the system under consideration is written in the form

$$\mathcal{H} = -\sum_{\mathbf{R}_i\Delta} J^{(\Delta)}(\Delta)\mathbf{S}_{\mathbf{R}_i}\mathbf{S}_{\mathbf{R}_i+\Delta} - \mu_B \mathbf{H}\sum_{\mathbf{R}} g^{(\mathbf{R})}\mathbf{S}_{\mathbf{R}}, \tag{3}$$

where

$$J^{(\Delta)}(\Delta) = \begin{cases} J'(\Delta), \\ \text{if} \quad \mathbf{R}_1 = 0, \\ J(\Delta), \ \text{if} \\ \mathbf{R}_1 \neq 0 \neq \mathbf{R}_1 + \Delta. \end{cases}$$

The ground state of the spin system can be obtained by minimizing the eigenvalue of the Hamiltonian (3). To determine the parameters of the spin system at $T \neq 0$ we use the molecular field approximation. In the case of an AFM impurity, introducing the proper coordinate systems for each spin and choosing the axis $\zeta_{\mathbf{R}}$ along the direction of the spin $\mathbf{S}_{\mathbf{R}}$, we obtain in the zeroth approximation in $\mathbf{S}_{\mathbf{R}} - \langle \mathbf{S}_{\mathbf{R}} \rangle$[12] the following expression for the free energy

$$F^{(0)} = 2\sum_{\mathbf{R}_i\Delta} |J^{(\Delta)}| \langle S^{\zeta}_{\mathbf{R}_i}\rangle \langle S^{\zeta}_{\mathbf{R}_i+\Delta}\rangle \cos(\theta_{\mathbf{R}_i} + \theta_{\mathbf{R}_i+\Delta}) - \frac{2}{\beta}\sum_{\mathbf{R}} \ln \frac{\operatorname{sh}(S_{\mathbf{R}} + 1/2)\, y_{\mathbf{R}}}{\operatorname{sh}(y_{\mathbf{R}}/2)}, \tag{4}$$

where

$$y_{\mathbf{R}} = \beta\Big[\sum_{\Delta} |J^{(\Delta)}| \langle S^{\zeta}_{\mathbf{R}+\Delta}\rangle \cos(\theta_{\mathbf{R}} + \theta_{\mathbf{R}+\Delta}) + \mu_B g^{(\mathbf{R})} H \sin\theta_{\mathbf{R}}\Big],$$
$$J^{(\Delta)} = \frac{1}{z}\sum_{\Delta} J^{(\Delta)}(\Delta), \quad \beta = \frac{1}{T}. \tag{5}$$

We introduce the indices i = 0, 1, 2, ... for the impurity, first coordination sphere, second coordination sphere, etc., respectively. Minimizing $F^{(0)}$ with respect to $\langle S^{\zeta}_i \rangle$ and θ_i, we obtain

$$\langle S_0^{\zeta}\rangle = b_0(y_0), \quad \langle S_1^{\zeta}\rangle = b_1(y_1), \ldots,$$
$$z|J'|\langle S_1^{\zeta}\rangle \sin(\theta_0 + \theta_1) = \mu_B g_0 H \cos\theta_0, \tag{6}$$

$$|J'|\langle S_0^{\zeta}\rangle \sin(\theta_0 + \theta_1) + (z-1)|J|\langle S_2^{\zeta}\rangle \sin(\theta_1 + \theta_2) = \mu_B g_1 H \cos\theta_1 \tag{7}$$

etc., where

$$b_i(y_i) = (S_i + 1/2)\operatorname{cth}(S_i + 1/2)y_i - 1/2 \operatorname{cth} 1/2 y_i$$

is the Brillouin function.

Confining ourselves to a case amenable to an investigation, when the perturbation is localized in the first coordination sphere, we put $\theta_i \approx \theta$ for $i > 2$ and, using the condition (1), find the solution of the system (7):

$$\sin\theta = H/2H_E,$$
$$\cos\theta_1 \approx \approx \Big[1 + \frac{z}{(z-1)^2}\Big(\frac{H}{H_E}\Big)^2\Big]^{-1/2}\cos\theta,$$
$$\cos\theta_0 \approx \Big[1 + \Big(\frac{H}{H_E'}\Big)^2 - 2\Big(\frac{H}{H_E'}\Big)\sin\theta_1\Big]^{-1/2}\cos\theta_1, \tag{8}$$

where

$$H_E = \frac{z|J|\langle S^{\zeta}\rangle}{\mu_B g}, \quad H_E' = \frac{z|J'|\langle S_1^{\zeta}\rangle}{\mu_B g_0}. \tag{9}$$

Under the chosen condition, θ_1 does not depend on the perturbation parameters and ranges from 0.9θ to 1.0θ, whereas θ_0 can differ noticeably from θ (Fig. 2). We shall show that for the perturbation to the localized in the first coordination sphere it is necessary to have $\theta_1 \approx \theta$, which is satisfied, in particular, under the condition (1).

To this end, we introduce single-particle, say retarded, Green's functions in the node representation

$$G^{ij}_{r\rho}(t-t') = -i\Theta(t-t')\langle[S^{+}_{ri}(t), S^{-}_{\rho j}(t')]\rangle,$$
$$\tilde{G}^{ij}_{r\rho}(t-t') = -i\Theta(t-t')\langle[S^{-}_{ri}(t), S^{-}_{\rho j}(t')]\rangle, \tag{10}$$

where

$$\Theta(t-t') = \begin{cases} 1, & t' > t, \\ 0, & t' < t, \end{cases} \quad S^{\pm} = (S^{\xi} \pm iS^{\eta})/\sqrt{2},$$

ξ, η, and ζ are the axes of the proper coordinate systems of each spin. Transforming the Hamiltonian by changing over to the proper systems of the spins and recognizing that

$$G_{r\rho}(t-t') = \frac{1}{2\pi}\int_{-\infty}^{\infty} G_{r\rho}(\varepsilon)\exp[-i\varepsilon(t-t')]\,d\varepsilon, \tag{11}$$

we obtain ultimately the equations of motion

$$\varepsilon G^{11}_{0,\rho} = [S_0^{+}, S_{\rho}^{-}]\,\delta_{0\rho} + |J'|\sum_{\Delta}\Big[\frac{1-\cos(\theta_0+\theta_{0+\Delta})}{2}\langle S_0^{\zeta}\rangle G^{21}_{0+\Delta,\rho} + \frac{1+\cos(\theta_0+\theta_{0+\Delta})}{2}\langle S_0^{\zeta}\rangle \tilde{G}^{21}_{0+\Delta,\rho} + \cos(\theta_0+\theta_{0+\Delta})\langle S^{\zeta}_{0+\Delta}\rangle G^{11}_{0\rho} - \frac{i}{\sqrt{2}}\langle S^{\zeta}_{0+\Delta}\rangle\langle S_0^{\zeta}\rangle \sin(\theta_0+\theta_{0+\Delta})\Big] + \mu_B g_0 H \sin\theta_0 G^{11}_{0\rho},$$

$$\varepsilon G^{21}_{0+\Delta,\rho} = |J|\sum_{\delta}\Big[\frac{1-\cos(\theta_{0+\Delta+\delta}+\theta_{0+\Delta})}{2}\langle S^{\zeta}_{0+\Delta}\rangle G^{11}_{0+\Delta+\delta,\rho} + \frac{1+\cos(\theta_{0+\Delta+\delta}+\theta_{0+\Delta})}{2}\langle S^{\zeta}_{0+\Delta}\rangle \tilde{G}^{11}_{0+\Delta+\delta,\rho} + \cos(\theta_{0+\Delta+\delta}+\theta_{0+\Delta})\langle S^{\zeta}_{0+\Delta+\delta}\rangle \cdot G^{21}_{0+\Delta,\rho} - \frac{i}{\sqrt{2}}\langle S^{\zeta}_{0+\Delta+\delta}\rangle\langle S^{\zeta}_{0+\Delta}\rangle \sin(\theta_{0+\Delta+\delta}+\theta_{0+\Delta})\Big] + |J'|\Big[\frac{1-\cos(\theta_0+\theta_{0+\Delta})}{2}\langle S^{\zeta}_{0+\Delta}\rangle G^{11}_{0\rho} + \frac{1+\cos(\theta_0+\theta_{0+\Delta})}{2}\langle S^{\zeta}_{0+\Delta}\rangle \tilde{G}^{11}_{0\rho} + \cos(\theta_0+\theta_{0+\Delta})\langle S_0^{\zeta}\rangle G^{21}_{0+\Delta,\rho} + \frac{i}{\sqrt{2}}\langle S_0^{\zeta}\rangle\langle S^{\zeta}_{0+\Delta}\rangle \sin(\theta_0+\theta_{0+\Delta})\Big] + \mu_B g H \sin\theta_{0+\Delta} G^{21}_{0+\Delta,\rho}, \tag{12}$$

where the summation over δ denotes summation over the nearest neighbors of the site of the first coordination sphere belonging to the second coordination sphere.

The perturbation in the first coordination sphere can be separated if the coefficients of $G^{11}_{0+\Delta+\delta,\rho}$ and $\tilde{G}^{11}_{0+\Delta+\delta,\rho}$ in (12) do not contain the parameters of the perturbation, i.e.,

$$[1 \pm \cos(\theta_1 + \theta_2)]\langle S_1^{\zeta}\rangle \approx [1 \pm \cos 2\theta]\langle S^{\zeta}\rangle. \tag{13}$$

Investigation of the system (6) and condition (13) lead to a condition for the localizability of the perturbation

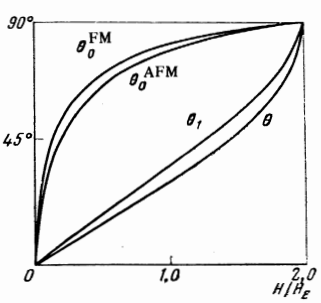

FIG. 2. Dependence of the angles θ_1 on the magnetic field for a body-centered cubic lattice.

in the first coordination sphere at arbitrary H:

$$|J'|\langle S_0^\zeta\rangle \lesssim 1{,}3|J|\langle S^\zeta\rangle. \qquad (14)$$

Allowance for the perturbation in the second coordination sphere leads to exceedingly cumbersome calculations (the number of atoms in the second coordination sphere is 18 at z = 8).

The limitation imposed on the perturbation parameters, with allowance for the fact that in the case of an AFM impurity the width $\delta\epsilon_0$ of the impurity level[9] becomes comparable with the energy ϵ_0 when $J'S_0 \sim JS$ (the impurity level then loses its distinguishing features), gives grounds for assuming that condition (1) determines the most interesting region of the values of the perturbation parameters J' and S_0.

The impurity-level energy is determined by the relation $\epsilon_0 \approx y_0/\beta$, from which we get when $J' < 0$, taking (5) into account,

$$\varepsilon_0 \approx \mu_B g_0[H_E' \cos(\theta_0+\theta_1) + H\sin\theta_0], \qquad (15)$$

where θ_0 and θ_1 are determined from (8).

In the case of an FM impurity we obtain for the energy of the impurity level (2) in place of (15)

$$\varepsilon_0 \approx \mu_B g_0[H_E' \cos(\theta_0-\theta_1) + H\sin\theta_0], \qquad (16)$$

where θ_0 and θ_1 are given by (8) with the sign of H_E' reversed.

When $H \ll H_E'$, formulas (15) and (16) can be represented, when account is taken of (8), in the form

$$\varepsilon_0 \approx \mu_B g_0\left[H_E' + \frac{1}{2}\left(\frac{1}{H_E'} \mp \frac{z+1}{z-1}\frac{1}{H_E}\right)H^2\right], \qquad (17)$$

where the upper sign corresponds to an AFM impurity.

When $H_E \gg H \gg H_E'$ we obtain $\epsilon_0 \approx \mu_B g_0 H$.

To calculate the temperature dependence of the impurity-level energy we note that the definitions of the exchange fields H_E and H_E'[9] contain the magnetizations of the matrix and impurity atoms. The temperature dependence of the magnetizations of all the atoms except the impurity atom is determined in the molecular-field approximation from the equation $\langle S^\zeta\rangle \approx b(y)$, with allowance for $y = y_{R>\Delta}$. The temperature dependence of the magnetization of the impurity atom, in view of the fact that y_0 does not depend on $\langle S_0^\zeta\rangle$, is determined by the formula $\langle S_0^\zeta\rangle = b_0(y_0)$. We note that Jaccarino, Walker, and Wertheim[13] obtained for an impurity in a ferromagnet, in the molecular-field approximation, a similar relation which has been experimentally confirmed in measurements performed by the nuclear magnetic resonance method on Mn nuclei dissolved in Fe[14].

3. The Hamiltonian of an antiferromagnet with an anisotropy of the "easy plane" type with an AFM impurity is given by

$$\begin{aligned}\mathcal{H} = {} & \sum_{R_i\Delta} |J(\Delta)|\,S_{R_i}S_{R_i+\Delta} + 2\sum_{R_i\Delta} D(\Delta)(S_{R_i}^z S_{R_i+\Delta}^y - S_{R_i}^y S_{R_i+\Delta}^z) \\ & + \sum_R P(S_R^x)^2 + \sum_{r,\,R\neq r} Q(\mathbf{R}-\mathbf{r})S_r^x S_R^x + \sum_\Delta |J'(\Delta)|\,S_0 S_{0+\Delta} \\ & + 2\sum_\Delta D'(\Delta)(S_0^z S_{0+\Delta}^y - S_0^y S_{0+\Delta}^z) + P_0(S_0^x)^2 \\ & + 2\sum_{R\neq 0} Q'(\mathbf{R}) S_0^x S_R^x - \mu_B \mathbf{H}\left(\sum_{R\neq 0} g S_R + g_0 S_0\right). \qquad (18)\end{aligned}$$

We introduce the angles θ_i between the spin S_i and the XY plane, φ_i between the projection of S_i on the XY plane and the Y axis, and ψ between H and the basal plane ZY.

From the minimum of the free energy in the molecular-field approximation, in analogy to the case of a body-centered cubic structure, we obtain the temperature dependence of the average spins in the form of Brillouin functions of the respectively more complicated arguments y_i and angles θ_i and φ_i under condition (1) and $\varphi_1 \approx \varphi$, $\theta_1 \approx \theta$.

Under condition (1), the interaction of the impurity spin with the nearest neighbors is taken into account by introducing an effective field. The energy of the impurity level is determined by the real part of the pole of the Green's function $G_{OR}^{11}(\epsilon)$ for the impurity spin, the system of equations for which at $\psi = 0$ and $P_0 > 0$ is of the form

$$\begin{aligned}&[\varepsilon - z|J'|\langle S_1^\zeta\rangle\cos(\theta_0+\theta_1) - 2zD'\langle S_1^\zeta\rangle\sin(\theta_0+\theta_1) - \mu_B g_0 H\sin\theta_0]G_{0,R}^{11} \\ &\quad = \text{const} + P_0\left[\left(\langle S_0^\zeta\rangle - \frac{1}{2}\right)G_{0R}^{11} + \frac{1}{2}\langle S_0^\zeta\rangle\tilde{G}_{0R}^{11}\right], \\ &[\varepsilon + z|J'|\langle S_1^\zeta\rangle\cos(\theta_0+\theta_1) + 2zD'\langle S_1^\zeta\rangle\sin(\theta_0+\theta_1) + \mu_B g_0 H\sin\theta_0]\tilde{G}_{0,R}^{11} \\ &\quad = \text{const} - P_0\left[\left(\langle S_0^\zeta\rangle - \frac{1}{2}\right)\tilde{G}_{0R}^{11} + \frac{1}{2}\langle S_0^\zeta\rangle G_{0R}^{11}\right]. \qquad (19)\end{aligned}$$

A. Case H = 0

We investigate the dependence of the angles φ_0 and φ_1 on the magnitude and sign of the anisotropy. From the conditions that the free energy $F^{(0)}$ be minimal we get

$$\begin{aligned}&\cos\varphi_0 \approx \left(1 + \frac{D'D}{J'J}\right)\left[\frac{(|J'|+2Q')^2\langle S_0^\zeta\rangle}{(z-1)JJ'\langle S^\zeta\rangle} - \frac{2P_0\langle S_0^\zeta\rangle}{z|J'|\langle S_1^\zeta\rangle}\right]^{-1}, \\ &\varphi_1 \approx -\frac{(|J'|+2Q')\langle S_0^\zeta\rangle}{(z-1)|J|\langle S^\zeta\rangle}\sin\varphi_0; \qquad (20) \\ &(1-\sin\varphi_0) \ll 1 \quad \text{for } P_0 < 0 \text{ и} \\ &2|P_0|\langle S_0^\zeta\rangle \gtrsim 3z|J'|\langle S_1^\zeta\rangle - \frac{z(|J'|+2Q')^2\langle S_1^\zeta\rangle\langle S_0^\zeta\rangle}{(z-1)|J|\langle S^\zeta\rangle}; \qquad (21)\end{aligned}$$

$\varphi_0 = 0$ at $P_0 > 0$ or

$$2|P_0|\langle S_0^\zeta\rangle < z|J'|\langle S_1^\zeta\rangle - \frac{z(|J'|+2Q')^2\langle S_1^\zeta\rangle\langle S_0^\zeta\rangle}{(z-1)|J|\langle S^\zeta\rangle}, \qquad (22)$$

in contrast to the usual

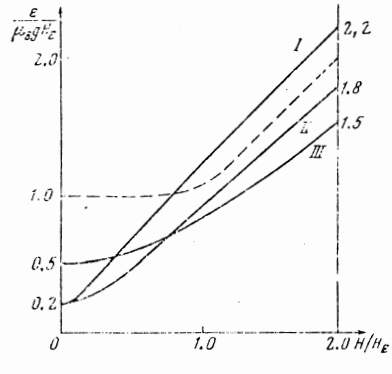

FIG. 3. Dependence of the energy of a virtual impurity level on the magnetic field for a body-centered cubic lattice in the case $g_0 = g$: I—FM impurity at $H_E' = 0.2H_E$, II—AFM impurity at $H_E' = 0.2H_E$, III—AFM impurity at $H_E' = 0.5H_E$. The accuracy with which ϵ is determined corresponds approximately to the accuracy with which the condition (1) is satisfied. The dashed curve is the upper limit of the spin-wave band. Under condition (1), local and quasilocal s_0 levels always exist for an FM impurity, but only a quasilocal level exists for an AFM impurity.

$$\varphi_{r_j}=(-1)^j\frac{\pi}{2} \text{ for } P-\sum_{\mathbf{R}\neq\mathbf{r}}Q(\mathbf{R}-\mathbf{r})<0,\quad j=1,2,$$
$$\varphi_r=0 \text{ for } P-\sum_{\mathbf{R}\neq\mathbf{r}}Q(\mathbf{R}-\mathbf{r})>0.$$

B. Case $(1-\sin\varphi_0)\ll 1$, $H\neq 0$

We shall investigate the dependence of the impurity-level energy on the field orientation for values of H such that all angles with the exception of φ_0 are small. No matter how the angle φ_0 varies, the expressions for θ, θ_1, φ, and φ_1 remain the same:

$$\theta\approx\frac{H+H_D}{2H_E},\quad \theta_1\approx\frac{H_D}{2H_E}+\frac{z+1}{z-1}\frac{H}{2H_E},$$
$$\varphi\approx\frac{H\psi}{2H_E},\quad \varphi_1\approx\frac{z+1}{z-1}\frac{H\psi}{2H_E}, \tag{23}$$

where $H_D = 2zD\langle S^\zeta\rangle/\mu_B g$.

For φ_0 and θ_0 at $H_D H_D' \ll H_E H_E'$, $H_3' \lesssim H_E'$, $H_2' \lesssim H_E'$, $H\psi \ll H_E'$ we obtain

$$\cos\varphi_0\approx|H_{10}|^{-1}\Big[H_E'+\Big(\psi-\frac{z+1}{z-1}\frac{H_D'}{2H_E}\Big)H\Big], \tag{24}$$

$$\theta_0\approx\frac{H_E'|H_{10}|}{H_E'^2+H_{10}^2}\Big[\frac{H_D}{2H_E}-\Big(\frac{1}{H_E'}-\frac{z+1}{z-1}\frac{1}{2H_E}\Big)H + \frac{H_D}{2H_E}\frac{H_E}{H_E'^2+H_{10}^2}\Big(1+\frac{z+1}{z-1}\frac{|H_{10}|}{2H_E}\Big)H\psi\Big], \tag{25}$$

where

$$H_D'=\frac{2zD'\langle S_1^\zeta\rangle}{\mu_B g_0},\quad H_{10}=\frac{2P_0\langle S_0^\zeta\rangle}{\mu_B g_0},$$
$$H_2'=\sum_{\Delta}\frac{2Q'(\Delta)\langle S_1^\zeta\rangle}{\mu_B g_0},\quad H_3'=\sum_{\mathbf{R}\neq 0,\,\Delta}\frac{2Q'(\mathbf{R})\langle S^\zeta\rangle}{\mu_B g_0}.$$

and $\theta_0<0$ in view of the smallness of H_D'.

We obtain the impurity-level energy in the form

$$\varepsilon_0\approx\mu_B g_0\sqrt{H_{\text{eff}}^2-H_{10}^2/16}, \tag{26}$$

where

$$H_{\text{eff}}\approx\frac{(H_E')^2}{|H_{10}|}-\frac{H_D}{2H_E}\frac{H_E'|H_{10}|}{(H_E')^2+H_{10}^2}H + \frac{|H_{10}|H_E'}{(H_E')^2+H_{10}^2}\Big(\frac{1}{H_E'}-\frac{z+1}{z-1}\frac{1}{2H_E}\Big)H^2 + \Big(1+\frac{H_E'}{|H_{10}|}-\frac{z+1}{z-1}\frac{H_E'}{2H_E}\Big)H\psi. \tag{27}$$

C. Case $|\varphi_0-\sin\varphi_0|\ll 1$, $H\neq 0$

In this case, for $H\ll H_E'$ and $\sin\psi\approx\psi$, we obtain the following expressions for the angles θ_0 and φ_0:

$$\theta_0\approx\Big(\frac{H_D'}{H_E'}-\frac{H_D}{2H_E}\Big)+\Big(\frac{1}{H_E'}-\frac{z+1}{z-1}\frac{1}{2H_E}\Big)H, \tag{28}$$
$$\varphi_0\approx H\psi/(H_E'+H_{10}). \tag{29}$$

The impurity level energy is determined by formula (26), where

$$H_{\text{eff}}\approx H_E'\Big[1+\frac{1}{2}\Big(\frac{H_D'}{H_E'}\Big)^2\Big]+\frac{1}{2}H_{10}+\Big(\frac{H_D'}{H_E'}-\frac{H_D}{2H_E}\Big)H + \frac{1}{2}\Big(\frac{1}{H_E'}-\frac{z+1}{z-1}\frac{1}{H_E}\Big)H^2+\frac{1}{2}\frac{H^2\psi^2}{H_E'+H_{10}}. \tag{30}$$

When $H_E \gg H \gg H_E'$ and $H^2\psi \ll H_E H_E'$, the dependence of the energy ϵ_0 on the field H is given by the following approximate formula

$$\varepsilon_0\approx\mu_B g_0\Big(\frac{1}{2}H_{10}+H\Big)\Big(1-\frac{\psi^2}{2}\Big). \tag{31}$$

4. It is of interest to investigate impurity complexes consisting of several impurity atoms. For a complex of two identical impurity atoms we set the constants J″, D″, and Q″ in correspondence with the interactions of the impurity spins with one another. In the case $J'<0$, $J''<0$, under condition (1), when the influence of the impurity spins on the spins of the first coordinations sphere can be neglected, we consider an isolated system of impurity spins, each of which is determined in the effective field by its interaction with the nearest environment and the external magnetic field. The validity of such an approach is based on the assumption that $J''S_0 \lesssim (z-2)J'S$. In the opposite case, it is necessary to assume the possibility of formation of a two-spin impurity molecule.

For the Green's functions of the system of impurity spins we obtain for $P_0-Q''>0$ and $\psi=0$ the following equations:

$$(\varepsilon-\varepsilon_{\vartheta\phi\phi})G_{0\mathbf{R}}^{11}=\text{const}+|J''|\langle S_0^\zeta\rangle[\sin^2\theta_0 G_{0+\Delta,\mathbf{R}}^{21}+\cos^2\theta_0\tilde{G}_{0+\Delta,\mathbf{R}}^{21}] + D''\langle S_0^\zeta\rangle\sin 2\theta_0[\tilde{G}_{0+\Delta,\mathbf{R}}^{21}-G_{0+\Delta,\mathbf{R}}^{21}]+Q''\langle S_0^\zeta\rangle[\tilde{G}_{0+\Delta,\mathbf{R}}^{21}+G_{0+\Delta,\mathbf{R}}^{21}] + P_0\Big[\Big(\langle S_0^\zeta\rangle-\frac{1}{2}\Big)G_{0\mathbf{R}}^{11}+\frac{1}{2}\langle S_0^\zeta\rangle\tilde{G}_{0\mathbf{R}}^{11}\Big] \tag{32}$$

(and analogously for G^{21} with the substitution $G^{11}\rightleftarrows G^{21}$, $\tilde{G}^{11}\rightleftarrows\tilde{G}^{21}$; for $\tilde{G}^{11}$ with the substitution $\epsilon\to-\epsilon$, $G^{11}\rightleftarrows G^{11}$, $G^{21}\rightleftarrows\tilde{G}^{21}$, and for $\tilde{G}^{21}$), where the angle θ_1 is determined for small values of θ_1 from the formulas (23) and

$$\varepsilon_{\vartheta\phi\phi}=\mu_B g_0\Big[\frac{z-1}{z}H_E'\cos(\theta_0+\theta_1)+\frac{1}{z}H_E''\cos 2\theta_0 + \frac{z-1}{z}H_D'\sin(\theta_0+\theta_1)+\frac{1}{z}H_D''\sin 2\theta_0+H\sin\theta_0\Big],$$
$$\theta_0\approx\frac{(z-1)H_D'+2H_D''-(z-1)H_E'(H_D/2H_E)+[z-(z+1)(H_E'/2H_E)]H}{(z-1)H_E'+4H_E''} \tag{33}$$

where

$$H_E''=\frac{z|J''|\langle S_0^\zeta\rangle}{\mu_B g_0},\quad H_D''=\frac{2zD''\langle S_0^\zeta\rangle}{\mu_B g_0}.$$

An analysis of the solution is made difficult by the abundance of constants, the choice of which is quite arbitrary. We therefore note the most significant prop-

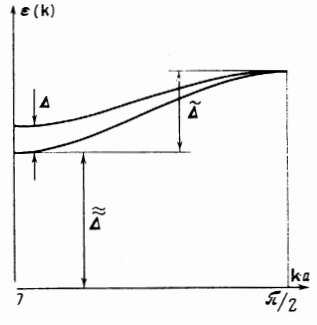

FIG. 4. Qualitative form of the spin-wave spectrum of a linear defect, $\tilde{\tilde{\Delta}}$ is determined approximately by formula (36).

erties of the two impurity levels that make up the solution of the system (32).

For H = 0, in the case when anisotropy can be neglected, the level energies are described by the expression

$$\varepsilon_{1,2} \approx \mu_B g_0 \frac{z-1}{z}\left[(H_E')^2 + \frac{2}{z-1} H_E' H_E''\right]^{1/2}. \quad (34)$$

The distance between the levels, neglecting the Dzyaloshinskiĭ interaction, was determined by the anisotropy, and when H = 0 and $P_0 - Q'' > 0$ it takes the form

$$\Delta_\varepsilon \approx \mu_B g_0 \frac{H_E''(H_{10} - 2H_2''/z) - 2(z-1)H_E' H_2''}{(z-1)\sqrt{H_E'^2 + 2H_E' H_E''/(z-1)}}, \quad (35)$$

where

$$H_2'' = 2zQ''\langle S_0^\xi\rangle / \mu_B g_0.$$

5. A natural generalization of the case of a two-atom impurity is, in particular, a linear defect whose axis coincides with the highest-order axis of the crystal, so that the impurity atoms are nearest neighbors. Unlike the two-atom impurity, a strong exchange coupling between the atoms with the defect is apparently permissible.

Use of translational symmetry along the defect axis makes it possible to solve the equations for the Green's function of the system of impurity spins in the case $J' < 0$, $J'' < 0$ under condition (1), when the influence of the impurity spins on the nearest non-impurity surrounding is negligibly small. Neglecting anisotropy we obtain at H = 0

$$\varepsilon_{1,2} \approx \mu_B g_0 \left[\left(\frac{z-2}{z}\right)^2 (H_E')^2 + 4\frac{z-2}{z^2} H_E' H_E'' + \frac{4}{z^2}(H_E'')^2 \sin^2 ka\right]^{1/2}, \quad (36)$$

where **k** is the wave vector of the spin wave propagating along the defect and a is the distance between the neighboring impurity atoms of the defect.

The distance between the impurity branches is determined by the anisotropy and has the following form at H = 0 and $P_0 - 2Q'' > 0$ in the absence of a Dzyaloshinskiĭ interaction:

$$\Delta_\varepsilon \approx \mu_B g_0 \frac{[H_E''(H_{10} - 8H_2''/z) - 2H_E' H_2''(z-2)/z]\cos ka}{[(z-2)^2(H_E')^2 + 4(z-2)H_E' H_E'' + 4(H_E'')^2 \sin^2 ka]^{1/2}}. \quad (37)$$

For the width of the impurity spin-wave band we obtain

$$\tilde{\Delta}_\varepsilon \approx \mu_B g_0 \frac{z-2}{z}\left[\left(H_E' + \frac{2}{z-2} H_E''\right) - \sqrt{(H_E')^2 + \frac{4}{z-2} H_E' H_E''}\right]. \quad (38)$$

The dependence on H agrees qualitatively with the case of a point-like defect.

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