SINGULARITIES IN THE STATE DENSITY OF QUASIPARTICLES IN A CRYSTAL

V. G. BAR'YAKHTAR, A. G. KVIRIKADZE, and V. A. POPOV

Physico-technical Institute, Ukrainian Academy of Sciences; Physico-technical Institute of Low Temperatures, Ukrainian Academy of Sciences

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We consider the state-density singularities connected with the fact that the quasiparticle effective masses become infinite near the faces of the Brillouin zone. We show that the state-density singularities $g(\omega)$ take the form $g(\omega) \sim |\omega|^{1/4}$ when one effective mass becomes infinite. A finite jump in $g(\omega)$ when $\omega = 0$ or a logarithmic singularity at $\omega = 0$, when two effective masses become infinite, and $g(\omega) \sim |\omega|^{-1/4}$ when three effective masses become infinite. The energies are reckoned from the critical value at which the topology of the surface $\epsilon(p, A) = \text{const}$ changes. By way of an example, we consider the density of states of a Heisenberg antiferromagnet in an external magnetic field. We calculate the values of the magnetic fields at which one, two, and three masses of the spin waves become infinite.

1. INTRODUCTION

It is well known that the density of states of the quasiparticles comes into play in a large number of thermodynamic and kinetic properties of crystals. For example, the cross section of inelastic incoherent scattering of slow neutrons in a crystal, accompanied by excitation of one phonon (or magnon), is proportional respectively to the density of states $g(\epsilon)$ of the phonons[1] (or magnons[2]). The coefficient of light absorption in a crystal, accompanied by excitation of two magnons or two phonons is also proportional to $g(\epsilon)$. Finally, the thermodynamic properties of metals in both the normal and in the superconducting state depend on the behavior of $g(\epsilon)$ at $\epsilon = \epsilon_F$, where ϵ_F is the electron Fermi energy. The possible manifestation of singularities of $g(\epsilon)$ in the thermodynamic and kinetic characteristics of a metal were apparently first pointed out by Jones[3]. It is therefore very important to investigate the general properties of the state density of quasiparticles in a crystal.

One of the most fundamental papers in this direction is one by Van-Hove[4], where it is shown, starting from general considerations of the translational symmetry of crystals, that there exist such values of the energy ϵ_q of a quasiparticle in a crystal, near which $g(\epsilon)$ has a singularity of the type $g(\epsilon) \approx g_{reg}(\epsilon) \pm B|\epsilon - \epsilon_q|^{1/2}$, where $g_{reg}(\epsilon)$ is continuous and has finite derivatives at $\epsilon = \epsilon_q$.

In an analysis of the properties of normal metals, I. Lifshitz[5] has shown that by applying external pressure (on the value of which the spectrum of the conduction electrons $\epsilon = \epsilon_e(p, P)$ obviously depends) it is possible to satisfy the condition $\epsilon_q = \epsilon_F$ when the singularities in the density of states are "taken out" on the Fermi surface, and this leads to anomalies in the dependence of the thermodynamic quantities and also of the galvanomagnetic characteristics on the pressure[5].

It was shown in[6-8] (theoretically and experimentally) that the Van-Hove singularities lead to a nonlinear dependence of the temperature of the superconducting transition on the pressure and the density of the impurities (acceptors or donors).

We consider in this paper the question of the singularities in the density of states of quasiparticles in a crystal, in the case when the quasiparticle spectrum $\epsilon(p, A)$ depends strongly on some external parameter A. In addition to the aforementioned pressure, such a parameter may be, for example, an external magnetic field for magnetically-ordered crystals and metals, or an external electric field for electrically-ordered dielectrics.

We shall show that at definite values of the external parameter $A = A_q$ there can appear in the density of states singularities of a new type, (for example, $g(\epsilon) = g_{reg}(\epsilon) + B|\epsilon - \epsilon_q|^{\pm 1/4}$). If the occurrence of the Van-Hove singularities is connected with the vanishing of the group velocity of the quasiparticle $v = (\partial\epsilon/\partial p) = 0$ at a certain $p = p_0$, then the singularities considered by us are connected with the fact that generally speaking one of the effective masses of the quasiparticle becomes infinite when $p = p_0$ and $A = A_q$. If the point $p = p_0$ coincides with one of the symmetrical points of the Brillouin cell, then it is possible to cause more than one of the effective masses to vanish with the aid of the external parameter.

It is clear from the foregoing that with the aid of an external pressure or a magnetic field (or some other external parameter) it is possible to exert a considerable influence on all the processes that depend on $g(\epsilon)$. In the case of metals, particular interest attaches to the case when the quasiparticle spectrum depends on two parameters. It is then possible to use one of them to bring the Van-Hove singularity to the Fermi surface, and to use the other to cause the effective mass to vanish[1)].

[1)]The joint action of impurities and pressure on a superconductor, considered in [7,8], cannot be a typical example of a two-parameter dependence of the quasiparticle spectrum, for in the main the impurities change the electron density in the metal, and have little effect on the electron spectrum.

2. SPECTRUM AND DENSITY OF STATES OF A QUASIPARTICLE NEAR THE SINGULAR POINTS

We consider a quasiparticle with a dispersion law $\epsilon = \epsilon(p, A)$, where p is the quasimomentum of the particle and A is an external parameter. By virtue of the periodicity $\epsilon(p, A) = \epsilon(p + b, A)$, where b is the reciprocal-lattice vector, there is always a value $p = p_0$ such that

$$(\partial \varepsilon / \partial \mathbf{p})_{\mathbf{p}=\mathbf{p}_0} = 0. \tag{2.1}$$

In particular, there are always points on the Brillouin-zone surface satisfying this condition.

Let us consider the spectrum of the quasiparticle at $p = p_0 + k$, $k \ll p_0$. Then

$$\begin{aligned}\varepsilon(\mathbf{p}_0 + \mathbf{k}, A) = \varepsilon(\mathbf{p}_0, A) + (k_1^2 / 2m_1) + (k_2^2 / 2m_2) \\ + (k_3^2 / 2m_3) + \psi(\mathbf{k}, A),\end{aligned} \tag{2.2}$$

where $\psi(k, A)$ tends to zero when $k \to 0$ no slower than k^3, and the effective masses $m_i = m_i(A)$ can be either positive or negative. On the other hand, if a symmetry axis passes through the point $p = p_0$, then two of the effective masses coincide (say $m_1 = m_2$); if the vicinity of the point $p = p_0$ has elements of cubic symmetry, then $m_1 = m_2 = m_3 = m(A)$.[2)]

Let us assume that the parameter A can be chosen such that one of the effective masses $m_1(A)$ becomes infinite, i.e.,

$$m_1^{-1}(A)\,|_{A=A_q} = 0. \tag{2.3}$$

Expanding $m_1^{-1}(A)$ near $A = A_q$, we obtain

$$\begin{aligned}\varepsilon(\mathbf{p}_0 + \mathbf{k}, A_q + a) = \varepsilon_q + \frac{1}{2} a k_1^2 \left(\frac{\partial}{\partial A} m_1^{-1}\right)_{A_q} \\ + (k_2^2/2m_2(A_q)) + (k_3^2/2m_3(A_q)) + \psi(\mathbf{k}, A_q),\end{aligned} \tag{2.4}$$

from which we readily obtain formulas similar to those of Van Hove

$$g(\varepsilon) = g_{\text{reg}}(\varepsilon) + \delta g(\varepsilon).$$

$$\delta g(\varepsilon) = \begin{cases} \mp \frac{1}{2} (m_2 m_3)^{1/2} \left(\frac{\partial}{\partial A} m_1^{-1}\right)_{A_q}^{-1/2} \left|\frac{\varepsilon_q - \varepsilon}{a}\right|^{1/2} \Theta(\varepsilon_q - \varepsilon) \\ \mp \frac{1}{2} (m_2 m_3)^{1/2} \left(\frac{\partial}{\partial A} m_1^{-1}\right)_{A_q}^{-1/2} \left|\frac{\varepsilon - \varepsilon_q}{a}\right|^{1/2} \Theta(\varepsilon - \varepsilon_q). \end{cases} \tag{2.5}$$

The upper line of the right-hand side of (2.5) pertains to the case when the closed constant-energy surface becomes open (with a minus sign) or when one of the cavities of the Fermi surface (with a plus sign) vanishes, while the lower line pertains to the opposite case; $\Theta(x) = 1$ if $x \geq 0$ and $\Theta(x) = 0$ if $x < 0$. We see from these formulas that at $a = A - A_q \to 0$ the singularity in the density of states becomes stronger and formally $\delta g(\epsilon, A)$ becomes infinite when $A = A_q$. The behavior of $\delta g(\epsilon, A)$ at $\epsilon \to \epsilon_q$ and $a \to 0$ depends on the manner in which ϵ approaches ϵ_q and a approaches zero. In order to investigate in greater detail the resultant $g(\epsilon, A)$ singularity at $A = A_q$, it is necessary to take into account the next higher terms of the expansion in $\mathbf{k}$ in formula (2.2), i.e., it is necessary to know the explicit form of the function ψ.

From the topological point of view, the singularities arise when the connectivity of the Fermi surface changes[5], namely, on going over from open Fermi surfaces to closed ones, or when a new cavity appears. Accordingly, we shall henceforth choose the simplest formulas, describing these topological changes, for the expansion of $\epsilon(p, A)$ near the critical point p_0.

1. Let us discuss first the case when one of the effective masses vanishes. A convenient expression for $\epsilon(p, A)$ and one sufficiently complete for the description of the possible types of the transitions, is[3)]

$$\varepsilon(\mathbf{p}, A_q) = \varepsilon_q + (k_1^2 / 2m_1) + (k_2^2 / 2m_2) + (\gamma k_3^4 / 4). \tag{2.6}$$

The density of states $g(\epsilon)$, as is well known, is defined by the formula

$$g(\omega) = \frac{g_0}{(2\pi)^3} \int d\mathbf{p}\, \delta(\omega - \varepsilon(\mathbf{p}, A_q) + \varepsilon_q) = \frac{g_0}{(2\pi)^3} \int\limits_{\varepsilon(\mathbf{p}, A_q) = \text{const}} \frac{ds}{v}, \tag{2.7}$$

where $\omega = \epsilon - \epsilon_q$, g_0 is the multiplicity of the degeneracy of the level with energy $\epsilon(p, A_q)$, and the volume of the system is assumed equal to unity, $v = |\nabla_p \epsilon(p, A_q)|$.

If the effective masses m_1 and m_2 and γ have the same sign, then

$$g(\omega) = \frac{g_0}{2\pi^2} (2m_1 m_2)^{1/2} \begin{cases} (\omega/\gamma)^{1/4} \Theta(\omega), & m_1,\ m_2,\ \gamma > 0; \\ (\omega/\gamma)^{1/4} \Theta(-\omega), & m_1,\ m_2,\ \gamma < 0. \end{cases} \tag{2.8}$$

The upper of these formulas describes the changes in the density of states upon formation of a new group of quasiparticles and the closed surface $\epsilon(p, A_q) = \text{const}$ corresponding to this group at $\omega > 0$, while the lower describes the changes upon formation of a new group of quasiparticles with $\omega < 0$.

If the effective masses m_1 and m_2 have the same sign, and the sign of γ is opposite to the sign of the effective masses, then a transition from closed surfaces $\epsilon(p, A_q) = \text{const}$ to open surfaces $\epsilon(p, A_q) = \text{const}$ takes place with changing sign of ω. The expression for $g(\omega)$ is in this case

$$g(\omega) = g_{\text{reg}}(\omega) - (g_0 / 2\pi^2)(2m_1 m_2)^{1/2} \begin{cases} (\omega/\gamma)^{1/4} \Theta(-\omega), & m_1,\ m_2 < 0,\ \gamma < 0, \\ (\omega/\gamma)^{1/4} \Theta(\omega), & m_1,\ m_2 < 0,\ \chi > 0. \end{cases} \tag{2.9}$$

The upper formula in (2.9) describes the changes in the density of states on going from a closed surface $\epsilon(p, A_q) = \text{const}$ when $\omega < 0$ to an open surface when $\omega > 0$. The lower formula of (2.9) describes the changes in $g(\omega)$ following a transition from a surface $\epsilon(p, A_q) = \text{const}$ that is open when $\omega < 0$ to a closed one when $\omega > 0$. (We do not present the expression for $g_{\text{reg}}(\omega)$, since its determination calls for a knowledge of the dispersion law $\epsilon(p, A_q)$ in the entire Brillouin zone, and not only near $p = p_0$.)

If the effective masses have opposite signs, then there is likewise a change in the topology of the surface $\epsilon(p, A_q)$, such as a transition from open surfaces to closed ones. (The open surface is oriented along the axis corresponding to the negative mass.) The changes in the density of state following such transitions are described by the formulas

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2)If the equal-energy surface $\epsilon(p, A) = \text{const}$ becomes tangent to one of the boundaries of the Brillouin zone at one point when the energy ϵ increases, then this will be a tangency in one of the symmetrical points of the Brillouin zone.

3)In this formula and from now on we use a system of units in which $\hbar = 1$.

$$g(\omega)=g_{\rm reg}(\omega)-$$
$$-Cg_0|m_1m_2|^{1/2}\begin{cases}(-\omega/\gamma)^{1/4}\Theta(-\omega), & m_1<0,\ m_2>0,\ \gamma>0;\\ (-\omega/\gamma)^{1/4}\Theta(\omega), & m_1<0,\ m_2>0,\ \gamma<0,\end{cases} \quad (2.10)$$

where

$$C=\frac{4\sqrt{2}}{(2\pi)^3}\Big[1-\frac{1}{2}\int_0^1\frac{dz}{\sqrt{1-z^4}}\int_0^1\frac{dt}{t^{3/2}}\frac{1-\sqrt[4]{1-t^2}}{\sqrt[4]{1-t^2}}\Big].$$

The upper of these formulas pertains to the case when the surface $\epsilon(p, A_q)$ const changes from an open one to a closed one on going from positive to negative ω, and the lower corresponds to the opposite case. We see from (2.8), (2.9), and (2.10) that in the case when one of the effective masses becomes infinite singularities of the type $\delta g(\omega) \sim |\omega|^{1/4}$ appear in the density of state when $|\omega| \ll \epsilon_q$.

2. We now proceed to consider the case when two of the effective masses become infinite. It is clear that this can occur if a symmetry axis, say of fourfold symmetry, passes through the point $p = p_0$. Therefore the expansion for $\epsilon(p, A_q)$ at $k \ll p_0$ takes the form

$$\varepsilon(\mathbf{p}_0+\mathbf{k}, A_q)=\varepsilon_q+(k_3^2/2m_3)+\gamma_1k_\perp^4+\gamma_2k_1^2k_2^2+\gamma_3k_3^2k_\perp^2, \quad (2.11)$$

where $k_\perp^2 = k_1^2 + k_2^2$ and the z axis coincides with the symmetry axis.

However, correct relations for the singularities in the density of states can be obtained also on the basis of simpler formulas for $\epsilon(p, A)$. Namely, in order to investigate the singularities of $g(\omega)$ upon occurrence (or vanishing) of a group of quasiparticles and of a corresponding closed surface $\epsilon(p, A_q) = \text{const}$ on going from $\omega < 0$ to $\omega > 0$, we can confine ourselves to the expression

$$\varepsilon(\mathbf{p}_0+\mathbf{k}, A_q)=\varepsilon_q+(k_3^2/2m_3)+\gamma_1k_\perp^4+\gamma_3k_3^2k_\perp^2. \quad (2.12)$$

Substituting this expansion for $\epsilon(p_0 + \mathbf{k}, A_q)$ in formula (2.7) and first integrating with respect to k_3 and then with respect to $k_\perp$, we obtain

$$g(\omega)=\frac{g_0}{4\pi}\Big(\frac{m_3}{2\gamma_1}\Big)^{1/2}\Big[1-\frac{4m_3\gamma_3}{\pi|\gamma_1|^{1/2}}\sqrt{|\omega|}\Big]\begin{cases}\Theta(\omega); & m_3,\gamma_1,\gamma_3>0\\ \Theta(-\omega); & m_3,\gamma_1,\gamma_3<0.\end{cases} \quad (2.13)$$

The upper of these formulas describes the occurrence of a group of quasiparticles at $\omega > 0$ and of the corresponding closed surface, and the lower describes the occurrence of a group of quasiparticles with $\omega < 0$.

To investigate the transitions from the open to the closed surfaces, we start from formula (2.11), in which we put $\gamma_2 = \gamma_3 = 0$. It is easy to verify that in this case

$$g(\omega)=g_{\rm reg}(\omega)-\frac{1}{8\pi^2}\Big(\frac{2|m_3|}{|\gamma_1|}\Big)^{1/2}\ln\Big|\frac{\omega}{\varepsilon'}\Big|^{1/2}; \quad (2.14)$$

when $m_3 > 0, \gamma_1 < 0$; when $m_3 < 0, \gamma_1 > 0, \epsilon'$ is a certain characteristic energy of the order of ϵ_q.

We see from (2.13) and (2.14) that in the case when two effective masses become infinite at the point $p = p_0$ (corresponding to a change in the topology of the surface $\epsilon(p, A_q) = \text{const}$), the density of states either changes jumpwise (see (2.13), or has a logarithmic singularity. We note that these singularities are stronger than those corresponding to the case when one of the effective masses becomes infinite.

3. Finally, let us consider the case when all three effective masses become infinite, so that there are not terms of second order of smallness in the expansion of $\epsilon(p_0 + \mathbf{k}, A_q)$ near $p = p_0$. With the aid of one external parameter it is possible to cause all three masses to vanish only if the point p_0 corresponds to a surrounding with cubic symmetry. In this case $\epsilon(p_0 + \mathbf{k}, A_q)$ can be represented in the form

$$\varepsilon(\mathbf{p}_0+\mathbf{k}, A_q)=\varepsilon_q+\gamma_1k^4+\gamma_2(k_1^2k_2^2+k_1^2k_3^2+k_2^2k_3^2) \quad (2.15)$$

in accordance with the fact that there are two invariants of fourth order relative to $\mathbf{k}$.

To investigate the singularities of $g(\omega)$ upon occurrence (vanishing) of a group of quasiparticles, it suffices to start from the expansion $\epsilon(p_0 + \mathbf{k}, A_q) = \epsilon_q + {}_1k^4$, i.e., to put $\gamma_2 = 0$. Integration with respect to $\mathbf{k}$ is trivial in this case, and we get

$$g(\omega)=(g_0)/(8\pi^2|\gamma_1|^{3/4}|\omega|^{1/4})\begin{cases}\Theta(\omega), & \gamma_1>0;\\ \Theta(-\omega), & \gamma_1<0.\end{cases} \quad (2.16)$$

The upper formula corresponds to the occurrence of a group of quasiparticles at $\omega > 0$, and the lower to $\omega < 0$.

To describe the transitions from open surfaces to closed ones following the reversal of the sign of ω, it is necessary to retain in (2.15) both terms. In this case, too, as shown by calculations, the singularities of $g(\omega)$ are of the form $\delta g(\omega) \sim |\omega|^{-1/4}$.

We see thus that the strongest singularities of $g(\omega)$ correspond to the case when three effective masses become infinite. The enhancement of the singularities of $g(\omega)$ can be represented schematically as follows: $\delta g(\omega) \sim |\omega|^{1/4}$, $m_1^{-1} = 0$; if $m_1^{-1} = m_2^{-2} = 0$, then $\delta g(\omega) \sim C\Theta(\omega)$ or $\ln|\omega$; if $m_1^{-1} = m_2^{-1} = m_3^{-1} = 0$, then $\delta g(\omega) \sim |\omega|^{-1/4}$.

We note that nowhere in the expansion of $\epsilon(p_0 + \mathbf{k}, A_q)$ near $p = p_0$ did we take into account the third-order terms. The reason is that we attempted to investigate the singularities of $g(\omega)$ following the occurrence of new closed surfaces $\epsilon(p, A_q) = \text{const}$ and following the transition from closed to open surfaces. The most general situation for the change of the topology of the surface $\epsilon(p, A_q) = \text{const}$ occurs when the point p_0 lies on one of the faces of the Brillouin zone, and then $\epsilon(p_0 + \mathbf{k}, A_q)$ is an even function of the deviations in the vicinity of $p = p_0$.

On the other hand, if the new closed surface is produced somewhere inside the Brillouin zone (such a situation occurs for conduction electrons in germanium and silicon, cf.[9,10]), then this surface is in general asymmetrical and to investigate the singularities in this case it is necessary to take into account third- and fourth-order terms. We shall not do this here, however.

3. DENSITY OF STATES OF SPIN WAVES IN ANTIFERROMAGNETS

In this section we consider the influence of an external magnetic field on the singularities in the density of states of spin waves in antiferromagnets. As will be shown below, the character of the singularities of $g(\omega)$ changes in fields on the order of the exchange field. We therefore discard beforehand, to simplify the calculation, all the interactions in the spin system, except the exchange interaction.

In this case the energy of the spin waves is[11]

$$\varepsilon_1^2(\mathbf{p}, H)=s^2[I(0)+I(\mathbf{p})+J(0)-J(\mathbf{p})][I(0)-I(\mathbf{p})+2I(\mathbf{p})\cos^2\theta+J(0)-J(\mathbf{p})],$$

$$\varepsilon_2^2(\mathbf{p}, H) = s^2[I(0) - I(p) + J(0) - J(p)][I(0) + I(p) - 2I(p)\cos^2\theta + J(0) - J(p)], \quad (3.1)$$

where

$$I(p) = \sum_m I(R_m)\exp(i\mathbf{p}\mathbf{R}_m), \quad J(p) = \sum_m J(R_m)\exp(i\mathbf{p}\mathbf{R}_m)$$

are the Fourier components of the exchange integrals between spins of different I(p) and identical J(p) sublattices, and $\cos\theta = (\mu H/sI(0))$. The first of these branches has activation at $p = 0$, and we shall call it "optical," while the second has no activation at $p = 0$, (acoustic branch).

To make the subsequent calculations concrete, we consider an antiferromagnet in which the structure of ordering of the magnetic moments in the absence of an external field is analogous to the structure of NaCl. The unit cell contains in this case two atoms with spin "up" and spin "down" and is the cell of the face-centered cubic lattice. Let the distance between two neighboring atoms with opposite spin orientation be a, and then we have in the nearest-neighbor approximation

$$I(\mathbf{p}) = 2I(\cos ap_1 + \cos ap_2 + \cos ap_3),$$
$$J(\mathbf{p}) = 4J(\cos ap_1\cos ap_2 + \cos ap_1\cos ap_3 + \cos ap_2\cos ap_3). \quad (3.2)$$

Using these formulas and (3.1), we can verify that the group velocities of the spin waves vanish at wave vectors corresponding to stars of six vectors p_{01} of the type $(\pi/a, 0, 0)$, $(0, \pi/a, 0)$ and $(0, 0, \pi/a)$. In addition, the group velocity of the optical branch vanishes at $p = 0$.

The star of wave vectors p_{01} represents wave vectors directed to the centers of the quadratic faces of the first Brillouin zone for an fcc lattice.

The expansions of $\epsilon_1(p, H)$ and $\epsilon_2(p, H)$ at p close to p_{01} are given by

$$\begin{aligned}\varepsilon_1^2(\mathbf{p}_{01} + \mathbf{k}, \mathbf{H}) &= \varepsilon_1^2(\mathbf{p}_{01}, \mathbf{H}) + \frac{\varepsilon_1(\mathbf{p}_{01}, \mathbf{H})}{m_{11}(H)}\left(x_1^2 - \frac{1}{12}x_1^4\right) + \frac{\varepsilon_1(\mathbf{p}_{01}, \mathbf{H})}{m_{12}(H)}\left(x_2^2 + x_3^2 - \frac{1}{12}x_2^4 - \frac{1}{12}x_3^4\right)\\ &+ s^2[4J + I(1 - 2\cos^2\theta)][4J - I]x_1^4 - (sI)^2(1 - 2\cos^2\theta)(x_2^2 + x_3^2)^2\\ &- 4s^2J[I\cos^2\theta + 3I + 8J]x_2^2x_3^2 + s^2[12IJ\cos^2\theta + 2I^2(1 - 2\cos^2\theta) + 4J(3I + 8J)]x_1^2(x_2^2 + x_3^2), \end{aligned} \quad (3.3)$$

$$\varepsilon_2^2(\mathbf{p}_{01} + \mathbf{k}, H) = \varepsilon_2^2(\mathbf{p}_{01}, H) + \frac{\varepsilon_2(\mathbf{p}_{01}, H)}{m_{21}(H)}x_1^2 + \frac{\varepsilon_2(\mathbf{p}_{01}, H)}{m_{22}(H)}(x_2^2 + x_3^2) + O(x^4),$$

where $x_i^2 = a^2k_i^2$,

$$\varepsilon_2^2(\mathbf{p}_{10}, H) = s^2[4I + 16J][8I + 16J - 4I\cos^2\theta],$$
$$\varepsilon_1^2(\mathbf{p}_{10}, H) = s^2[8I + 16J][4I + 16J + 4I\cos^2\theta],$$

and

$$\varepsilon_1(\mathbf{p}_{01}, H)m_{11}^{-1}(H) = -4s^2I(5I + 4J)\left[\frac{I^2 + 4J(3I + 8J)}{I(5I + 4J)} - \cos^2\theta\right],$$
$$\varepsilon_1(\mathbf{p}_{01}, H)m_{12}^{-1}(H) = 4s^2(5I + 8J)[I(5I + 8J)^{-1} - \cos^2\theta],$$
$$\varepsilon_2(\mathbf{p}_{02}, H)m_{21}^{-1}(H) = -4s^2[4J(3I + 8J) + I^2 + I(I + 4J)\cos^2\theta],$$
$$\varepsilon_2(\mathbf{p}_{01}, H)m_{22}^{-1}(H) = 4s^2I[I + (I + 8J)\cos^2\theta]. \quad (3.4)$$

We see therefore that $m_{21} < 0$ and $m_{22} > 0$ at any value of the magnetic field, and the effective masses m_{11} and m_{12} become infinite at magnetic field values H_1 and H_2, respectively,

$$\mu H_1 = 6sI\sqrt{\frac{I^2 + 4J(3I + 8J)}{I(5I + 4J)}}, \quad \mu H_2 = 6sI\sqrt{\frac{I}{5I + 8J}} \quad (3.5)$$

(we recall that I and J are positive, and note that the solution for H_1 exists if the corresponding radicand in (3.5) is smaller than unity). It is easy to verify that $H_1 > H_2$ and therefore $m_{11}(H) < 0$ and $m_{12}(H) > 0$ when $H < H_2$; when $H_2 \le H \le H_1$ both effective masses $m_{11}(H)$ and $m_{12}(H)$ are negative, and when $H > H_1$ we have $m_{11}(H) > 0$ and $m_{12}(H) < 0$.

To find the singularities of $g(\omega)$ at $H = H_2$ it suffices to use in lieu of (3.3) the expansion

$$\varepsilon_1^2(\mathbf{p}_{01} + \mathbf{k}, H_2) = \varepsilon_1^2(\mathbf{p}_{01}, H_2) + \frac{\varepsilon_1(\mathbf{p}_{01}, H_2)}{m_{11}(H_2)}x_1^2 - s^2I^2(1 - 2\cos^2\theta)\cdot(x_2^2 + x_3^2)^2 - 4s^2J(I\cos^2\theta + 3I + 8J)x_2^2x_3^2. \quad (3.6)$$

Since $m_1(H_2) < 0$ and $\cos^2\theta < 1/5$ at $H = H_2$, the negative values of the difference $\omega = \epsilon - \epsilon_1(p_{01}, H_2)$ corresponds to the closed surface $\epsilon_1(p, H_2) = \text{const}$ (there exists no surface $\epsilon_1(p, H_2) = \text{const}$ when ω is positive). In accordance with formula (2.13), the density of states $g(\omega)$ is proportional to $\theta(-\omega)$. Assuming that $I \gg J$, we get

$$g(\omega) \approx \frac{6}{4\pi a^3}\left(\frac{-m_{11}(H_2)\varepsilon_1(\mathbf{p}_{01}, H_2)}{0{,}6s^2I^2}\right)^{1/2}\Theta(-\omega). \quad (3.7)$$

If $H = H_1$, then the effective mass $m_{11}(H_1)$ vanishes, and we can calculate the singularities of the density of states $g(\omega)$ by starting from the formula

$$\varepsilon_1^2(\mathbf{p}_{01} + \mathbf{k}, H_1) = \varepsilon_1^2(\mathbf{p}_{01}, H_1) + \frac{\varepsilon_1(\mathbf{p}_{01}, H_1)}{m_{12}(H_1)}(x_2^2 + x_3^2) - 3s^2(I - 4J)^2(I + 4J)(5I + 4J)^{-1}x_1^4. \quad (3.8)$$

When $H = H_1$ the effective mass $m_{12}(H)$ is negative. Since the coefficient of x_1^4 is also negative, we deal in this case with the occurrence of a closed surface at small negative values of the difference $\omega = \epsilon - \epsilon_1(p_{01}, H_1)$. In accordance with (2.8), we have for the density of states

$$g(\omega) = \frac{6|m_{12}(H_1)|}{2\pi^2a^3}\left[\frac{8\varepsilon_1(\mathbf{p}_{01}, H_1)(5I + 4J)}{3(I - 4J)^2(I + 4J)s^2}\right]^{1/4}(-\omega)^{1/4}\Theta(-\omega). \quad (3.9)$$

Formulas (3.7) and (3.9) describe the density-of-states singularities connected with the spin-wave branch $\epsilon_1(p, H)$ at $H = H_1$ or $H = H_2$ and at energies close to $\epsilon_1(p_{01}, H_1)$ or $\epsilon_1(p_{01}, H_2)$. On the other hand, if we consider $g(\omega)$ at $\omega = |\epsilon - \epsilon_2(p_{01}, H)| \ll \epsilon_2(p_{01}, H)$, then $g(\omega)$ has Van-Hove singularities.

We proceed now to consider $g(\omega)$ at energies corresponding to small wave vectors. The expansions for $\epsilon_1(p, H)$ and $\epsilon_2(p, H)$ have at small p the form

$$\begin{aligned}\varepsilon_1^2(\mathbf{p}, H) &= (12sI\cos\theta)^2 + 12s^2I(3I - 4J)\left[\frac{I + 4J}{3I - 4J} - \cos^2\theta\right](ap)^2\\ &- s^2[6IJ + I^2 - (4J)^2 + 2I(7J - I)\cos^2\theta](ap)^4\\ &+ s^2[(3I + 2J)\cos^2\theta - I + 2J]Ia^4(p_1^4 + p_2^4 + p_3^4), \end{aligned}\quad (3.10)$$
$$\varepsilon_2^2(\mathbf{p}, H) = s^2(I + 4J)[12I\sin^2\theta - (I - 4J - 2I\cos^2\theta)(ap)^2](ap)^2.$$

We see from these formulas that the effective masses in $\epsilon_1(p, H)$ become infinite at $H = H_1^*$

$$\mu H_1^* = 6sI[(I + 4J)/(3I - 4J)]^{1/2}, \quad (3.11)$$

and the dispersion law of the second of the branches changes from linear to quadratic in a field $H = H_2^*$,

$$\mu H_2^* = 6sI. \quad (3.12)$$

(It follows from (3.11) that the effective masses in $\epsilon_1(p, H)$ can become infinite when the magnetic field changes only if $I > 4J$.)

Let us consider first the singularities in the density of states at $H = H_1^*$. These singularities are connected with the branch $\epsilon_1(p, H)$, which can be represented in the form

$$\varepsilon_1^2(\mathbf{p}, H_1^*) = \varepsilon_1^2(0, H_1^*) + \frac{24s^2I^2J}{3I-4J}a^4(p_1^4+p_2^4+p_3^4) - \frac{s^2}{3I-4J}[(I+4J)^2 - 4I(4J)^2](ap)^4. \quad (3.13)$$

The character of the topological transition for the constant-energy surface at $|\omega| = |\epsilon - \epsilon_1(0, H_1^*)| \ll \epsilon_1(0, H_1^*)$ depends on the ratio of the exchange integrals I and J. Let us consider the limiting case $I \gg J$. If $I \gg J$, then

$$\varepsilon_1^2(\mathbf{p}, H_1^*) \approx (4sI)^2 - {}^1/_3 s^2I^2(ap)^4.$$

In this case there is formed at negative ω a spherical surface of constant energy with radius $\sim\omega^{1/4}$ [12], and

$$g(\omega) \approx \frac{g_0}{8\pi^2a^3}\left(\frac{24}{sI}\right)^{3/4}(-\omega)^{-1/4}\Theta(-\omega). \quad (3.14)$$

Let us examine now the state-density singularities connected with the spin-wave branch $\epsilon_2(p, H)$ at $H = H_2^*$. In this case

$$\varepsilon_2(\mathbf{p}, H_2^*) \approx s(I+4J)(ap)^2 \quad (3.15)$$

and

$$g(\omega) = \frac{g_0}{4\pi^2a^3}[s(I+4J)]^{-3/2}\sqrt{\omega}\,\Theta(\omega).$$

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