Effect of magnetic ordering on interband transitions of electrons in crystals

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The temperature behavior of threshold singularities of the high frequency conductivity of magnetic crystals is investigated. It is shown that in ferromagnets and antiferromagnets with two magnetic ions per unit cell the shift and the smearing of these singularities near the transition point T_c are of a critical nature, i.e., they are proportional to $(T-T_c)^{-x}$, and the exponent x depends both on the type of the singular point of the spectrum and on the magnitude of the critical exponent of the correlator of the angular momenta. Similar anomalies also occur in the refractive index.

Optical properties of crystals are determined to a large extent by interband transitions which depend to a significant extent both on the spectrum of Bloch electrons and on electron interactions (among themselves, with phonons, etc.)[1,2]. The interaction of electrons with a magnetic system leads to a change in their spectra[3] and to additional scattering[4,5] by the fluctuations of the magnetic moment.

In the present paper we consider the manner in which the ferro- or antiferromagnetic ordering and the large scale fluctuations near the Curie (Neel) temperature[1)] T_c affect the Van Hove singularities in the frequency dependence of the electrical conductivity tensor. These singularities appear as the result of singular points of interband or intraband spectral densities[2,6]. The interaction with the spin system splits, shifts and smears out such singularities. The temperature dependence of these changes in the spectrum has anomalies at the Curie point.

1. CHOICE OF MODEL

We consider a system of conduction electrons in a crystalline lattice which undergo interband transitions under the action of the electric field of a light wave. These electrons interact with the system of spins $\mathbf{S}_n$ localized at the sites $\mathbf{r}_n$ of the lattice. Such a model corresponds well to f-metals.

We describe the electron transitions by introducing the single-particle density matrix

$$\rho_{p's',ps}(t)=\langle a^{+}_{p's'}(t)a_{ps}(t)\rangle. \tag{1}$$

Here $a^{+}_{ps}(t)$ and $a_{ps}(t)$ are the Heisenberg creation and annihilation operators for a Bloch electron in a state characterized by a quasimomentum $\mathbf{p}$ and spin $s = \pm 1/2$. Just as in the paper by Kopeliovich[1], in the present problem it is also convenient to utilize the "expanded band" scheme. In such a scheme the quasimomentum vector $\mathbf{p}$ varies over the whole reciprocal space, while an interband transition is a transition in $\mathbf{p}$-space with a change of the quasimomentum into some other vector of the reciprocal lattice $\mathbf{g}$.

We write the complete Hamiltonian for the system in the form

$$H=H_0+H_n+H_{sf}+H', \quad H_0=\sum_{p,s}\xi_p a^{+}_{ps}a_{ps}, \tag{2}$$

where $\xi_p = \epsilon(\mathbf{p}) - \mu_0$ is the excitation energy of a conduction electron, $\epsilon(\mathbf{p})$ is the dispersion law, μ_0 is the chemical potential. The Hamiltonian for the interaction with the electromagnetic field is

$$H_n=-\frac{e}{c}\mathbf{A}\sum_{p_1,p_2,s}\mathbf{v}_{p_1p_2}a^{+}_{p_1s}a_{p_2s}, \quad \mathbf{A}=\frac{ic}{\omega}\mathbf{E}=\frac{ic}{\omega}\mathbf{E}_0e^{i\omega t}.$$

Here the matrix elements of the velocity $\mathbf{v}_{p_1p_2}$ differ from zero under the condition $\mathbf{p}_1 - \mathbf{p}_2 = \mathbf{g}$, $\mathbf{E}$ is the intensity of the electric field in a wave of frequency ω.

The Hamiltonian H_{sf} describes the exchange interaction between the subsystems of unlocalized conduction s-electrons and magnetic f-electrons localized at the sites of the lattice, and has the form[7]

$$H_{sf}=\sum_{\mathbf{p},\mathbf{p}',n}J_n(\mathbf{p},\mathbf{p}')\{(a^{+}_{p+}a_{p'+}-a^{+}_{p-}a_{p'-})S_n^{z}+a^{+}_{p+}a_{p'-}S_n^{-}+a^{+}_{p-}a_{p'+}S_n^{+}\},$$
$$J_n(\mathbf{p},\mathbf{p}')=-(1/N)\exp[i(\mathbf{p}'-\mathbf{p})\mathbf{r}_n]J(\mathbf{p},\mathbf{p}'). \tag{3}$$

Here the sum over n is taken over all the N lattice points, the components of the spin operator S^z, $S^{\pm} = S^x \pm iS^y$ satisfy the well-known commutation relation[7], while the quasimomenta $\mathbf{p}$ and $\mathbf{p}'$ take on all values in reciprocal space. The quantity $J(\mathbf{p}, \mathbf{p}')$ determines the energy of the exchange interaction. The ratio J/ϵ_0, where ϵ_0 is the characteristic band energy, is a small parameter. As a result of H_{sf} a splitting and a shift of energies $\Delta\xi^{\pm}$ as well as a damping $\Delta\gamma$ appear, which will be the subject of our investigation. On the other hand, H_{sf} leads to an indirect spin exchange between the spins of the f-system and to magnetic ordering.

We include in the term H' the remaining (Coulomb) interaction of electrons with each other, and also the interaction of electrons with phonons. The effect of these interactions on the interband transitions has been examined in detail by Kopeliovich in[1] where it was shown that such interactions lead to a renormalization of the spectrum $\Delta\xi_0$ and to an effective damping of electron states $\gamma_0 \sim \hbar/\tau_0$, where τ_0 is the lifetime of an excitation of the type electron-hole which appears as a result of photon absorption. Generally speaking, $\Delta\xi_0$ and γ_0 are of the same order as the analogous quantities $\Delta\xi^{\pm}$ and $\Delta\gamma$ associated with the exchange interaction. But in the principal approximation $\Delta\xi_0$ and γ_0 are smooth functions of the temperature in the region of the phase transition. Since we are interested in temperature anomalies near the Curie point, we shall take $\Delta\xi_0$ and γ_0 to be constant and include $\Delta\xi_0$ in ξ. Thus, we take H' into account by introducing into the spectrum the damping γ_0.

2. THE EQUATION FOR THE DENSITY MATRIX

We carry out a detailed investigation for the case of a ferromagnetic. We differentiate the density matrix (1) with respect to time and utilize the equations of motion for the operators $a^+_{ps}(t)$ and $a_{ps}(t)$ obtained in the usual manner by commuting with the Hamiltonian H. Since the effects in which we are interested appear in second order with respect to the exchange interaction we must retain the two first equations of the chain of equations of motion for the correlators.

$$\hat{T}_{p'p}\langle a_{p's}a_{ps}\rangle + \frac{e}{c}\mathbf{A}\mathbf{v}_{pp'}(n_{p's}-n_{ps}) \tag{4}$$
$$= \pm\sum_{n\mathbf{p}_1}[J_n(\mathbf{p},\mathbf{p}_1)(\langle a^+_{p's}a_{p_1s}\delta S_n{}^z\rangle \pm \langle a^+_{p's}a_{p_1-s}\delta S_n{}^{\mp}\rangle)$$
$$-J_n(\mathbf{p}_1,\mathbf{p}')(\langle a^+_{p_1s}a_{ps}\delta S_n{}^z\rangle \pm \langle a^+_{p_1-s}a_{ps}\delta S_n{}^{\pm}\rangle)],$$

$$\hat{T}_{p_1p_2}\langle a^+_{p_1s}a_{p_2s}\delta S_n{}^z\rangle = \pm\sum_{n_1\mathbf{p}_3}[J_{n_1}(\mathbf{p}_2,\mathbf{p}_3)\langle a^+_{p_1s}a_{p_3s}\delta S_n{}^z\,\delta S_{n_1}{}^z\rangle$$
$$-J_{n_1}(\mathbf{p}_3,\mathbf{p}_1)\langle a^+_{p_3s}a_{p_2s}\delta S_n{}^z\,\delta S_{n_1}{}^z\rangle],$$

$$\hat{T}_{p_1p_2} = i\hbar\frac{\partial}{\partial t} + \xi_{p_1p_2} + \Delta\xi^{(1)}_{p_1p_2s} + i\gamma_0, \qquad n_{ps} = \langle a_{ps}{}^+a_{ps}\rangle, \tag{5}$$

$$\xi_{p'p} = \xi_{p'} - \xi_p, \qquad \Delta\xi^{(1)}_{p'ps} = \pm(J(\mathbf{p},\mathbf{p}) - J(\mathbf{p}',\mathbf{p}'))\langle S\rangle. \tag{6}$$

Here the upper sign corresponds to $s = 1/2$, and the lower sign corresponds to $s = -1/2$, $\delta\mathbf{S}_n = \mathbf{S}_n - \langle\mathbf{S}\rangle$ and $\langle\mathbf{S}\rangle$ is the average value of the spin at a lattice point. Near the Curie point the magnetization $\langle\mathbf{S}\rangle \sim |\tau|^\beta$ with $\tau \equiv (T - T_c)/T_c < 0$ is small and $\langle\mathbf{S}\rangle = 0$ for $\tau > 0$. The equations of motion for $\langle a^+a\delta S^{\pm}_n\rangle$ have a form similar to (5).

The chain becomes closed if in (5) we pick out the part $\langle\delta S_n\delta S_{n_1}\rangle$ averaged over the ensemble from $\delta S_n\delta S_{n_1}$ and neglect the deviation from this average. It is not difficult to understand that the domain of applicability of the approximation made by us above is

$$|\tau| \gg J/\varepsilon_0. \tag{7}$$

Linearizing the equations obtained above with respect to the small deviation from equilibrium proportional to the electromagnetic field we obtain from the system of equations for the linear addition to the density matrix $\rho^{(1)}_{\mathbf{p}'s,\mathbf{p}s}$ the integral equation

$$T_{p'p}(\omega)\rho^{(1)}_{p's,ps} + \frac{e}{c}\mathbf{A}\mathbf{v}_{pp'}(n_{p's}-n_{ps}) = -\Xi\rho^{(1)}_{p's,ps} + \hat{I}\rho^{(1)}_{p_1s_1,p_2s_2}, \tag{8}$$

$$\Xi = -N\sum_{n\mathbf{p}_1}\left[\frac{J_n(\mathbf{p}_1,\mathbf{p})J(\mathbf{p},\mathbf{p}_1)}{T_{p'p_1}(\omega)} + \frac{J_n(\mathbf{p}',\mathbf{p}_1)J_0(\mathbf{p}_1,\mathbf{p}')}{T_{p_1p}(\omega)}\right]\langle\delta S_0\,\delta S_n\rangle, \tag{9}$$

$$T_{p'p}(\omega) = -\hbar\omega + \xi_{p'p} + \Delta\xi^{(1)}_{p'ps} + i\gamma_0.$$

For the derivation of (4)—(8) we utilized the identity

$$(1/N)\sum_n e^{-i\mathbf{k}\mathbf{r}_n} = \sum_{\mathbf{g}}\delta_{\mathbf{k},\mathbf{g}}$$

and in the resultant sum over the vectors of the reciprocal lattice $\mathbf{g}$ we have retained only the term with $\mathbf{g} = 0$, since, as will be clear from what follows, the addition to the density matrix near the singularities of the spectrum at appropriate frequencies has a singularity at $\mathbf{p}' = \mathbf{p} + \mathbf{g}_0$, where $\mathbf{g}_0$ is the vector of the reciprocal lattice which describes within the expanded band scheme the given interband transition[2)]. Moreover, we have neglected terms arising due to the noncommutativity of the spin components, since such terms in the principal approximation are $\sim\langle\mathbf{S}\rangle$, just as $\Delta\xi^{(1)}$, but at the same time are smaller than $\Delta\xi^{(1)}$ by a factor of ϵ_0/J, and we also neglect terms describing electron transitions accompanied by spin flip since $\rho^{(1)}_{\mathbf{p}'s,\mathbf{p}-s} \sim (J/\epsilon_0)\rho^{(1)}_{\mathbf{p}'s,\mathbf{p}s}$.

Further simplification is associated with the fact that the integral term in (8) can be neglected[1]. The physical meaning of such neglect consists of the fact that the addition to the density matrix has a resonance character for each value of the momentum (this can be seen by neglecting the right hand side part in (8)). We shall be interested in those cases when the frequency is close to the resonance frequency for one of the singular points of the interband density of states. Then the contribution to all the quantities in which we are interested is made by a small region in the neighborhood of the singular point in a manner similar to what happens, for example, in the case of cyclotron resonance[2]. For this reason we shall not in future take the term $\hat{I}\rho^{(1)}$ into account. From equation (8) we obtain

$$\rho^{(1)}_{p's,ps} = \frac{ie\mathbf{E}\mathbf{v}_{pp'}(n_{p's}-n_{ps})}{\omega[T_{p'p}(\omega) + \Delta\xi^{(2)}_{p'ps} + i\Delta\gamma_{p'ps}]}, \tag{10}$$

$$\Delta\xi^{(2)}_{p'ps} = \mathrm{Re}\,\Xi, \qquad \Delta\gamma_{p'ps} = \mathrm{Im}\,\Xi. \tag{11}$$

We utilize formulas (9)—(11) to calculate the interband part $\sigma^{\alpha\beta}_i(\omega)$ of the high frequency conductivity.

3. THE HIGH FREQUENCY CONDUCTIVITY

In order to calculate $\sigma^{\alpha\beta}_i(\omega)$ we obtain the interband current $\mathbf{j}_i(\omega)$ in accordance with the formula

$$\mathbf{j}_i(\omega) = \frac{e}{V}\mathrm{Sp}\,\rho^{(1)}\mathbf{v}, \tag{12}$$

where V is the volume of the system. Substituting (10) into (12) and taking into account the fact that $j^\alpha_i = \sigma^{\alpha\beta}_i E^\beta$, we obtain for $\sigma^{\alpha\beta}_i(\omega)$ the following expression:

$$\sigma_i{}^{\alpha\beta}(\omega) = \sum_{\mathbf{g}}\sigma^{\alpha\beta}_{i\mathbf{g}}(\omega),$$

$$\sigma^{\alpha\beta}_{i\mathbf{g}}(\omega) = \frac{ie^2}{(2\pi)^3\omega}\sum_s\int d\zeta\oint_{\xi_{\mathbf{g}s}(\mathbf{p})=\zeta}\frac{dS}{|\nabla_{\mathbf{p}}\xi_{\mathbf{g}s}(\mathbf{p})|}\frac{v^\alpha_{\mathbf{p}+\mathbf{g}}v^\beta_{\mathbf{p}+\mathbf{g}p}(n_{ps}-n_{p+gs})}{-\hbar\omega+\zeta+i\gamma_{gs}},$$

$$\xi_{gs}(\mathbf{p}) = \xi_{p+g,p} + \Delta\xi^{(1)}_{p+g,ps} + \Delta\xi^{(2)}, \qquad \gamma_{gs} = \gamma_0 + \Delta\gamma,$$

$$\Delta\xi^{(2)} \equiv \Delta\xi^{(2)}_{p+g,ps}, \qquad \Delta\gamma \equiv \Delta\gamma_{p+g,ps}. \tag{13}$$

As is well known, the real part of the conductivity $\sigma^{\alpha\beta}(\omega)$ has smeared out singularities at frequencies for which the equation $\nabla_{\mathbf{p}}\xi_{\mathbf{g}s}(\mathbf{p}) = 0$ is satisfied at some point $\mathbf{p}_0$ on the surface $\hbar\omega = \xi_{\mathbf{g}s}(\mathbf{p})$, and the existence of such points leads to the appearance of the so-called Van Hove singularities in the interband density of states[2]

$$\nu_{gs}(\zeta) = \frac{1}{(2\pi)^3}\oint_{\xi_{gs}(\mathbf{p})=\zeta}\frac{dS}{|\nabla_{\mathbf{p}}\xi_{gs}(\mathbf{p})|}. \tag{14}$$

In order to determine the analytic behavior of the function $\nu_{\mathbf{g}s}(\zeta)$ near a singularity of the Van Hove type $\xi_{\mathbf{g}s}(\mathbf{p})$ is usually expanded into a Taylor series near the critical point $\mathbf{p}_0$:

$$\xi_{gs}(\mathbf{p}) = \hbar\omega_0 + \frac{1}{2}\sum_{j=1}^{3}M_j{}^{-1}(p_j-p_{0j})^2,$$
$$\hbar\omega_0 \equiv \xi_{gs}(\mathbf{p}_0), \qquad M_j{}^{-1} \equiv \partial^2\xi_{gs}(\mathbf{p}_0)/\partial p_j{}^2. \tag{15}$$

Depending on the set of signs of the coefficients of M^{-1}_j the point $\mathbf{p}_0$ can either be an extremum or a saddle point. Calculation according to formula (14) shows that the singular part of $\nu_{\mathbf{g}s}(\zeta)$ for $\eta(\zeta - \hbar\omega_0) > 0$ has the form

$$\pm 2^{-1/2}\pi^{-2}[\eta(\zeta-\hbar\omega_0)|M_1M_2M_3|]^{1/2}, \qquad \eta = \frac{M_1}{|M_1|},$$

i.e., it has divergent derivatives: the plus sign here refers to the case of an extremum (threshold), the minus

sign refers to a saddle point (ridge), the axes in the expansion (15) are always so chosen that M_2 and M_3 have the same sign.

With the aid of (13), taking out the smooth functions from under the integrals, and utilizing the form of the anomalous part of $\nu_{gs}(\zeta)$, it can be easily shown that

$$\operatorname{Re}\sigma_{ig}^{\alpha\beta}(\omega)=\operatorname{Re}\sigma_0^{\alpha\beta}(\omega)\pm L\sum_s\{\eta(\omega-\omega_{0s})+[(\omega-\omega_{0s})^2+\gamma_{gs}^2(\mathbf{p}_0)/\hbar^2]^{1/2}\}^{1/2},$$

$$L=e^2v^{\alpha}_{\mathbf{p}_0\mathbf{p}_0+\mathbf{g}}v^{\beta}_{\mathbf{p}_0+\mathbf{g}\mathbf{p}_0}|M_1M_2M_3|^{1/2}\hbar^{1/2}/2\pi\omega. \tag{16}$$

Here $\sigma_0^{\alpha}\beta(\omega)$ is a smooth function of the frequency, the plus sign refers to an extremum, and the minus refers to a saddle point.

The derivative $d\operatorname{Re}\sigma(\omega)/d\omega$ has peaks in the neighborhood of the frequencies ω_{0s}. The quantities that are experimentally measurable are the positions of these peaks, their width and their height. We denote the width of the peaks measured at half height by Γ_1. In some experimental papers the magnitude of the smearing out of a singularity is characterized by the difference in the positions of the extrema of the second derivative $d^2\operatorname{Re}\sigma(\omega)/d\omega^2$; we denote this difference by Γ_2. In future we shall everywhere state values both of Γ_1 and of Γ_2.

Since ω_{0s} is different for $s=+1/2$ and $s=-1/2$, then from formula (16) it can be seen that magnetic ordering leads to a splitting of the singularities by an amount Δ which in accordance with (6) is equal to

$$\Delta=2(J_1-J_2)\langle S\rangle\sim|\tau|^{\beta},\quad \tau<0,$$
$$J_1\equiv J(\mathbf{p}_0,\mathbf{p}_0),\quad J_2\equiv J(\mathbf{p}_0+\mathbf{g},\mathbf{p}_0+\mathbf{g}). \tag{17}$$

This result agrees with the usual phenomenological discussion [3] of the effect of magnetic ordering on a spectrum.

In order to calculate the smearing out and the shift arising in second order with respect to the exchange interaction we write (9), (11) in the form

$$\Delta\xi^{(2)}+i\Delta\gamma=(\Delta\xi_1^{(2)}+i\Delta\gamma_1)+(\Delta\xi_2^{(2)}+i\Delta\gamma_2), \tag{18}$$

$$\Delta\xi_1^{(2)}+i\Delta\gamma_1=-\int\frac{d^3r}{(2\pi)^3}\int d^3p\,\frac{J(\mathbf{p}_0,\mathbf{p})J(\mathbf{p},\mathbf{p}_0)}{-\beta+\xi_{\mathbf{p}_0}-\xi_{\mathbf{p}}+i\gamma_g(\mathbf{p}_0)}\exp[i(\mathbf{p}_0-\mathbf{p})\mathbf{r}]g(\mathbf{r}),$$

$$\Delta\xi_2^{(2)}+i\Delta\gamma_2=-\int\frac{d^3r}{(2\pi)^3}\int d^3p\,\frac{J(\mathbf{p},\mathbf{p}_0+\mathbf{g})J(\mathbf{p}_0+\mathbf{g},\mathbf{p})}{-\beta+\xi_{\mathbf{p}}-\xi_{\mathbf{p}_0+\mathbf{g}}+i\gamma_g(\mathbf{p}_0)}\exp[i(\mathbf{p}-\mathbf{p}_0-\mathbf{g})\mathbf{r}]g(\mathbf{r}),$$

where $g(\mathbf{r})=\langle\delta\mathbf{S}_0\delta\mathbf{S}_{\mathbf{r}}\rangle$ is an irreducible correlator, $\beta=\hbar(\omega-\omega_0)$, where in the denominators we have taken into account in a self-consistent manner terms of the next order in J/ϵ_0. As will be seen from the following, the circumstance that $\Delta\xi^{(2)}$ and $\Delta\gamma$ are functions of the frequency can have a significant effect on the shape of the curve $\operatorname{Re}\sigma(\omega)$.

At a frequency close to ω_0, as a result of the resonance nature of the denominators of the integrand the principal contribution to the integrals over $\mathbf{p}$ in (18) must come from the immediate neighborhood of the points $\mathbf{p}_0$ for the first term (the contribution of the lower band) and $\mathbf{p}_0+\mathbf{g}$ for the second term (the contribution of the upper band). Near these points we can carry out an expansion of $\xi_{\mathbf{p}}$. Thus, in the neighborhood of $\mathbf{p}_0$ we obtain

$$\xi_{\mathbf{p}}=\xi_{\mathbf{p}_0}+\mathbf{v}_{\mathbf{p}_0}(\mathbf{p}-\mathbf{p}_0)+\frac{1}{2}\sum_{j=1}^{3}m_{\mathbf{p}_0j}^{-1}(p_j-p_{0j})^2,$$
$$\mathbf{v}_{\mathbf{p}_0}=\nabla_{\mathbf{p}}\xi_{\mathbf{p}}(\mathbf{p}_0),\quad m_{\mathbf{p}_0j}^{-1}=\partial^2\xi_{\mathbf{p}}(\mathbf{p}_0)/\partial p_j^2. \tag{19}$$

An analogous expression can also be written for the neighborhood of the point $\mathbf{p}_0+\mathbf{g}$.

In accordance with the theory of second-order phase transitions based on the hypothesis of the similarity of correlations the function $g(\mathbf{r})\sim 1/r^{\nu_1}$ for $r_c\gg r\gg a$ and falls off rapidly for $r\gg r_c$. Here a is the interatomic distance, r_c is the range of correlation. As we approach the critical point $\tau\to 0$, while $r_c\sim\tau^{-\mu}$ increases. For the sake of simplicity we shall approximate the cut-off factor in $g(\mathbf{r})$ by the exponential $\exp(-r/r_c)$. The exact form of this smooth function has no significant effect on the results of the calculation.

It turns out that, depending on the structure of each of the two bands, the results in the neighborhood of their interband critical point will be significantly different in the following characteristic cases:

I. The usual critical point: $\mathbf{v}_{\mathbf{p}_0}=\mathbf{v}_{\mathbf{p}_0+\mathbf{g}}=\mathbf{v}_0\neq 0$. In this case in the expansion (19) it is sufficient to restrict ourselves to the approximation linear in $\mathbf{p}-\mathbf{p}_0\equiv\mathbf{q}$.

We substitute (19) into (18) and we choose the direction of the z-axis along $\mathbf{v}_0$. Then we have

$$\Delta\xi^{(2)}+i\Delta\gamma=\frac{J_1^2+J_2^2}{(2\pi)^3}\int_{-\infty}^{\infty}\frac{dx\,dy\,dz}{(r/a)^{\nu_1}}\int_{-\infty}\frac{\exp(-r/r_c-iq_zz)\,dq_z}{\beta+v_0q_z-i\gamma}$$
$$\times\int\exp(-iq_xx-iq_yy)\,dq_x\,dq_y=i\frac{J_1^2+J_2^2}{v_0}a\Gamma(1-\nu_1)\left(\frac{a}{l}+i\frac{\beta a}{v_0}\right)^{\nu_1-1},$$
$$1/l=1/r_c+\gamma/v_0,\quad r=(x^2+y^2+z^2)^{1/2}. \tag{20}$$

In evaluating (20) we utilize the fact that in integration over q_x and q_y the contribution to the integrals from the limits $|q_{x\max}|$, $|q_{y\max}|\sim 1/a$ is small in terms of the parameter a/l_{eff}, where $l_{\text{eff}}=\min\{r_c, v_0/\beta, v_0/\gamma\}$, so that these integrals can be replaced by $\delta(x)\delta(y)$.

It can be shown that within the domain of applicability of our theory because of the inequality (7) we have $l\approx r_c$. It is also not difficult to verify that the position of the maximum β_m and the values of β which determine the widths Γ_1 and Γ_2 fall in the region $\beta r_c/v_0\ll 1$. At the same time we have

$$\Delta\gamma=\frac{J_1^2+J_2^2}{v_0}a\Gamma(1-\nu_1)\left(\frac{r_c}{a}\right)^{1-\nu_1},$$
$$\Delta\xi^{(2)}=\frac{J_1^2+J_2^2}{v_0}\frac{\beta a^2}{v_0}\Gamma(2-\nu_1)\left(\frac{r_c}{a}\right)^{2-\nu_1}. \tag{21}$$

For $\nu_1=1$ the anomalous part of γ varies logarithmically $\sim\ln(r_c/a)$. Such a behavior is quite close to the behavior of the specific heat of magnetic materials near the Curie point. The shift $\Delta\xi^{(2)}$ is small in this case.

From formula (16) it follows that the position of $\eta\beta_m$, the quantity $(d\operatorname{Re}\sigma/d\eta\beta)_m$ and the widths Γ_1 and Γ_2 of the extremum of the derivative $d\operatorname{Re}\sigma/d\eta\beta$ are given by

$$\eta\beta_m=0.58\gamma,\quad (d\operatorname{Re}\sigma/d\eta\beta)_m=0.57L\gamma^{-1/2},\quad \Gamma_1=1{,}1\gamma,\quad \Gamma_2=1{,}7\gamma. \tag{22}$$

Thus, the position, width and height of the peaks have in the present case the same temperature anomaly $\sim\tau^{-\mu(1-\nu_1)}$ (for $\nu_1=1$ the anomaly is $\sim\ln|\tau|$).

II. The symmetric critical point: $\mathbf{v}_{\mathbf{p}_0}=\mathbf{v}_{\mathbf{p}_0+\mathbf{g}}=0$. There are no linear terms in the expansion (19). At the same time in each of the two bands participating in this transition the critical point has, in its turn, the nature of an extremum or a saddle point, while the combination between them can be arbitrary. For the sake of simplicity we assume that all the intraband effective masses in (19) are equal in absolute value, and this does not qualitatively affect the nature of the anomalies.

We quote the results of calculations in accordance with (18) of the contribution of the lower band.

1. If the point $\mathbf{p}_0$ is an extremal intraband critical point, then the constant energy surfaces near it are spheres. Then we have

$$\xi_p=\xi_{p_0}+\frac{q^2}{2m_{p_0}},\quad \Delta\xi_1^{(2)}+i\Delta\gamma_1=\frac{J_1^2}{(2\pi)^3}\int\frac{d^3r}{(r/a)^{\nu_1}}\int\frac{\exp(-r/r_c-iqr)}{\beta+q^2/2m_{p_0}-i\gamma}d^3q. \tag{23}$$

Integration in (23) can be carried out in an elementary manner. As a result we obtain

$$\Delta\xi_1^{(2)}+i\Delta\gamma_1=\frac{2J_1^2m_{p_0}a^2\Gamma(2-\nu_1)}{[a/r_c+a(\varkappa+m_{p_0}\beta)^{1/2}-i(\operatorname{sign}m_{p_0})a(\varkappa-m_{p_0}\beta)^{1/2}]^{2-\nu_1}},$$
$$\varkappa=|m_{p_0}|(\beta^2+\gamma^2)^{1/2}. \tag{24}$$

The region which is of the greatest interest to us is the one in which the inequality

$$r_c\varkappa^{1/2}\ll 1.$$

is satisfied. In that range we have

$$\Delta\gamma_1=2J_1^2|m_{p_0}|a^3\Gamma(3-\nu_1)(r_c/a)^{3-\nu_1}(\varkappa-m_{p_0}\beta)^{1/2}, \tag{25}$$

$$\Delta\xi_1^{(2)}=2J_1^2m_{p_0}a^2\Gamma(2-\nu_1)(r_c/a)^{2-\nu_1}. \tag{26}$$

2. If the point $\mathbf{p}_0$ is an intraband critical saddle point, then the constant energy surfaces near it are the hyperboloids

$$\xi_p=\xi_{p_0}+\frac{1}{2}m_{p_0}^{-1}[q_x^2+q_y^2-q_z^2].$$

Substituting ξ_p into (18) and introducing spherical coordinates we have

$$\Delta\xi_1^{(2)}+i\Delta\gamma_1=\frac{J_1^2}{2\pi}\int\frac{r^2dr\,d\cos\varphi}{(r/a)^{\nu_1}}\int\frac{q^2dq\,d\cos\theta\exp(-r/r_c-iqr\cos\varphi)}{\beta+(q^2/2m_{p_0})(1-2\cos^2\theta)-i\gamma}$$

We break up the integral over $\cos\theta = u$ into two regions: $u^2 < 1/2$ and $u^2 > 1/2$. In the former we carry out the replacement $1-2u^2 = 1/t^2$, and in the latter $2u^2-1 = 1/t^2$. Integrating over φ and q we obtain

$$\Delta\xi_1^{(2)}+i\Delta\gamma_1=2^{1/2}J_1^2m_{p_0}\int_0^\infty\frac{r\,dr}{(r/a)^{\nu_1}}\Big(\int_1^\infty\frac{dt}{(t^2-1)^{1/2}}\exp(iq_0^{(1)}rt)$$
$$-\int_1^\infty\frac{dt}{(t^2+1)^{1/2}}\exp(iq_0^{(2)}rt)\Big)\exp(-r/r_c),$$

$$q_0^{(1)}=(\operatorname{sign}m_{p_0})(\varkappa-m_{p_0}\beta)^{1/2}+i(\varkappa+m_{p_0}\beta)^{1/2},\quad q_0^{(2)}=i(\operatorname{sign}m_{p_0})q_0^{(1)}. \tag{27}$$

In particular, for $r_c\varkappa^{1/2}\ll 1$ we have

$$\Delta\gamma_1=(2\pi)^{1/2}J_1^2|m_{p_0}|a^2\Gamma(2-\nu_1)(r_c/a)^{2-\nu_1}, \tag{28}$$

$$\Delta\xi_1^{(2)}=2(2/\pi)^{1/2}\ln(1+2^{1/2})J_1^2m_{p_0}a^2\Gamma(2-\nu_1)(r_c/a)^{2-\nu_1}. \tag{29}$$

Substituting ξ_p into (18) it can be easily seen that the contribution of the upper band is obtained from expressions (25)—(29) by means of the following replacement in them

$$m_{p_0}\to -m_{p_0+g},\quad J_1\to J_2.$$

We describe the frequency behavior of the conductivity near the singularity by the function

$$\Sigma(\eta\beta)\equiv\operatorname{Re}(\sigma_i^{\alpha\beta}-\sigma_0^{\alpha\beta})/L.$$

The shape of the curve $\Sigma(\eta\beta)$ depends on the combination of the intraband points and is obtained by substituting into (16) the solutions of the system

$$\Delta\gamma=\Delta\gamma_1(\gamma,\beta)+\Delta\gamma_2(\gamma,\beta),\quad \gamma=\gamma_0+\Delta\gamma, \tag{30}$$

where $\Delta\gamma_1$ and $\Delta\gamma_2$ are determined by means of formulas (25) and (28).

a) For transitions of the type saddle point—saddle point, saddle point—extremum or extremum—saddle point the principal contribution to $\Delta\gamma$ is made by the saddle points. In this case $(d\Sigma/d\eta\beta)_m$, β_m, Γ_1, Γ_2 are determined by formulas (22), (28) with $\Delta\gamma\sim|\tau|^{-\mu(2-\nu_1)}$, i.e., the temperature anomaly is considerably stronger than in the case of the ordinary critical point.

b) For transitions between two extremal points with intraband masses which coincide with respect to their sign with the interband mass, it is possible to obtain a function reciprocal to $\Sigma(\eta\beta)$:

$$\eta\beta(\Sigma)=\tfrac{1}{2}\Sigma^2-\tfrac{1}{2}B^2(1+\gamma_0/B\Sigma)^2,\quad B=B_1+B_2,$$
$$B_i=2J_i^2|m_{p_i}|^{3/2}a^3\Gamma(3-\nu_i)(r_c/a)^{3-\nu_i}\sim\varepsilon_0^{1/2}(J/\varepsilon_0)^2(r_c/a)^{3-\nu_i}, \tag{31}$$

where one of the vectors $\mathbf{p}_1$, $\mathbf{p}_2$ is equal to $\mathbf{p}_0$, and the other is equal to $\mathbf{p}_0+\mathbf{g}$.

c) If the signs of the intraband masses are the same and do not coincide with the sign of the interband mass

$$\eta\beta(\Sigma)=\tfrac{1}{2}\Sigma^2-\tfrac{1}{2}\gamma^2/(\Sigma-B)^2,\quad \Sigma>B. \tag{32}$$

d) If the transition occurs between two extremal points with effective masses of opposite sign, then we have

$$\eta\beta(\Sigma)=\frac{1}{2}\Sigma^2-\frac{1}{2}\left(\frac{\gamma_0+B_1\Sigma}{\Sigma-B_2}\right)^2,\quad \Sigma>B_2; \tag{33}$$

here $\eta = \operatorname{sign} m_{p_1}$.

Formulas (31)—(33) completely determine the shape of $\Sigma(\eta\beta)$ and its temperature behavior and enable us to find temperature dependences of $(d\Sigma/d\eta\beta)_m$, β_m, Γ_1 and Γ_2 in terms of $B_i(\tau)\sim|\tau|^{-\mu(3-\nu_1)}\sim\chi(\tau)$, where $\chi(\tau)$ is the magnetic susceptibility). The effective parameter is the quantity B^2/γ_0. In particular, for

$$\frac{B^2}{\gamma_0}\ll 1,\ \text{i.e.,}\left(\frac{J^2}{\varepsilon_0\gamma_0}\left(\frac{J}{\varepsilon_0}\right)^2\right)^{1/2\mu(3-\nu_1)}\ll\tau.$$

we obtain that

$$(d\Sigma/d\eta\beta)_m=0.57\gamma_0^{-1/4},\quad \eta\beta_m=0.58\gamma_0,\quad \Gamma_1=1.1\gamma_0,\quad \Gamma_2=1.7\gamma_0 \tag{34}$$

have a weak temperature dependence near T_c.

In the opposite limiting case $B^2/\gamma_0\gg 1$ for transitions of type b) we have

$$\left(\frac{d\Sigma}{d\eta\beta}\right)_m=0.53\left(\frac{\gamma_0}{B^2}\right)^{1/4}\gamma_0^{-1/4}\sim\chi^{-1/4}(\tau),\quad \eta\beta_m=-\frac{1}{2}B^2\sim\chi^2(\tau),$$
$$\Gamma_1=1.6\left(\frac{B^2}{\gamma_0}\right)^{1/3}\gamma_0\sim\chi^{2/3}(\tau),\quad \Gamma_2=0.8\Gamma_1\sim\chi^{2/3}(\tau). \tag{35}$$

For transitions of type c) we have

$$\left(\frac{d\Sigma}{d\eta\beta}\right)_m=\frac{1}{B}\sim\chi^{-1}(\tau),\quad \eta\beta_m=\frac{1}{2}B^2\sim\chi^2(\tau),$$
$$\Gamma_1=\frac{2}{3}B^2\sim\chi^2(\tau),\quad \Gamma_2=1.3\left(\frac{B^2}{\gamma}\right)^{3/4}\gamma_0\sim\chi^{3/2}(\tau). \tag{36}$$

For transitions of type d) we have

$$\left(\frac{d\Sigma}{d\eta\beta}\right)_m=\frac{1}{B_2}f_1\left(\frac{B_1}{B_2}\right)\sim\chi^{-1}(\tau),\quad \eta\beta_m=B_2^2f_2\left(\frac{B_1}{B_2}\right)\sim\chi^2(\tau),$$
$$\Gamma_1=B_2^2f_3\left(\frac{B_1}{B}\right)\sim\chi^2(\tau),\quad \Gamma_2=B_2^2f_4\left(\frac{B_1}{B_2}\right)\sim\chi^2(\tau), \tag{37}$$

where f_α (α = 1, 2, 3, 4) are functions which do not depend on τ with $f_\alpha\sim 1$ for $B_1\sim B_2$.

The experimentally measured anomaly in the position of the extremum of $d\,\mathrm{Re}\,\sigma/d\omega$ is described by the quantity $\Delta\omega_0 = \Delta\xi^{(2)} + \beta_m$, where $\Delta\xi^{(2)}$ is defined by formulas (21), (26), (29).

4. ANTIFERROMAGNETICS

In the case of antiferromagnetics the investigation is carried out in an analogous manner. It is not difficult to verify in this case that if in an elementary crystal cell there is present only one magnetic ion, then no splitting into subbands with oppositely oriented spin occurs (we do not touch upon the effects of exchange splitting associated with a doubling of the period below the Neel point), and the shift which appears in second order is proportional to $\langle \mathbf{S} \rangle^2$, where $\langle \mathbf{S} \rangle$ is the magnetization of the sublattice, while the fluctuation smearing out and shift are small and do not undergo anomalous growth as $T \to T_c$ due to the fact that the correlation function $g(\mathbf{r}) = \langle \delta \mathbf{S}_0 \delta \mathbf{S}_r \rangle$ is of an oscillatory nature.

However, if in a unit cell of the crystal there is present more than one magnetic ion, then a splitting, smearing out and shift can arise with a behavior analogous to the one in the ferromagnetic case, since in (3) the integrals for the exchange interaction $J(\mathbf{p}, \mathbf{p}')$ for a Bloch electron with ions localized on different sublattices can become different. For the case of a two-sublattice antiferromagnetic in distinction from a ferromagnetic the parameter $J(\mathbf{p}_0, \mathbf{p}_0)$ in the results is replaced by $J_I(\mathbf{p}_0, \mathbf{p}_0) - J_{II}(\mathbf{p}_0, \mathbf{p}_0)$, i.e., by the difference between the exchange integrals for the first and the second sublattice; the anomalous quantity $\chi(\tau) \sim |\tau|^{-\mu(3-\nu_1)}$ no longer has the meaning of the static magnetic susceptibility.

5. CONCLUSION

An investigation of the temperature behavior of the frequency dependent characteristics of crystals near the Curie point is of interest both for the theory of phase transitions, and also for the study of electron spectra [2,9-11], since a possibility appears to distinguish by the nature of the temperature behavior of the anomalies near T_c the type of critical points in the electron spectrum. However, we do not know of sufficiently accurate data on the temperature dependences of the optical properties of transition metals in the neighborhood of the point of magnetic ordering.

Generally speaking, our results are valid both for metals and for dielectrics to the extent to which a Hamiltonian of the type (3) is applicable to describe the interaction of Bloch electrons with localized spins. In this case it is of interest to calculate the magnetic addition $\Delta n_M^{\alpha\beta}$ to the index of refraction, which was recently studied in experiments on double refraction [12] in the fluorides of transition metals (MnF_2, NiF_2, CoF_2) which are two-sublattice antiferromagnetics with two magnetic ions in an elementary cell. For this it is necessary to evaluate the imaginary part of the conductivity. Near the threshold for self-absorption we obtain with the aid of (13)

$$\mathrm{Im}\,\sigma_{ig}^{\alpha\beta}(\omega) = \mathrm{Im}\,\sigma_0^{\alpha\beta}(\omega) + L\sum_{\mathbf{g}_s} \{\eta(\omega_{0s} - \omega) + [(\omega_{0s} - \omega)^2 + \gamma_{\mathbf{g}_s}^2(\mathbf{p}_0)/\hbar^2]^{1/2}\}^{1/2}. \tag{38}$$

If the frequency is such that $|\xi_{\mathbf{p}_0+\mathbf{g},\mathbf{p}_0} - \hbar\omega| \gg \Delta\xi$, $\Delta\gamma$, then for antiferromagnetics with two magnetic ions per cell we have

$$\Delta n_M^{\alpha\beta} = A_1^{\alpha\beta}\langle \mathbf{S} \rangle^2 + A_2^{\alpha\beta}(r_c/a)^{2-\nu_1}, \tag{39}$$

where $\langle \mathbf{S} \rangle$ is the magnetization of the sublattice. We note that far from the threshold for self-absorption it is not possible, strictly speaking, to neglect the integral term in (8) and perturbation theory should be used for the solution. However, it can be shown that the result (39) remains valid as long as the parameter

$$r_c(|M(\xi_{\mathbf{p}_0+\mathbf{g},\mathbf{p}_0} - \hbar\omega)|)^{1/4} \ll 1,$$

is small, and for this it is required that the frequency should be not too far from the threshold frequency. In the opposite limiting case the dependence on r_c disappears. Such behavior of $\Delta n_M^{\alpha\beta}$ agrees with experimental results [12] in which it is found that for MnF_2 for $\tau > 0.1$ a growth of $\Delta n_M^{\alpha\beta}$ is observed according to a law close to

$$r_c^{2-\nu_1} \sim \tau^{-\mu(2-\nu_1)}, \quad \nu_1 \approx 1, \quad \mu \approx 2/3$$

with an asymptotic approach to a constant value for $\tau \sim 0.1$ (and this, apparently, corresponds to a comparatively large distance to the nearest threshold). It would be of interest to obtain analogous data for NiF_2, for which the operating light frequency lies near the threshold of the absorption band, and this means that the growth of $\Delta n_M^{\alpha\beta} \sim \tau^{-2/3}$ ought to be observed down to considerably smaller values of τ. The same should also occur in MnF_2 at frequencies close to the threshold frequency.

In conclusion we note that temperature singularities analogous to those discussed above must also occur in photoemission, and this was observed in the paper of Rowe and Trasy [13].

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[1] Below for the sake of brevity we shall always speak of the Curie temperature.

[2] In this paper we shall not discuss cases when the singular point $\mathbf{p}_0$ is a point of band degeneracy.

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22