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The Temperature Dependence of the Absorption Bands Intensities of the Spectra of Molecular Crystals at Fermi Resonance

II. The Mass Operator. The Band Shape

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Abstract—The mass operator for the system of intramolecular oscillations interacting with the lattice phonons is calculated. With the use of a linear chain model it was shown that the frequency dependence of the mass operator causes a deviation of the shape of the absorption curve from the Lorentzian one and an appearance of additional maxima on the tails of absorption bands.

1. The General Expression

It was noted in Part 1 that the frequency dependence of the imaginary part of the mass operator causes a different temperature dependence of the intensities of the components of the Fermi-doublet. To clarify the character of the frequency dependence indicated, we shall calculate the mass operator of the system for some model. We assume that the excitons interact only with the optical lattice phonons, predominantly with one certain type of phonon of frequency Ω . With these restrictions,

$$M_{\pm}^{ff'}(\mathbf{k}, \omega) = \nu_0 \mp \sum_{f, q'} \frac{1}{N} \sum_{\mathbf{q}'} F^{*f'f}(\mathbf{k}, \mathbf{q}') F^{f, f'}(\mathbf{k}, \mathbf{q}') \frac{\Delta_{1, \pm}^{f, q'}(\mathbf{k}, \mathbf{q}', \omega)}{\Delta_{1, \pm}(\mathbf{k}, \mathbf{q}', \omega)} \quad (1)$$

All the notations are the same as in (Part I). To be definite, we calculate $M_{+}^{ff'}(\mathbf{k}, \omega)$, since the transition to the $M_{-}^{ff'}(\mathbf{k}, \omega)$ demands only the change of the sign before Ω . The determinant $\Delta_{1, +}(\mathbf{k}, \mathbf{q}', \omega)$

is a quadratic triplex in relation to the frequency ω and it can be represented as a product

$$\Delta_{1,+}(\mathbf{k}, \mathbf{q}', \omega) = [\omega - \omega_-(\Omega)][\omega - \omega_+(\Omega)] \quad (2)$$

$$\omega_{\pm}(\Omega) = \omega_{\pm}^0 - \Omega \quad (3a)$$

$$\omega_{\pm}^0 = \frac{1}{2}[Z^{11}(\mathbf{k} + \mathbf{q}') + Z^{22}(\mathbf{k} + \mathbf{q}')] \quad (3b)$$

$$\pm \frac{1}{2} \sqrt{[Z^{11}(\mathbf{k} + \mathbf{q}') - Z^{22}(\mathbf{k} + \mathbf{q}')]^2 + 4[Z^{12}(\mathbf{k} + \mathbf{q}')]^2} \quad (3b)$$

$$Z_{1,+}^{q'f'}(\mathbf{k} + \mathbf{q}', \omega) = (\omega + \Omega)\delta_{q'f'} - Z^{q'f'}(\mathbf{k} + \mathbf{q}') \quad (4a)$$

$$\Delta_{1,+}(\mathbf{k} + \mathbf{q}', \omega) = \det \| Z_{1,+}^{q'f'}(\mathbf{k} + \mathbf{q}', \omega) \| \quad (4b)$$

$\Delta_{1,+}^{f'g}(\mathbf{k}, \mathbf{q}', \omega)$ as before denotes corresponding algebraic complements to the determinant $\Delta_{1,+}$. Having introduced (2) and (4a) into (1), we get

$$M_{+}^{ff'}(\mathbf{k}, \omega) = \frac{\nu_0^-}{N} \sum_{\mathbf{q}'} \frac{1}{\omega_{+}^0 - \omega_{-}^0} \left[\frac{A^{ff'}(\omega_{+}^0)}{\omega - \omega_{+}(\Omega)} - \frac{A^{ff'}(\omega_{-}^0)}{\omega - \omega_{-}(\Omega)} \right] \quad (5)$$

where

$$\begin{aligned} A^{ff'}(\omega_{\pm}^0) = & F^{*1f}(\mathbf{k}, \mathbf{q}') F^{1f'}(\mathbf{k}, \mathbf{q}') [\omega_{\pm}^0 - Z^{22}(\mathbf{k} + \mathbf{q}')] \\ & + F^{*2f}(\mathbf{k}, \mathbf{q}') F^{1f'}(\mathbf{k}, \mathbf{q}') Z^{21}(\mathbf{k} + \mathbf{q}') + F^{*1f}(\mathbf{k}, \mathbf{q}') F^{2f'}(\mathbf{k}, \mathbf{q}') Z^{12}(\mathbf{k} + \mathbf{q}') \\ & + F^{*2f}(\mathbf{k}, \mathbf{q}') F^{2f'}(\mathbf{k}, \mathbf{q}') [\omega_{\pm}^0 - Z^{11}(\mathbf{k} + \mathbf{q}')] \end{aligned} \quad (6)$$

All the subsequent calculations we shall make for a special model, namely the linear chain. The scheme used by Davydov⁽¹⁾ will be employed. To do this, we look for an obvious form of the binding function $F^{fg}(\mathbf{k}, \mathbf{q}')$ and of the values $Z^{fg}(\mathbf{k} + \mathbf{q}')$. According to our previous paper,⁽²⁾

$$Z^{fg}(\mathbf{k} + \mathbf{q}') = \Delta \epsilon^f \delta_{fg} + D^{fg} + \tilde{M}^{fg}(\mathbf{k} + \mathbf{q}') \quad (7a)$$

$$\tilde{M}^{fg}(\mathbf{k} + \mathbf{q}') = \sum_{\mathbf{m}} M_{0\mathbf{m}}^{fg} e^{i(\mathbf{k} + \mathbf{q}') \cdot \mathbf{m}} \quad (7b)$$

D^{fg} is a constant independent on the wave vector: at the dipole approximation for the molecules with a centre of inversion it is equal to zero. For the sake of simplicity, we assume $D^{fg} = 0$ though its account will introduce no qualitative specialities into the calculation $M_{0\mathbf{m}}^{fg}$ is a matrix element of the transfer of the excitation from the molecule at the site o to the molecule at the site \mathbf{m} .

We consider a linear chain orientated along the Z axis and composed of molecules at a distance a from each other. They can

perform translational motions and rotations around the equilibrium position. We take that an exact Fermi-resonance is observed. Then⁽³⁾

$$\mathbf{d}' \approx \mathbf{d}'' = \frac{\mathbf{d}}{\sqrt{2}} \quad (8)$$

where \mathbf{d} is the dipole momentum of the transition in the molecule for the main tone in absence of the resonance. In this case both the transitions are connected with the same dipole momentum, which we consider to be orientated in the plane XZ at the angle v with the Z axis. Taking account of (8) and having confined ourselves to the first term of the sum in (7b), we get

$$\tilde{M}'^g(\mathbf{k} + \mathbf{q}') = \frac{Z}{4} \cos(\mathbf{k} + \mathbf{q}')a \quad (9)$$

Here

$$Z = \frac{4d^2(1 - 3\cos^2 v)}{a^3}$$

The absolute value of Z gives the width of the exciton band. As we see from formulae (9) there is no dependence on indexes f and g in the right hand part, which simplifies the subsequent calculations.

Similarly, we can get the functions of interactions of excitons with the photons

$$\begin{aligned} F'^g(\mathbf{k}, \mathbf{q}') = (2I\Omega)^{-1/2} & \left\{ \frac{3A^*iZ}{4a} [\sin \mathbf{k}a - \sin(\mathbf{k} + \mathbf{q}')a] \right. \\ & \left. + \frac{3A^vZ \sin 2v}{8(1 - 3\cos^2 v)} [\cos \mathbf{k}a + \cos(\mathbf{k} + \mathbf{q}')a] \right\} \end{aligned} \quad (10a)$$

where I is the momentum of inertia of a molecule, A^v and A^*/a are the relative amplitudes showing the contributions of rotations and of shifts along Z axis into the optical branch correspondingly. We assume that the first terms of the sum in (10a) is small, thus taking that the optical branch is caused by the rotations of molecules relative to the equilibrium position. Such an approximation does not affect the qualitative results of the theory.

In the following we shall use the notation

$$\beta = \frac{3A^vZ \sin 2v}{8\sqrt{2I\Omega}(1 - 3\cos^2 v)} \quad (10b)$$

If we introduce (7a), (9), (10a) and (10b) into (6) and take account of (3b), then we obtain

$$A'''(\omega_{\pm}^0) = \beta^2 [\cos \mathbf{k}\mathbf{a} + \cos (\mathbf{k} + \mathbf{q}')\mathbf{a}]^2 \times \left[\pm \sqrt{\delta^2 + \frac{Z^2}{4} \cos^2 (\mathbf{k} + \mathbf{q}')\mathbf{a}} + \frac{Z}{2} \cos (\mathbf{k} + \mathbf{q}')\mathbf{a} \right] \quad (6b)$$

where

$$\delta = \Delta\epsilon^1 - \Delta\epsilon^2 \quad (11)$$

$$\omega_+^0 - \omega_-^0 = \sqrt{\delta^2 + \frac{Z^2}{4} \cos^2 (\mathbf{k} + \mathbf{q}')\mathbf{a}} \quad (12a)$$

$$\omega - \omega_{\pm}(\Omega) = \epsilon - \frac{1}{2} \left[\frac{Z}{2} \cos (\mathbf{k} + \mathbf{q}')\mathbf{a} \pm \sqrt{\delta^2 + \frac{Z^2}{4} \cos^2 (\mathbf{k} + \mathbf{q}')\mathbf{a}} \right] \quad (12b)$$

$$\epsilon = \omega + \Omega - \frac{\Delta\epsilon^1 + \Delta\epsilon^2}{2} \quad (12c)$$

It will be convenient for the subsequent analyses to express all the quantities as the width of exciton bands. Assuming $Z > 0$ we introduce the notations

$$\epsilon_0 = \frac{4\epsilon}{Z}; \quad \delta_0 = \frac{2\delta}{Z}; \quad \beta_0 = \frac{\beta^2}{Z}. \quad (13)$$

Using instead of summation at \mathbf{q}' an integration with the help of the equation

$$\frac{1}{N} \sum_{\mathbf{q}'} \dots = \frac{1}{2\pi} \int dz \dots \quad (14)$$

where

$$z = (\mathbf{k} + \mathbf{q}')\mathbf{a}; \quad x = \mathbf{k}\mathbf{a}$$

and having introduced (6b), (12a–12c) and (13) into (5), we get a final expression for the mass operator

$$M_+(\mathbf{k}, \omega) = \frac{2\nu_0 \beta_0}{\pi} \int_{-\pi}^{\pi} \frac{(\cos x + \cos z)^2}{\sqrt{\delta_0^2 + \cos^2 z}} \left\{ \frac{\sqrt{\delta_0^2 + \cos^2 z} + \cos z}{\epsilon_0 - \sqrt{\delta_0^2 + \cos^2 z} - \cos z + i\eta} + \frac{\sqrt{\delta_0^2 + \cos^2 z} - \cos z}{\epsilon_0 + \sqrt{\delta_0^2 + \cos^2 z} - \cos z + i\eta} \right\} dz \quad (15)$$

The value $i\eta$ which has appeared in the denominator is caused by the necessity of the substitution of ω for $\omega + i\eta$ in the finite expressions, to show the rule of the rounding of the poles. Besides, we

take $\cos x = 1$ since the momentum of a photon is small. The mass operator is a complex quantity which determines the width of the absorption bands and their shift caused by the interactions of intramolecular vibrations with the lattice phonons. Let us calculate the real and imaginary parts separately. For this we use the relation

$$\frac{1}{x + i\eta} = P \frac{1}{x} - i\pi\delta(x) \quad (16)$$

2. The Imaginary Part

After the introduction of (16) into (15), we get

$$\begin{aligned} \text{Im} M_+(\mathbf{k}, \omega) = & -2\nu_0^{-}\beta_0 \int_{-\pi}^{\pi} \frac{(1 + \cos z)^2}{\sqrt{\delta_0^2 + \cos^2 z}} \\ & \times \{ (\sqrt{\delta_0^2 + \cos^2 z} + \cos z) \delta(\epsilon_0 - \sqrt{\delta_0^2 + \cos^2 z} - \cos z) \\ & + (\sqrt{\delta_0^2 + \cos^2 z} - \cos z) \delta(\epsilon_0 + \sqrt{\delta_0^2 + \cos^2 z} - \cos z) \} dz. \end{aligned} \quad (17)$$

The δ function entering the expression (17) is a complex one, and integration with its help can be done with the use of equation⁽⁴⁾

$$\delta[\phi(z)] = \sum_i \frac{1}{|\phi'(z_i)|} \delta(z - z_i) \quad (18a)$$

where z_i are the roots of the equation $\phi(z) = 0$. It is easily seen that these roots are determined by the equation.

$$z = \pm \arccos \frac{\epsilon_0^2 - \delta_0^2}{2\epsilon_0} \quad (18b)$$

and depending on the sign of the ϵ_0 the contribution into the solution is made either by the first or by the second term of a sum in expression (17). If we introduce (18a) and (18b) into (17) and take into account that $\cos z$ is even function, we get

$$\text{Im} M_+(\mathbf{k}, \omega) = -4\nu_0^{-}\beta_0 \frac{[1 \pm (\epsilon_0^2 - \delta_0^2)/(2|\epsilon_0|)]^2}{\sqrt{1 - [(\epsilon_0^2 - \delta_0^2)/(2|\epsilon_0|)]^2}} \quad (19)$$

The signs \pm are related to inequalities $\epsilon_0 \gtrless 0$ correspondingly.

3. The Real Part

$$\begin{aligned} \operatorname{Re} M_+(\mathbf{k}, \omega) &= \frac{2\nu_0^{-}\beta_0}{\pi} \int_{-\pi}^{\pi} \frac{(1 + \cos z)^2}{\sqrt{\delta_0^2 + \cos^2 z}} \\ &\times \left\{ \frac{\sqrt{\delta_0^2 + \cos^2 z} + \cos z}{\epsilon_0 - \sqrt{\delta_0^2 + \cos^2 z} - \cos z} \right. \\ &\left. + \frac{\sqrt{\delta_0^2 + \cos^2 z} - \cos z}{\epsilon_0 + \sqrt{\delta_0^2 + \cos^2 z} - \cos z} \right\} dz \end{aligned} \quad (20a)$$

Here the dash near the sign of the integral means that the latter must be calculated in a sense of the principal value. It will be convenient to introduce a new variable

$$\sqrt{\delta_0^2 + \cos^2 z} = \cos z + x \quad (21a)$$

If we also take into account that the even function of z is under the sign of the integral (20a), than after the simple transformations we get

$$\operatorname{Re} M_+(\mathbf{k}, \omega) = \frac{2\nu_0^{-}\beta_0}{\pi} \int_{x_H}^{x_b} \frac{(2x + \delta_0^2 - x^2)^2 dx}{x^2 \sqrt{(x_b^2 - x^2)(x^2 - x_H^2)}} \left[\frac{\delta_0^2}{\epsilon_0 x - \delta_0^2} + \frac{x}{\epsilon_0 + x} \right] \quad (20b)$$

where

$$x_b = \sqrt{\delta_0^2 + 1} + 1 \quad (21b)$$

$$x_H = \sqrt{\delta_0^2 + 1} - 1$$

It is evident from Eq. (20b) that this integral cannot be taken in algebraic form since it is the elliptical integral. Subsequent simplifications of expression (20b) can be made by separating the odd and even parts of the function $f(x)$ under the integral sign according to the relation

$$f(x) = \frac{f(x) + f(-x)}{2} + \frac{f(x) - f(-x)}{2} \quad (22)$$

If we rewrite (20b) as

$$\operatorname{Re} M_+(\mathbf{k}, \omega) = J_1 + J_2 \quad (23)$$

where J_1 and J_2 are connected with the even and the odd parts of $f(x)$ correspondingly, then

$$J_2 = \frac{\nu_0^{-1}\beta_0}{\pi} \int_{x_H^2}^{x_b^2} \frac{dy}{y\sqrt{(x_b^2 - y)(y - x_H^2)}} \left[\frac{(\delta_0^2 - y)^2\epsilon_0 + 4(\delta_0^2 - y)\delta_0^2 + 4y\epsilon_0\delta_0^2}{\epsilon_0^2 y - \delta_0^2} - \frac{(\delta_0^2 - y)^2\epsilon_0 - 4y(\delta_0^2 - y) + 4y\epsilon_0}{y - \epsilon_0^2} \right] \quad (24a)$$

where $y = x^2$. The sub-integral function (24a) can be represented in simple fractions, which gives a set of integrals of a form

$$\int_{x_H^2}^{x_b^2} \frac{dy}{(y - a_i)^k \sqrt{(x_b^2 - y)(y - x_H^2)}} \quad (24b)$$

where $k = 0, 1$; $i = 1, 2, 3$. They can be easily calculated with the help of a simple substitution of the variable

$$\sqrt{(x_b^2 - y)(y - x_H^2)} = \nu(y - x_H^2) \quad (24c)$$

The values a_i in (24b) are determined as follows

$$a_1 = 0; a_2 = \frac{\delta_0^4}{\epsilon_0^2}; a_3 = \epsilon_0^2 \quad (25)$$

and a_2, a_3 are frequency-dependent, according to (12c) and (13), so that the value of the integral (24b) depends upon the frequency interval where it is calculated. The result of the calculation is

$$J_2 = \nu_0^{-1}\beta_0 \left[\frac{2\delta_0^2}{\epsilon_0} - 2\epsilon_0 - 5 + \phi(\epsilon_0, \delta_0) \right] \quad (26a)$$

where

$$\begin{aligned} \phi(\epsilon_0, \delta_0) = & \mu \left[\frac{4\epsilon_0^2 - 4\delta_0^2\epsilon_0 - 2\delta_0^2\epsilon_0^2 + \delta_0^4 + \epsilon_0^4 + \epsilon_0^3}{\epsilon_0^3} \right. \\ & \times \frac{1}{\sqrt{[x_b^2 - (\delta_0^4/\epsilon_0^2)][x_H^2 - (\delta_0^4/\epsilon_0^2)]}} \\ & + \frac{4\epsilon_0^2 - 4\delta_0^2\epsilon_0 - 2\delta_0^2\epsilon_0^2 + \epsilon_0^4 + 4\epsilon_0^3 + \delta_0^4}{\epsilon_0} \\ & \left. \times \frac{1}{\sqrt{(x_b^2 - \epsilon_0^2)(x_H^2 - \epsilon_0^2)}} \right] \quad (26b) \end{aligned}$$

$$\mu = \begin{cases} -1 & \text{for } |\epsilon_0| \leq x_H \\ +1 & \text{for } |\epsilon_0| \geq x_b \\ 0 & \text{for } x_H < |\epsilon_0| < x_b \end{cases} \quad (26c)$$

It is seen from (26a) and (26b) that the integral goes to 0 when $\epsilon_0 \rightarrow 0$; $\pm \infty$; its sign being determined by the signs of ϵ_0 and μ . Inside the interval $[x_H, x_b]$ J_2 will be a smooth function; when we approach the boundaries of this interval from the outside J_2 goes to infinite.

$$J_1 = \frac{\nu_0 - \beta_0}{\pi} \int_{x_H}^{x_b} \frac{dx}{x^2 \sqrt{(x_b^2 - x^2)(x^2 - x_H^2)}} \times \left[\frac{(\delta_0^2 - x^2)^2 \delta_0^2 + 4\epsilon_0 x^2 (\delta_0^2 - x^2) + 4x^2 \delta_0^2}{\epsilon_0^2 x^2 - \delta_0^2} + \frac{(\delta_0^2 - x^2)^2 x^2 - 4x^2 (\delta_0^2 - x^2) \epsilon_0 + 4x^2}{x^2 - \epsilon_0^2} \right] \quad (27a)$$

The sub-integral function can be also expanded in fractions relative to x^2 so that the integral J_1 will take a form⁽⁵⁾

$$J_1 = \frac{\nu_0 - \beta_0}{\pi x_b} \left[\left(\frac{\delta_0^2}{\epsilon_0^2} - \frac{4}{\epsilon_0} + \epsilon_0^2 + 4\epsilon_0 + 4 - 2\delta_0^2 \right) F\left(\frac{\pi}{2}; k\right) + x_b^2 E\left(\frac{\pi}{2}; k\right) - \frac{\delta_0^2}{x_b^2} \Pi\left(\frac{\pi}{2}; -k^2; k\right) + \frac{4\epsilon_0^3 \delta_0^2 + 4\delta_0^2 \epsilon_0^2 - 2\delta_0^4 \epsilon_0^2 + \delta_0^6 - 4\delta_0^4 \epsilon_0 + \epsilon_0^4 \delta_0^2}{\epsilon_0^4 (x_b^2 - (\delta_0^4 / \epsilon_0^2))} \times \Pi\left(\frac{\pi}{2}; n_1; k\right) + \frac{\epsilon_0^4 + 4\epsilon_0^3 + 4\epsilon_0^2 - 2\delta_0^2 \epsilon_0^2 - 4\delta_0^2 \epsilon_0 + \delta_0^4}{x_b^2 - \epsilon_0^2} \times \Pi\left(\frac{\pi}{2}; n_2; k\right) \right] \quad (27b)$$

where

$$F\left(\frac{\pi}{2}; k\right); E\left(\frac{\pi}{2}; k\right); \Pi\left(\frac{\pi}{2}; n; k\right)$$

are the full elliptical integrals of the 1st, 2nd, and 3rd type correspondingly.

Here

$$k^2 = \frac{x_b^2 - x_H^2}{x_b^2}; n_1 = \frac{x_b^2 - x_H^2}{(\delta_0^4 / \epsilon_0^2) - x_b^2}; n_2 = \frac{x_b^2 - x_H^2}{\epsilon_0^2 - x_b^2}. \quad (28)$$

The value of J_1 , at large and small frequencies goes to the constant determined by the second member of the expression (27b). Near the values $|\epsilon_0| = x_H$ and $|\epsilon_0| = x_b$ in this expression also the specialities arise connected with the last two members. Their analyses show that J_1 is a smooth function inside the interval $[x_H, x_b]$ while outside of it (near x_H and x_b) it goes to infinity.

All the calculations made so far were related to the value $M_+(\mathbf{k}, \omega)$ of the mass operator. They will be held also for $M_-(\mathbf{k}, \omega)$, one should only change the sign before Ω in finite expressions and substitute ν_0^- for ν_0^+ .

The real and imaginary parts of the mass operator are presented in Fig. 1a.

If no interaction with phonons took place, there should be two sharp maxima in Fig. 1a with the peak frequencies ω_{\pm}^0 .

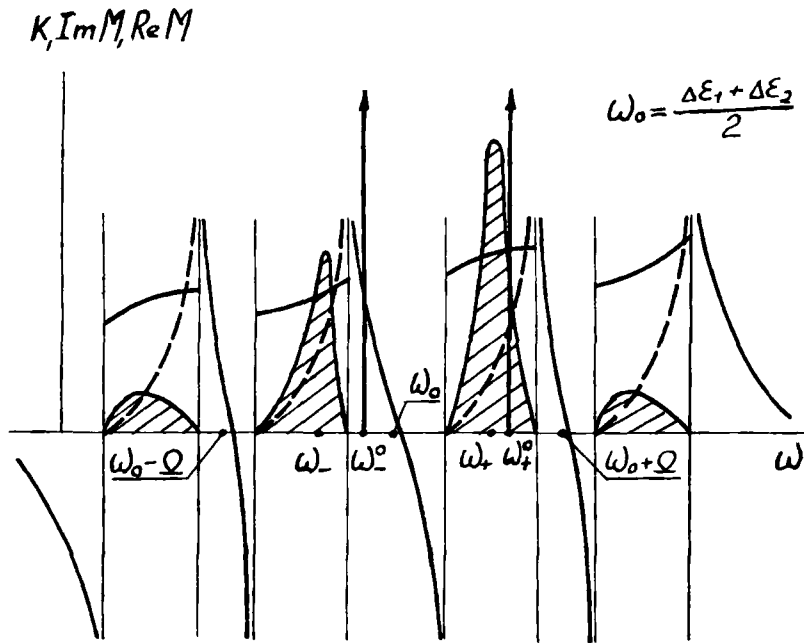


Figure 1a. The mass operator and the shape of the absorption band for the case of linear chain at presence of the Fermi-resonance.

The dashed line gives the imaginary part, the solid line the real part, the crossed regions the absorption bands. To the left from $\omega_0 M(\mathbf{k}, \omega) \sim \nu_0$ to the right from $\omega_0 M(\mathbf{k}, \omega) \sim (1 + \nu_0)$.

The participation of the phonons leads to the shift and broadening of these bands. It is also seen from Fig. 1a that there will be four bands instead of two.

This is apparently caused by the fact that the processes accompanied by an absorption as well as those accompanied by an emission of lattice phonons both contribute to the mass operator. Then even for one level we must expect an appearance of two peaks separated by the distance $\sim 2\Omega$ (which depends also upon the structure of exciton bands). These peaks will be different since an absorption band is determined not only by the mass operator (see (10c) Part I) but also by the values of $\omega - \omega_{\pm}$. In the frequency region where $\text{Im}M(\mathbf{k}, \omega) \neq 0$ and $\omega - \omega_{+(-)} = 0$ the peak will be sharp, but when also $\omega - \omega_{+(-)} \neq 0$, it will be essentially weaker. An account of the next approximation will make the sharp edges of the bands more smooth⁽⁶⁾ and the absorption spectra will become similar to that shown in Fig. 1b. It

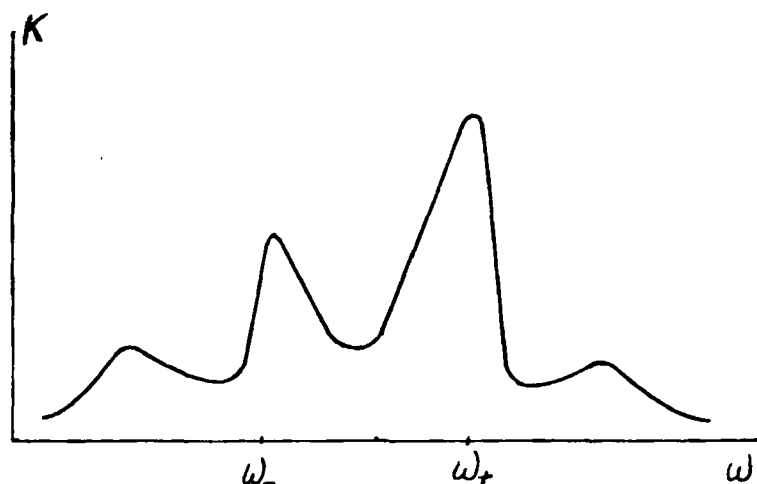


Figure 1b. The shape of the absorption band at account in the mass operator of the corrections of the higher order.

may be possible that the additional maxima will be very weak or even completely absent; this depends on the parameters Ω , δ_0 and β_0 of the substance. Thus, in addition to the effect of the resonant over-lapping of the bands (see Part I), when the half-width of the bands is comparable to the distance between the maxima, the

frequency dependence of $M''(\mathbf{k}, \omega)$ given an extra distortion leading to the appearance of an excess absorption maxima.

If $\delta_0 \rightarrow 0$ as it is evident from (15), one of the members of the sum in the mass operator will disappear and we come to the case of one band.⁽⁶⁾ At an increase of δ_0 the frequencies ω_-^0 and ω_+^0 drift from each other, and the absorption spectrum will consist of two isolated bands. It is also seen from Fig. 1a that upon decrease of the temperature, the intensity of the component ω_- will surpass the absorption in the maximum for the component ω_+ , i.e. for the values of the parameters chosen the case *c* is realized (see Part I, Fig. 1). The change of these parameters can lead to the other behaviour of the components of the doublet examined.

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