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A THEORY OF THE DISPERSION OF THE HIGH-FREQUENCY EXCITON CONDUCTIVITY OF A CRYSTAL

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We have applied the diagram technique developed in reference 5 to the evaluation of the high-frequency conductivity. We obtain exciton states with large radii which occur near the threshold for the direct transition, whatever the position of the band extrema. We determine the exciton absorption spectrum and show that the fine structure of the exciton absorption lines is connected with a Doppler shift.

1. CLASSIFICATION OF THE DIRECT TRANSITIONS

THE absorption spectrum connected with the excitation of large radius excitons is a set of lines near the red limit of the main absorption of the crystal. The structure of the exciton states is connected in an essential way with the character of the interband transition responsible for the main absorption. The character of the interband transition is in turn determined by the relative position of the energy surfaces of the valence band and the conduction band in the Brillouin zone. The transitions that occur without the participation of phonons (direct transitions) are usually considered for the case (case a) where the extrema of the valence band and of the conduction band lie in the same point in momentum space. A number of authors[1-3] have considered the exciton states accompanying such a direct transition.

In the case when the energy maximum of the valence band and the minimum of the conduction band are in different points of **p**-space (case b), one usually only pays attention to the indirect transitions that involve the participation of a phonon.[1] The exciton spectrum accompanying a direct transition of this latter type is of some interest. The absorption coefficient connected with the main transition is an increasing function of the frequency. The initial section of this curve is determined in case b by the indirect transition. The absorption coefficient is relatively small in this section. It increases steeply near the frequency ω_0 at which the direct transition becomes possible. The exciton absorption spectrum due to the direct transition will lie in the region of the indirect transition. It is the purpose of the present paper to study exciton states of this latter type.

The direct transition proceeds in case b from a point on the slope of the energy surface of the valence band to a point on the slope of the energy surface of the conduction band in such a way that these points correspond to the same wave vector apart from the small wave vector of the light. It is clear that such a transition occurs first at a frequency ω_0 corresponding to the minimum value for the difference between the energies in the bands at the same electron wave vector. Because of the crystal symmetry there will be in **p**-space several such completely identical threshold points for the direct transition $\mathbf{K}_1, \ldots, \mathbf{K}_i, \ldots$.

We shall show that an exciton is formed near each threshold point for a direct transition $\mathbf{K}_i$. These excitons are equivalent, and their spectra are the same if we neglect the wave vector of the light. Each of them, however, is formed by the absorption of light by an electron which has a non-vanishing average velocity $\mathbf{v}_i = \partial\epsilon_{\mathbf{p}}/\partial\mathbf{p}\,|_{\mathbf{p}=\mathbf{K}_i}$. It is clear that such an electron perceives the light with a Doppler shift $\Delta\omega_i = \boldsymbol{\kappa}\cdot\mathbf{v}_i$ where κ is the wave vector of the light. Since the velocities of the electrons in the different points $\mathbf{K}_i$ are in different directions, the exciton absorption line will be split into several components corresponding to the excitons in the different points $\mathbf{K}_i$, while the position of these components will depend on the orientation of the wave vector of the light with respect to the crystal axes. This effect is specific for the exciton absorption spectrum.

2. THE DIAGRAM TECHNIQUE FOR THE EVALUATION OF THE HIGH-FREQUENCY ELECTRON CONDUCTIVITY OF THE CRYSTAL

We construct the solution of the problem by using the simple model of an electron gas located in a periodic field, and we assume that the interaction between the electrons is sufficiently weak so that the effective interaction energy can be assumed to be much less than the width of the forbidden band. A phenomenological approach of this kind is the usual one in the theory of the Mott excitons.[1-3]

We consider a system of electrons in the periodic field of the lattice which fills the valence band. The Hamiltonian H of the system is of the form

$$H = H_0 + U; \qquad H_0 = \sum_{j\mathbf{p}} \varepsilon_{j\mathbf{p}} a^+_{j\mathbf{p}} a_{j\mathbf{p}},$$

$$U = \sum U^{j_3\mathbf{p}_3,\ j_4\mathbf{p}_4}_{j_1\mathbf{p}_1,\ j_2\mathbf{p}_2} a^+_{j_3\mathbf{p}_3} a^+_{j_4\mathbf{p}_4} a_{j_2\mathbf{p}_2} a_{j_1\mathbf{p}_1},$$

$$U^{j_3\mathbf{p}_3,\ j_4\mathbf{p}_4}_{j_1\mathbf{p}_1,\ j_2\mathbf{p}_2} = \sum_{\gamma,n,m} \frac{4\pi e^2}{\varepsilon\gamma^2 V} \delta_{\gamma+\mathbf{p}_1,\ \mathbf{p}_3+\mathbf{b}n} \delta_{\gamma+\mathbf{p}_4,\mathbf{p}_2+\mathbf{b}_m} \Gamma_{j_1j_3}$$
$$\times (\mathbf{p}_1; \mathbf{p}_3, \gamma) \Gamma_{j_2j_4} (\mathbf{p}_2, \mathbf{p}_4, -\gamma),$$

$$\Gamma_{j_1j_3} (\mathbf{p}_1, \mathbf{p}_3, \gamma) = \int_{V_0} e^{i\gamma\mathbf{x}} \psi^*_{j_3\mathbf{p}_3}(\mathbf{x}) \psi_{j_1\mathbf{p}_1}(\mathbf{x})\, d\mathbf{x}. \tag{1}$$

Here $a^+_{j\mathbf{p}}$ and $a_{j\mathbf{p}}$ are respectively the creation and the annihilation operators of an electron in a state in the j-th band with a quasi-momentum $\mathbf{p}$, which is described by a Bloch wave function $\psi_{j\mathbf{p}}(\mathbf{x})$; $\epsilon_{j\mathbf{p}}$ is the energy of this state; V is the normalizing volume; V_0 the volume of the elementary cell in the crystal; $\mathbf{b}_m$ and $\mathbf{b}_n$ are vectors which are multiples of the reciprocal lattice vector; the summation in the equation for U is over all the encountered band numbers and quasi-momenta. The quantity ϵ is the dielectric constant, which decreases the electron-electron interaction; we assume it to be a scalar for the sake of simplicity, although one can easily generalize the final result to the case where ϵ is a tensor.

We use Eq. (4a) of reference 5 to find a correction to the single-particle density matrix $f_{j\mathbf{p},j'\mathbf{p}'}$ which is proportional to the intensity of the applied electrical field $E_\mu(\mathbf{x}, t) = E_\mu(\kappa, s) \exp(i\kappa \cdot \mathbf{x} + st)$, where $s = -i\omega + \nu$, κ and ω are the wave vector and the frequency of the light, and ν is an adiabatic parameter (in the final equations $\nu \to 0$). We have, indeed,

$$f_{j\mathbf{p},\ j'\mathbf{p}'}(t)$$
$$= E_\mu(\mathbf{x}, s)\, e^{st} \sum_{i\mathbf{k},\ i'\mathbf{k}'} G^{i'\mathbf{k}',\ j'\mathbf{p}'}_{i\mathbf{k},\ j\mathbf{p}}(s, \beta) \int e^{i\kappa\mathbf{x}} j_\mu(\mathbf{x})_{i\mathbf{k},i'\mathbf{k}'} d\mathbf{x}; \tag{2a}$$

$$G^{i'\mathbf{k}',\ j'\mathbf{p}'}_{i\mathbf{k},\ j\mathbf{p}}(s, \beta) = Z^{-1} \int_{-\infty}^{0} e^{s\tau} d\tau \int_0^\beta d\lambda\, \mathrm{Sp} \left\{ e^{-\beta H} \exp\left[\frac{H(\tau + i\hbar\lambda)}{i\hbar}\right] a^+_{j\mathbf{p}} a_{j'\mathbf{p}'} \right.$$
$$\left. \times \exp\left[-\frac{H(\tau + i\hbar\lambda)}{i\hbar}\right] a^+_{i\mathbf{k}} a_{i'\mathbf{k}'} \right\}, \tag{2b}$$

$$(j_\mu(\mathbf{x}))_{i\mathbf{k},\ i'\mathbf{k}'}$$
$$= (e/2m) [\psi^*_{i\mathbf{k}}(\mathbf{x}) \hat{\mathbf{P}}_\mu \psi_{i'\mathbf{k}'}(\mathbf{x}) - \psi_{i'\mathbf{k}'}(\mathbf{x}) \hat{\mathbf{P}}_\mu \psi^*_{i\mathbf{k}}(\mathbf{x})], \tag{2c}$$

$Z = \mathrm{Sp}\, e^{-\beta H}$, $\beta = T^{-1}$, T is the absolute temperature in energy units.

To evaluate the function $G^{i'\mathbf{k}',j'\mathbf{p}'}_{i\mathbf{k},j\mathbf{p}}(s, \beta)$ we use a diagram technique.[5] The feature of our case is that we have chosen the Bloch wave functions as the single-electron states. It is clear that in that case each line corresponds to the combination of the indices j and $\mathbf{p}$. The vertex describing the electron-electron interaction is drawn in Fig. 1; it corresponds to the factor

$$\pm (i\hbar)^{-1} \sum_{mn} \frac{4\pi e^2 \varepsilon^{-1}}{V(\mathbf{p}_3 - \mathbf{p}_1 + \mathbf{b}_n)^2} \Gamma_{j_1j_3} (\mathbf{p}_1, \mathbf{p}_3, \mathbf{p}_3 - \mathbf{p}_1 + \mathbf{b}n)$$
$$\times \Gamma_{j_2j_4} (\mathbf{p}_2, \mathbf{p}_4, \mathbf{p}_2 - \mathbf{p}_4 - \mathbf{b}_m) \delta_{\mathbf{p}_1+\mathbf{p}_2-\mathbf{p}_3-\mathbf{p}_4,\ \mathbf{b}_m-\mathbf{b}_n}.$$

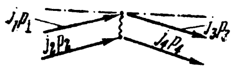

FIG. 1

The absolute magnitude of the quasi-momentum of any line is less than half a reciprocal lattice vector. Because of this, the quantity $\mathbf{b}_n - \mathbf{b}_m$ is less than a reciprocal lattice vector. It is clear that a factor $1 - n_{j\mathbf{p}}$ or $n_{j\mathbf{p}}$, where $n_{j\mathbf{p}}$ is a Fermi function, will correspond to a line. We shall consider the case $T \ll \hbar\omega_0'$; then $n_{j\mathbf{p}} = 0$, if j is an index of an unfilled band, and $n_{j\mathbf{p}} = 1$ if j is the index of a filled band.

We consider successively different approximations of perturbation theory. In Fig. 2 we give the zeroth order term. This diagram corresponds to the expression

$$\delta_{ij'}, \delta_{i'j} \delta_{\mathbf{p}\mathbf{k}'} \delta_{\mathbf{k}\mathbf{p}'} \sigma^{-1} (\sigma + \varepsilon_{j'\mathbf{p}'} - \varepsilon_{j\mathbf{p}})^{-1} [s + i\hbar^{-1} (\varepsilon_{j\mathbf{p}} - \varepsilon_{j'\mathbf{p}'})]^{-1}.$$

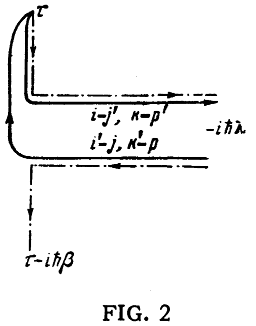

FIG. 2

The index j refers to a filled band and the index j′ to an empty band.

Since the frequency of the light is close to the threshold frequency ω_0 for a direct transition, the dominant zeroth order term will be the one where the index j is the same as the index v, referring to the valence band and when the index j′ is the same as the index c referring to the conduction band. For that term the denominator is a minimum. The threshold frequency for a direct transition is given by $\omega_0 = \mathrm{Min}(\epsilon_{c\mathbf{p}+\kappa} - \epsilon_{v\mathbf{p}})$. From the condition

$$\frac{\partial}{\partial p_\nu}(\varepsilon_{c\mathbf{p}+\varkappa} - \varepsilon_{v\mathbf{p}})\big|_{\mathbf{p}=\mathbf{K}_i(\varkappa)} = 0$$

we can determine the momentum $\mathbf{K}_i(\kappa)$ of the electrons which undergo a direct transition at the absorption threshold. It will be clear that only the two above-mentioned bands will be important. We introduce the notation

$$\int e^{i\varkappa \mathbf{x}}(j_\mu(\mathbf{x}))_{c\mathbf{k},\,v\mathbf{k}'}d\mathbf{x} = \delta_{\mathbf{k},\,\mathbf{k}'+\varkappa}\, j_\mu(\mathbf{k}',\varkappa),$$

$$j_\mu(\mathbf{k}',\varkappa) \equiv \int\limits_{V_0} e^{i\varkappa\mathbf{x}}(j_\mu(\mathbf{x}))_{c\mathbf{k}'+\varkappa,\,v\mathbf{k}'}d\mathbf{x}. \qquad (3)$$

One sees easily that

$$\int e^{-i\xi\mathbf{x}}(j_\nu(\mathbf{x}))_{v\mathbf{p},\,c\mathbf{p}'}\,d\mathbf{x} = \delta_{\mathbf{p}',\,\mathbf{p}+\xi}\; j_\nu^*(\mathbf{p},\,\xi).$$

We have not considered here the possibility of an Umklapp process for which $\mathbf{k}' + \kappa - \mathbf{k}' = \mathbf{b}$ ($\mathbf{b}$ is the reciprocal lattice vector), since the limits between which κ can vary are limited to a very small region of order κ near the edge of the Brillouin zone and the corresponding integral over $\mathbf{k}'$ will be small.

3. ELIMINATION OF SINGULAR DIAGRAMS

Some first-order diagrams are drawn in Fig. 3. We note a characteristic singularity of the diagram 3a. To do this we write down the contribution $J_\nu^{(1)}(\mathbf{y})$ to the average current density of the system in the point y:

$$J_\nu^{(1)}(\mathbf{y}) = \sum_{\mathbf{pp}'} f^{(1)}_{v\mathbf{p},\,c\mathbf{p}'}(j_\nu(\mathbf{y}))_{v\mathbf{p},\,c\mathbf{p}'}. \qquad (4a)$$

Here

$$j_\nu(\mathbf{y})_{v\mathbf{p},\,c\mathbf{p}'} = \frac{1}{V}\sum_\xi e^{i\xi\mathbf{y}} j_\nu^*(\mathbf{p},\,\xi)\,\delta_{\mathbf{p}',\,\mathbf{p}+\xi}, \qquad (4b)$$

and $j_\nu(\mathbf{p},\xi)$ is defined by Eq. (3b);

$$f^{(1)}_{v\mathbf{p},\,c\mathbf{p}'} = -(i\hbar)^{-1}\sum_{\mathbf{kk}'}\sum_{mn}\frac{E_\mu(\varkappa,\,s)\,e^{st}}{\varepsilon_{c\mathbf{k}} - \varepsilon_{v\mathbf{k}'}}\,\frac{\delta_{\mathbf{k},\,\mathbf{k}'+\varkappa}}{s + i(\varepsilon_{c\mathbf{k}} - \varepsilon_{v\mathbf{k}'})/\hbar}$$

$$\times\left[s + \frac{i}{\hbar}(\varepsilon_{c\mathbf{p}'} - \varepsilon_{v\mathbf{p}})\right]^{-1}\frac{4\pi e^2\varepsilon^{-1}}{V(\mathbf{k}' - \mathbf{p} + \mathbf{b}_n)^2}\Gamma_{vv}$$

$$\times(\mathbf{p},\,\mathbf{k}',\,\mathbf{k}' - \mathbf{p} + \mathbf{b}_n)\,\Gamma_{cc}(\mathbf{k},\,\mathbf{p}',\,\mathbf{k} - \mathbf{p}' - \mathbf{b}_m)\,\delta_{\varkappa-\xi,\,\mathbf{b}_m-\mathbf{b}_n}. \qquad (4c)$$

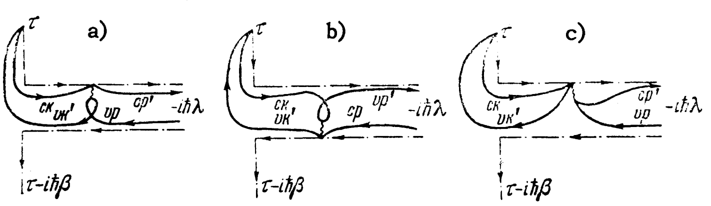

FIG. 3

The most important term in Eq. (4a) is, when we take (4b) and (4c) into account, the term with $\mathbf{b}_m = \mathbf{b}_n = 0$, in which there occurs an integral of the type

$$\int\frac{d\mathbf{k}'\,d\mathbf{p}}{(\mathbf{k}' - \mathbf{p})^2}A(\mathbf{k}',\,\mathbf{p})\left[s + \frac{i}{\hbar}(\varepsilon_{c\mathbf{k}'+\varkappa} - \varepsilon_{v\mathbf{k}'})\right]^{-1}$$

$$\times\left[s + \frac{i}{\hbar}(\varepsilon_{c\mathbf{p}+\varkappa} - \varepsilon_{v\mathbf{p}})\right]^{-1}.$$

The denominator in the integrand has at $\omega = \omega_0$ the form

$$s + i\hbar^{-1}(\varepsilon_{c\mathbf{p}+\varkappa} - \varepsilon_{v\mathbf{p}}) = \nu - \mu_{\alpha\beta}[\mathbf{p} - \mathbf{K}_i(\varkappa)]_\alpha[\mathbf{p} - \mathbf{K}_i(\varkappa)]_\beta$$

if p is near $\mathbf{K}_i(\kappa)$; $A(\mathbf{k}',\mathbf{p})$ is a function which is finite for $\mathbf{k}' = \mathbf{p} = \mathbf{K}_i(\kappa)$. It is clear that the integral diverges logarithmically as $\nu \to 0$. The terms connected with Umklapp processes for which $\mathbf{b}_m$ or $\mathbf{b}_n$ are different from zero are finite and small, since we have assumed that the reciprocal of the dielectric constant is sufficiently small. We shall therefore not consider Umklapp processes in the following, and put $\mathbf{b}_m = \mathbf{b}_n = 0$ at each vertex. Similarly we shall not take into account the diagrams of Figs. 3b and 3c. In these diagrams there is no divergence near the points $\mathbf{K}_i(\kappa)$: in diagram 3b the denominator corresponding to the last section on the right does not tend to zero, while in diagram 3c the interaction matrix element does not tend to infinity.

Turning to higher-order approximations in the perturbation theory, we shall retain only those terms which have the largest singularity for a given power of the small parameter ϵ^{-1}. Such terms are drawn in Fig. 4a. Other terms, even though they diverge for $\epsilon^{-1} \ll 1$, can be neglected in comparison with the ones taken into account. One can, for instance, neglect the diagram of Fig. 5 in comparison with the diagram 4a, since it has an extra small factor ϵ^{-2} for the same degree of divergence.

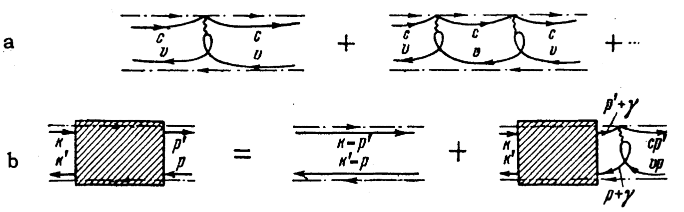

FIG. 4

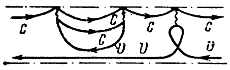

FIG. 5

All diagrams of Fig. 4a have a common factor corresponding to the horizontal section on the left so that it is convenient to introduce instead of the sum of the diagrams $G_{\mathbf{kp}}^{\mathbf{k'p'}}(s,\sigma)$ a quantity $F_{\mathbf{kp}}^{\mathbf{k'p'}}(s)$ such that

$$G_{\mathbf{kp}}^{\mathbf{k'p'}}(s,\sigma)=\frac{1}{\sigma}\frac{\delta_{\mathbf{k}+\mathbf{p},\,\mathbf{k}'+\mathbf{p}'}}{\sigma+\varepsilon_{c\mathbf{k}}-\varepsilon_{v\mathbf{k}'}}F_{\mathbf{kp}}^{\mathbf{k'p'}}(s). \tag{5}$$

We write down for the function $F_{\mathbf{kp}}^{\mathbf{k'p'}}(s)$ the equation depicted in Fig. 4b

$$F_{\mathbf{kp}}^{\mathbf{k'p'}}(s)=\delta_{\mathbf{k'p}}\left[s+i\hbar^{-1}(\varepsilon_{c\mathbf{p}'}-\varepsilon_{v\mathbf{p}})\right]^{-1}$$
$$-(i\hbar)^{-1}\sum_{\boldsymbol{\gamma}}F_{\mathbf{k},\,\mathbf{p}+\boldsymbol{\gamma}}^{\mathbf{k}',\,\mathbf{p}'+\boldsymbol{\gamma}}(s)\frac{4\pi e^2\varepsilon^{-1}}{V\gamma^2}\Gamma_{cc}(\mathbf{p}+\boldsymbol{\gamma},\mathbf{p},\boldsymbol{\gamma})$$
$$\times\Gamma_{vv}(\mathbf{p}',\mathbf{p}'+\boldsymbol{\gamma},-\boldsymbol{\gamma})\left[s+\frac{i}{\hbar}(\varepsilon_{c\mathbf{p}'}-\varepsilon_{v\mathbf{p}})\right]^{-1}. \tag{6}$$

One should note that the interaction matrix element has in that equation the opposite sign, because of the intersection on the line v. The potential energy term in Eq. (6) describes therefore an attraction. When $\epsilon^{-1}\ll 1$ only small momentum transfers γ are important in Eq. (6).

The quantities Γ_{cc} and Γ_{vv} are equal to unity for small γ. If we take this into account and also the fact that $\mathbf{p}'=\mathbf{p}+\boldsymbol{\kappa}$ and $\mathbf{k}=\mathbf{k}'+\boldsymbol{\kappa}$ we can write Eq. (6) in the form

$$(-i\hbar s+\varepsilon_{c\mathbf{p}+\boldsymbol{\varkappa}}-\varepsilon_{v\mathbf{p}})\,R(\mathbf{p},\mathbf{k}')$$
$$-\frac{4\pi e^2}{V}\sum_{\boldsymbol{\gamma}}\frac{\varepsilon^{-1}}{\gamma^2}R(\mathbf{p}+\boldsymbol{\gamma},\mathbf{k}')=-i\hbar\delta_{\mathbf{p},\,\mathbf{k}'}, \tag{7}$$

$$R(\mathbf{p},\mathbf{k}')\equiv F_{\mathbf{k}'+\boldsymbol{\varkappa},\,\mathbf{p}}^{\mathbf{k}',\,\mathbf{p}+\boldsymbol{\varkappa}}. \tag{8}$$

We have already pointed out that the difference $\epsilon_{c\mathbf{p}+\boldsymbol{\kappa}}-\epsilon_{v\mathbf{p}}$ is a minimum in a few points $\mathbf{K}_i(\boldsymbol{\kappa})$. The function $R(\mathbf{p},\mathbf{k}')$ can be seen to be large for large radius excitons only when $\mathbf{p}$ and $\mathbf{k}'$ are little different from $\mathbf{K}_i(\boldsymbol{\kappa})$. We shall find the function $R(\mathbf{p},\mathbf{k}')$ in the neighborhood of the point $\mathbf{K}_i(\boldsymbol{\kappa})\equiv\mathbf{K}_i+\boldsymbol{\lambda}$, $\mathbf{K}_i\equiv\mathbf{K}_i(0)$. In that region Eq. (7) is of the form

$$\Big\{-i\hbar s+\varepsilon_{c\mathbf{K}_i+\boldsymbol{\lambda}+\boldsymbol{\varkappa}}-\varepsilon_{v\mathbf{K}_i+\boldsymbol{\lambda}}+\frac{1}{2}\left[\frac{\partial^2}{\partial p_\nu\,\partial p_\mu}(\varepsilon_{c\mathbf{p}+\boldsymbol{\varkappa}}-\varepsilon_{v\mathbf{p}})\right]_{\mathbf{p}=\mathbf{K}_i+\boldsymbol{\lambda}}$$
$$\times(p-K_i-\lambda)_\nu(p-K_i-\lambda)_\mu\Big\}R(\mathbf{p},\mathbf{k}')$$
$$-\sum_{\boldsymbol{\gamma}}\frac{4\pi e^2\varepsilon^{-1}}{\gamma^2V}R(\mathbf{p}+\boldsymbol{\gamma},\mathbf{k}')=-i\hbar\delta_{\mathbf{p},\,\mathbf{k}'}. \tag{9}$$

We use the fact that $\boldsymbol{\kappa}$ and the quantity λ which is proportional to $\boldsymbol{\kappa}$ are small, and expand the kinetic energy (the sum within the square brackets) in Eq. (9), retaining no terms beyond those quadratic in $\boldsymbol{\kappa}$ and $\mathbf{p}-\mathbf{K}_i$. Equation (9) then becomes

$$\{-i\hbar s+E_0+\hbar\mathbf{v}^i\boldsymbol{\varkappa}+\tfrac{1}{2}M_{\alpha\beta}^{-1}\hbar^2\varkappa_\alpha\varkappa_\beta+\tfrac{1}{2}\mu_{\alpha\beta}^{-1}\hbar^2(p-K_i-\lambda)_\alpha$$
$$\times(p-K_i-\lambda)_\beta\}\,R(\mathbf{p},\mathbf{k}')$$
$$-\sum_{\boldsymbol{\gamma}}\frac{4\pi e^2\varepsilon^{-1}}{\gamma^2V}R(\mathbf{p}+\boldsymbol{\gamma},\mathbf{k}')=-i\hbar\delta_{\mathbf{p},\,\mathbf{k}'}, \tag{10}$$
$$E_0=\hbar\omega_0,\ \lambda_\alpha=-\left[(m_c^{-1}+m_v^{-1})^{-1}m_c^{-1}\right]_{\alpha,\,\beta}\varkappa_\beta,$$

$$M_{\alpha\beta}^{-1}=\left[m_c^{-1}(m_c^{-1}+m_v^{-1})^{-1}m_v^{-1}\right]_{\alpha\beta},\quad \mu_{\alpha\beta}^{-1}=(m_c^{-1}+m_v^{-1})_{\alpha\beta}, \tag{11}$$

where

$$(m_c^{-1})_{\alpha\beta}=\frac{1}{\hbar^2}\frac{\partial^2\varepsilon_{c\mathbf{p}}}{\partial p_\alpha\,\partial p_\beta}\bigg|_{\mathbf{p}=\mathbf{K}_i},\quad (m_v^{-1})_{\alpha\beta}=-\frac{1}{\hbar^2}\frac{\partial^2\varepsilon_{v\mathbf{p}}}{\partial p_\alpha\,\partial p_\beta}\bigg|_{\mathbf{p}=\mathbf{K}_i}$$

$$v_\alpha^i=\frac{1}{\hbar}\frac{\partial\varepsilon_{c\mathbf{p}}}{\partial p_\alpha}\bigg|_{\mathbf{p}=\mathbf{K}_i}=\frac{1}{\hbar}\frac{\partial\varepsilon_{v\mathbf{p}}}{\partial p_\alpha}\bigg|_{\mathbf{p}=\mathbf{K}_i}. \tag{12}$$

One checks easily that the solution of Eq. (10) is of the form

$$R(\mathbf{p},\mathbf{k}')=\begin{cases}\dfrac{1}{V}\displaystyle\sum_n\frac{\varphi_n(\mathbf{p}-\mathbf{K}_1-\boldsymbol{\lambda})\,\varphi_n^*(\mathbf{k}'-\mathbf{K}_1-\boldsymbol{\lambda})}{s+i(\omega_n+\mathbf{v}^i\boldsymbol{\varkappa})}, & \mathbf{p},\ \mathbf{k}'\sim\mathbf{K}_1+\boldsymbol{\lambda},\\[2ex] \dfrac{1}{V}\displaystyle\sum_n\frac{\varphi_n(\mathbf{p}-\mathbf{K}_i-\boldsymbol{\lambda})\,\varphi_n^*(\mathbf{k}'-\mathbf{K}_i-\boldsymbol{\lambda})}{s+i(\omega_n+\mathbf{v}^i\boldsymbol{\varkappa})}, & \mathbf{p},\ \mathbf{k}'\sim\mathbf{K}_i+\boldsymbol{\lambda}.\end{cases} \tag{13}$$

In all other cases R vanishes. In (13) $\hbar\omega_n=E_0+\tfrac{1}{2}M_{\alpha\beta}^{-1}\hbar^2\kappa_\alpha\kappa_\beta+\epsilon_n$ and the wave function $\varphi_n(\mathbf{q})$ of the n-th exciton state satisfies the equation

$$\mu_{\alpha\beta}^{-1}\frac{\hbar^2}{2}q_\alpha q_\beta\varphi_n(\mathbf{q})-\sum_{\boldsymbol{\gamma}}\frac{4\pi e^2}{\gamma^2}\frac{\varepsilon^{-1}}{V}\varphi_n(\mathbf{q}+\boldsymbol{\gamma})=\varepsilon_n\varphi_n(\mathbf{q}) \tag{14}$$

with eigenvalue ϵ_n.

If we take the Fourier transform of Eq. (14) we arrive at the normal Schrödinger equation, in coordinate representation, describing the internal motion of the exciton. $\varphi_n(\mathbf{q})$ turns out then to be the Fourier component of the normalized wave function $\tilde{\varphi}_n(\mathbf{r})$ in coordinate representation:

$$\varphi_n(\mathbf{q})=\int e^{i\mathbf{qr}}\tilde{\varphi}_n(\mathbf{r})\,d\mathbf{r},\quad \int|\tilde{\varphi}_n(\mathbf{r})|^2\,d\mathbf{r}=1. \tag{15}$$

4. THE HIGH-FREQUENCY CONDUCTIVITY AND THE ABSORPTION COEFFICIENT

Using Eqs. (13), (8), (5), (2a) and equations similar to (4a) and (4b), we find the high-frequency conductivity $\sigma_{\nu\mu}(\boldsymbol{\kappa},\omega)$

$$\sigma_{\nu\mu}(\boldsymbol{\varkappa},\omega)=E_0^{-1}(2\pi)^{-6}$$
$$\times\sum_{n,i}\int d\mathbf{p}\,d\mathbf{k}'\,\frac{\varphi_n(\mathbf{p}-\mathbf{K}_i-\boldsymbol{\lambda})\,\varphi_n^*(\mathbf{k}'-\mathbf{K}_i-\boldsymbol{\lambda})}{s+i(\omega_n+\mathbf{v}^i\boldsymbol{\varkappa})}j_\mu(\mathbf{k}',\boldsymbol{\varkappa})j_\nu^*(\mathbf{p},\boldsymbol{\varkappa}). \tag{16}$$

For allowed transitions, when $j_\mu(\mathbf{K}_i, 0) \neq 0$, the expression for $\sigma_{\nu\mu}$ can be simplified, since $\varphi(\mathbf{p} - \mathbf{K}_i - \boldsymbol{\lambda})$ is different from zero for large radius excitons only in a small region of **p**-space near the point $\mathbf{K}_i + \boldsymbol{\lambda}$. One can then neglect the $\mathbf{k}'$ dependence of the quantity $j_\mu(\mathbf{k}', \boldsymbol{\kappa})$, and remove it from under the integral sign at the point $\mathbf{K}_i$. The exciton high-frequency polarizability $\chi_{\nu\mu}(\boldsymbol{\kappa}, \omega) = \sigma_{\nu\mu}(\boldsymbol{\kappa}, \omega)/i\omega$ is then of the form

$$\chi_{\nu\mu}(\boldsymbol{\varkappa}, \omega) = \frac{e^2}{\hbar} \sum_n |\widetilde{\varphi}_n(0)|^2 \sum_j \frac{r^\nu_{vc}(\mathbf{K}_j)\, r^\mu_{cv}(\mathbf{K}_j)}{(\omega - \omega_n - \mathbf{v}^j \boldsymbol{\varkappa}) + i\nu},$$

$$r^\nu_{vc}(\mathbf{K}_j) = \int\limits_{V_0} \psi^*_{v\mathbf{K}_j}(\mathbf{r})\, r^\nu\, \psi_{c\mathbf{K}_j}(\mathbf{r})\, d\mathbf{r}. \tag{17}$$

This expression has the same form as the equation for the polarizability of a gas, with this difference that the quantity $|\widetilde{\varphi}_n(0)|^2$ plays the part of the concentration of the gas, so that the average distance between the "gas molecules" is equal to the exciton radius.

If we take relaxation processes into account we are led to a finite value of ν in Eq. (17). ν is then the reciprocal of the relaxation time. One obtains easily from Eq. (17) in that case an estimate for an expression for the exciton polarizability χ_l in one of the exciton absorption lines

$$\chi_l \sim (\omega_0/\nu)\,(r_a/r_e)^3, \tag{18}$$

where r_a is a quantity of the order of the interatomic distance and r_e the exciton radius.

If $\chi_l \geq (4\pi)^{-1}\epsilon$ one must solve a dispersion equation to find κ as a function of ω and take the exciton polarizability into account. The picture of the propagation of light through the crystal becomes then complicated (see references 6 and 7). In the present paper we restricted ourselves to the case $\chi_l \ll (4\pi)^{-1}\epsilon$. In that case $\kappa = (\omega/c)\sqrt{\epsilon}$. One obtains easily from Eq. (17) the absorption coefficient $\mathscr{K}_x(\boldsymbol{\kappa}, \omega)$ for an electromagnetic wave which is polarized along the x axis

$$\mathscr{K}_x(\boldsymbol{\varkappa}, \omega) = \frac{4\pi e^2}{\hbar c}\, \omega_0 \sum_n |\widetilde{\varphi}_n(0)|^2 \sum_j \frac{|r^x_{vc}|^2_j\, \nu}{\nu^2 + (\omega - \omega_n + \mathbf{v}^j \boldsymbol{\varkappa})^2}. \tag{19}$$

As before, we have assumed here that $\epsilon \gg 1$.

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