

The Mean Free Path of a Non-Localized Exciton in an Atomic Crystal

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The mean free path of a non-localized exciton in an atomic crystal is calculated under the assumption of interaction with thermal lattice vibrations.

INTRODUCTION

FRENKEL¹ first introduced the concept of excited electrons of dielectric crystals, which are not accompanied by a current of charged carriers, and formulated a quantitative theory of that phenomenon. Thus, the excited electron, by virtue of the translational symmetry of the crystal, does not remain bound to a particular point in the lattice, but can behave as a quasi-particle, possessing a wave vector \mathbf{k} and a certain quasi-momentum $\mathbf{p} = \hbar\mathbf{k}$. Frenkel called these quasi-particles excitons.

Frenkel² also introduced the concept of existence of two types of excitons, non-localized and localized. Non-localized excitons may be characterized as those that move in the excited crystal not accompanied by a localized or bound deformation of the lattice. Conversely, the localized exciton behaves as if, to quote Frenkel's figurative expression, "it were carrying the heavy burden of atomic displacements". Quite recently, Dykman and Pekar³ have shown that states corresponding to non-localized and localized excitons are obtained automatically if one takes into account the polarization conditions in an ionic crystal. It has also been found that the localized excitons are formed in an ionic crystal only if fairly rigid conditions are satisfied, namely, if the ratio of the effective masses of the hole and the electron is larger than ten. After the appearance of Frenkel's original work, a number of research papers devoted to the theory of the exciton were published. These papers dealt mainly with the basic point of the theory of the exciton — the conditions for its existence⁴. Wannier⁵ has shown that the states of a non-local-

ized exciton can be regarded as similar to the bound hydrogen-like states of an electron and a hole experiencing mutual Coulomb attraction. However, this condition may be regarded as a direct consequence of the effective mass method. One should not neglect to mention the investigations of Davydov⁶, who generalized the concept of the exciton and applied it to the study of spectra of molecular crystals.

In studying the internal photoelectric effect in copper oxide, Zhuze and Ryvkin⁷ arrived at the conclusion that their observations could not be interpreted without the introduction of the exciton concept. Further, the experimental investigations of the external photoelectric effect, conducted by Apker and Taft⁸ should be mentioned; the exciton concept is necessary, in the authors' opinion, to explain their results adequately. Finally, the work of Gross⁹ and his co-workers permits us, apparently, to speak of a direct experimental proof of the existence of the exciton. Thus, the excitons are becoming not merely theoretically permissible states of a crystal, but, evidently, ones that can be observed experimentally. It thus appears timely to conduct a more detailed study of the properties of the exciton; attention should first be given to the determination of the mean free path of the exciton, which determines the speed of migration of energy excitation in a crystal. The paper dealing with the interactions of the excitons and the phonons¹⁰, published some time ago, contains only numerical values of the mean free path of the exciton in various crystals. In the present study, the mean free path of a non-localized exciton is computed, on the basis of its interaction with the acoustic

¹I. A. Frenkel, Phys. Rev. 37, 17, 1276 (1931)

²I. A. Frenkel, J. Exper. Theoret. Phys. USSR 6, 647 (1936)

³I. M. Dikman and S. I. Pekar, Trudy In. Fiz. Akad. Nauk SSSR 3, 92 (1952)

⁴J. C. Slater and W. Shockley, Phys. Rev. 50, 705 (1936); W. R. Heller and A. Marcus, Phys. Rev. 84, 809 (1951)

⁵G. H. Wannier, Phys. Rev. 52, 191 (1937)

⁶A. S. Davydov, *Theory of the Absorption of Light in Molecular Crystals*, Kiev (1951)

⁷V. P. Zhuze and S. M. Ryvkin, Izv. Akad. Nauk SSSR, Ser. Fiz. 16, 93 (1952)

⁸L. Apker and E. Taft, Phys. Rev. 72, 964 (1950); Phys. Rev. 81, 698 (1951); Phys. Rev. 82, 814 (1951)

⁹E. F. Gross and I. A. Karryev, Doklady Akad. Nauk SSSR 84, 471 (1952)

¹⁰P. Leurgans and J. Bardeen, Phys. Rev. 87, 200 (1952)

branch of vibrations. It is assumed here that the internal state of the exciton is not changed by either its emission or absorption of phonons. We are not considering any of the competing processes, such as the disappearance of the non-localized exciton by the way of transition into a localized state, or the recombination of an electron and a hole accompanied by the transformation of the excitation energy into heat and light.

WAVE FUNCTION OF THE EXCITON AND ITS INTERACTION WITH PHONONS

Using the approximate method of effective mass, the wave function of a non-localized exciton of lowest excited state can be given by

$$\psi_{\text{exc}} = \frac{1}{V} e^{i\mathbf{k}\mathbf{R}} \frac{1}{V\pi a_{\text{exc}}^3} e^{-\rho/a_{\text{exc}}} \quad (1)$$

Here V is the fundamental cell of the crystal, \mathbf{k} is the wave vector of forward motion of the exciton, \mathbf{R} and ρ are the radius vectors of the center of inertia of the exciton and position of the electron with respect to the hole, that is,

$$\mathbf{R} = \frac{\mu_1 \mathbf{r}_1 + \mu_2 \mathbf{r}_2}{\mu_1 + \mu_2}, \quad \vec{\rho} = \mathbf{r}_1 - \mathbf{r}_2, \quad (2)$$

where μ_1 , μ_2 and \mathbf{r}_1 , \mathbf{r}_2 are the effective masses and radius vectors of the electron and hole (in what follows, the index 1 will refer to the electron and 2 to the hole), a_{exc} is the "radius of the exciton"

$$a_{\text{exc}} = \kappa \hbar^2 / \mu e^2, \quad (3)$$

where κ is the optical dielectric constant and $\mu = \mu_1 \mu_2 / (\mu_1 + \mu_2)$ is the reduced mass. If $\mu_1 = \mu_2 = m_e$ is the mass of the free electron, then a_{exc} is 2κ times as large as the atomic unit of length, equal to 0.53×10^{-8} cm. The large size of the ψ -cloud of the exciton justifies the approximate method of the effective mass. The state of the exciton [Eq. (1)] corresponds to an energy

$$E_0 = \frac{\hbar^2 k^2}{2\mu_{\text{exc}}} - \frac{\mu e^4}{2\kappa \hbar^2} = \varepsilon - \Delta E, \quad (4)$$

where the mass of the exciton $\mu_{\text{exc}} = \mu_1 + \mu_2$. The internal energy of the exciton ΔE is $2\kappa^2$ times (for $\mu_1 = \mu_2 = m_e$) lower than the ionization energy of a hydrogen atom, that is, it is comparable to thermal energies, even for not too high temperatures.

In what follows we will be interested only in such collisions between excitons and phonons for which

internal excitation or dissociation of the exciton will not occur. For collisions of the exciton, possessing a wave vector \mathbf{k} , with a phonon having a wave vector \mathbf{q} , and for minimal internal excitation of the exciton, we have the conservation laws

$$\mathbf{k} \pm \mathbf{q} = \mathbf{k}', \quad (5)$$

$$\frac{\hbar^2 k^2}{2\mu_{\text{exc}}} \pm \hbar v_0 q = \frac{\hbar^2 k'^2}{2\mu_{\text{exc}}} + \frac{3}{4} \Delta E, \quad (6)$$

where v_0 is the velocity of sound, and the upper sign corresponds to absorption, the lower to emission of a phonon.

From Eqs. (5) and (6) follows

$$q = \mp \left(k \cos \theta - \frac{\mu_{\text{exc}} v_0'}{\hbar} \right) \pm \sqrt{\left(k \cos \theta - \frac{\mu_{\text{exc}} v_0}{\hbar} \right)^2 - \frac{3\mu_{\text{exc}} \Delta E}{2\hbar^2}},$$

where θ is the angle between \mathbf{k} and \mathbf{q} . It is easy to see that for absolute temperatures of more than a few degrees, θ not too near $\pi/2$, $k \cos \theta \gg \mu_{\text{exc}} v_0 / \hbar$ for the overwhelming majority of excitons which are in thermal equilibrium with the lattice, and, consequently,

$$q = \mp k \cos \theta \pm \sqrt{k^2 \cos^2 \theta - (3\mu_{\text{exc}} \Delta E / 2\hbar^2)}.$$

In order that excitation may not take place, it is necessary that the expression occurring under the radical be negative, that is,

$$\frac{8}{3} \frac{\kappa^2 \hbar^2 \varepsilon}{\mu e^4} = \gamma \leq 1. \quad (7)$$

For the overwhelming number of excitons we can substitute $\varepsilon \approx k_0 T$ in this expression. Then a criterion of the applicability of the theory can be seen to be

$$\bar{\gamma} = \frac{8}{3} \frac{\kappa^2 \hbar^2 k_0 T}{\mu e^4} \leq 1. \quad (7a)$$

If $\mu_1 = \mu_2 = m_e$ and $\kappa = 15$, then $\bar{\gamma} = k_0 T / 0.023$ eV, from which it can be seen that this theory is applicable only for temperatures lower than room temperature.

Considering such collisions of excitons with phonons, for which excitation (dissociation) of the excitons does not occur, we must set $\Delta E = 0$ in Eq. (6), whence

$$q = \mp 2k \cos \theta \pm 2\mu_{\text{exc}} v_0 / \hbar.$$

If we again neglect the term $2\mu_{\text{exc}} v_0 / \hbar$, then

$$\cos \theta = \mp q / 2k, \quad (8)$$

where the upper sign corresponds to the absorption, the lower to the emission, of a phonon. From Eq. (8) it can be seen that phonons with wave vectors $\mathbf{q} \approx \mathbf{k}$ in general interact with the excitons. As q is positive by definition, it follows from Eq. (8) that the wave vector of the phonons can vary between the limits of $q_{\min} = 0$ to $q_{\max} = 2k$.

PROBABILITY OF TRANSITION OF AN EXCITON $\Psi_{\mathbf{k}\mathbf{k}'}$ BY ABSORPTION AND EMISSION OF PHONONS

For the calculation of the probability of transition of an exciton from a state with wave vector \mathbf{k} to a state \mathbf{k}' by collision with a phonon, we assume as the perturbation energy the deformation potential of Bardeen and Shockley¹¹

$$U(\mathbf{r}_1, \mathbf{r}_2) = C_1 \Delta(\mathbf{r}_1) - C_2 \Delta(\mathbf{r}_2). \quad (9)$$

Here C_1 and C_2 are constants of the order of magnitude of the energy of the atom, that is, 1 - 10 V and $\Delta(\mathbf{r}) = \text{div } \mathbf{u}$, the relative contraction, where $\mathbf{u}(\mathbf{r})$ is the displacement of a given point of the isotropic continuum. We will assume $C_1 > 0$ and $C_2 > 0$, and generally $C_1 \neq C_2$.

We investigate the elastic harmonic wave (phonon)

$$\mathbf{u}(\mathbf{r}) = \frac{1}{\sqrt{N}} \mathbf{e}_{\mathbf{q}j} [a_{\mathbf{q}j} e^{i(\mathbf{q}\mathbf{r})} + a_{\mathbf{q}j}^* e^{-i(\mathbf{q}\mathbf{r})}]. \quad (10)$$

Here N is the number of atoms in the unit volume of the crystal, $\mathbf{e}_{\mathbf{q}j}$ is the vector of polarization, $a_{\mathbf{q}j}$ and $a_{\mathbf{q}j}^*$ are the normal coordinates (amplitudes) of the vibrations.

Substituting Eq. (10) in Eq. (9), transforming from the coordinates \mathbf{r}_1 and \mathbf{r}_2 to $\vec{\rho}$ and \mathbf{R} , we obtain

$$U(\mathbf{r}_1, \mathbf{r}_2) = U_{\rho}(\vec{\rho}, \mathbf{R}) \quad (11)$$

$$= \frac{1}{\sqrt{N}} a_{\mathbf{q}j} e^{i(\mathbf{q}\mathbf{R})} \left[C_1 \exp \left\{ i \frac{\mu_2}{\mu_1 + \mu_2} (\mathbf{q}\vec{\rho}) \right\} - C_2 \exp \left\{ - \frac{\mu_1}{\mu_1 + \mu_2} (\mathbf{q}\vec{\rho}) \right\} \right] + \text{compl. conj.}$$

where we have made use of the fact that only longitudinal elastic waves interact with the exciton. The complete unperturbed wave function of the crystal has the form

$$\Psi(\mathbf{k}, N_q) = \frac{1}{\sqrt{V}} e^{i(\mathbf{k}\mathbf{R})} \frac{1}{\sqrt{\pi a_{\text{exc}}^3}} e^{-\rho/a_{\text{exc}}} \prod_{\mathbf{q}} \psi_{N_q}(a_{\mathbf{q}}), \quad (12)$$

where $\psi_{N_q}(a_{\mathbf{q}})$ is the oscillator wave function of the normal vibrations of the crystal (N_q is the quantum number of the oscillator with frequency $\omega_{\mathbf{q}} = \nu_0 q$).

The matrix elements of the transition are

$$M_{\mathbf{k}\mathbf{k}'} = \int \Psi^*(\mathbf{k}', N'_q) U_{\rho}(\vec{\rho}, \mathbf{R}) \quad (13)$$

$$\Psi(\mathbf{k}, N_q) da_{\mathbf{q}} d\mathbf{R} d\vec{\rho}.$$

Integration over $da_{\mathbf{q}}$ and $d\mathbf{R}$ gives

$$(a_{\mathbf{q}})_{N_q-1, N_q} = \sqrt{\frac{\hbar}{2M\omega_{\mathbf{q}}}} N_q; \quad (14)$$

$$(a_{\mathbf{q}}^*)_{N_q+1, N_q} = \sqrt{\frac{\hbar}{2M\omega_{\mathbf{q}}}} (N_q + 1);$$

$$\frac{1}{V} \int e^{i(\mathbf{k} \pm \mathbf{q} - \mathbf{k}', \mathbf{R})} d\mathbf{R} = \begin{cases} 1, & \text{if } \mathbf{k}' = \mathbf{k} \pm \mathbf{q}, \\ 0, & \text{if } \mathbf{k}' \neq \mathbf{k} \pm \mathbf{q}. \end{cases} \quad (15)$$

Here M is the mass of an atom of the crystal. It can be seen that Eq. (15) expresses the law of conservation of momentum [Eq. (5)] for the collision of an exciton and a phonon.

The integral remaining over $d\vec{\rho}$ from Eq. (13) can be seen to be

$$I = \frac{1}{\pi a_{\text{exc}}^3} \int \exp \left\{ \pm i \frac{\mu_{1,2}}{\mu_1 + \mu_2} (\mathbf{q}\vec{\rho}) \right\} \quad (16)$$

$$\times \exp \left\{ - \frac{2\rho}{a_{\text{exc}}} \vec{\rho} \right\} d\vec{\rho}$$

$$= \frac{1}{\pi a_{\text{exc}}^3} \int \exp \{ i(\mathbf{q}_1 \vec{\rho}) \} \exp \left\{ - \frac{2\rho}{a_{\text{exc}}} \right\} \rho^2 d\rho d\Omega,$$

where $\mathbf{q}_1 = \pm \frac{\mu_{1,2}}{\mu_1 + \mu_2} \mathbf{q}$ and $d\Omega$ is the element of solid angle.

For integration over $d\rho$ the function $\rho^2 \exp \left\{ - \frac{2\rho}{a_{\text{exc}}} \right\}$ has a maximum of $\rho = a_{\text{exc}}$. Consequently it is desirable to evaluate the magnitude of the quantity

$$|q_1 a_{\text{exc}}| = \frac{\mu_{1,2}}{\mu_1 + \mu_2} q \frac{\chi \hbar^2}{\mu e^2} \approx \frac{\sqrt{3}}{2} \frac{\mu_{1,2}}{\sqrt{\mu_1 \mu_2}} \sqrt{\gamma}, \quad (17)$$

where we have used the condition that in general excitons interact with phonons with $q \approx k$.

Equation (17) shows that in the limits of applicability of the theory ($\gamma \leq 1$) the magnitude $|q_1 a_{\text{exc}}|$ is of the order of unity. It can be seen that it may be equal to 2 - 3, depending on the ratio between μ_1 and μ_2 , the effective masses of the

¹¹ J. Bardeen and W. Shockley, Phys. Rev. 80, 72 (1950)

electrons and holes; therefore, in the general case it is impossible to assume $|q_1 a_{\text{exc}}| \ll 1$, if $q_1 a_{\text{exc}} \ll 1$, which does not contradict the conditions of applicability of the theory, then $l = 1$ and the matrix element $M_{\mathbf{k}\mathbf{k}'}$ has the same appearance, both for electron and hole separately. It can easily be seen that for this case the mean free path of the exciton is equal to

$$l = \frac{\pi M v_0^2 \hbar^4}{\Omega_0 \mu_{\text{exc}}^2 (C_1 - C_2)^2 k_0 T} = l_0, \quad (18)$$

where Ω_0 is the volume of the crystal cell. This expression is analogous to the expression for the mean free path of an electron hole¹², if one merely replaces μ_1 (μ_2) and C_1 (C_2) by $\mu_{\text{exc}} = \mu_1 + \mu_2$ and $C_1 - C_2$. It is obvious that $q_1 a_{\text{exc}} \ll 1$ is realized for the great majority of excitations with $\bar{\gamma} \ll 1$, that is with low temperatures and small dielectric constant κ .

Carrying out the integration of Eq. (16) we obtain

$$I = [1 + \beta_{1,2}^2 q^2]^{-2}, \quad (19)$$

where

$$\beta_1 = \frac{1}{4} \frac{\kappa \hbar^2}{\mu_1 e^2} = \left[\frac{\mu_2}{2(\mu_1 + \mu_2)} \right] a_{\text{exc}}, \quad (19a)$$

and similarly for β_2 . Thus $\beta_{1,2}$ is of the order of magnitude of a_{exc} . As a result, the probability of transition of an exciton, coupled with emission of absorption of a phonon, contains the factor

$$\begin{aligned} \Phi(q) &= \left\{ \frac{C_1}{[1 + \beta_1^2 q^2]^2} - \frac{C_2}{[1 + \beta_2^2 q^2]^2} \right\}^2 \quad (20) \\ &= \frac{C_1^2}{[1 + \beta_1^2 q^2]^4} + \frac{C_2^2}{[1 + \beta_2^2 q^2]^4} \\ &\quad - \frac{2C_1 C_2}{[1 + \beta_1^2 q^2]^2 [1 + \beta_2^2 q^2]^2}. \end{aligned}$$

Calculating by the usual method¹³, we obtain for the probability of transition, with absorption and emission of a phonon, the expressions

$$W_{\mathbf{k}\mathbf{k}'}^+ = \pi \frac{\Phi(q) q}{NM v_0} N_q \delta(\varepsilon_{\mathbf{k}'} - \varepsilon_{\mathbf{k}} - \hbar v_0 q); \quad (21)$$

$$W_{\mathbf{k}\mathbf{k}'}^- = \pi \frac{\Phi(q) q}{NM v_0} (N_q + 1) \delta(\varepsilon_{\mathbf{k}'} - \varepsilon_{\mathbf{k}} + \hbar v_0 q), \quad (21a)$$

where δ is the delta function, expressing the law of conservation of energy for the collision.

MEAN FREE PATH OF AN EXCITON

For high temperatures (for our case exceeding several degrees Kelvin) the relaxation time τ may be calculated from the formula¹⁴

$$\frac{1}{\tau} = - \sum_{\mathbf{k}} \frac{\Delta k_x(q)}{k_x} [W_{\mathbf{k}\mathbf{k}'}^+ + W_{\mathbf{k}\mathbf{k}'}^-] \quad (22)$$

where $\Delta k_x = k_x' - k_x$ is the change in the component of the wave vector due to the collision.

We substitute in Eq. (21) N for the mean number of phonons in equilibrium. From the Planck formula we have

$$\bar{N}_q = [\exp(\hbar v_0 q / k_0 T) - 1]^{-1}. \quad (23)$$

Taking into account that for the phonons, which mainly interact with excitons, $\hbar v_0 q / k_0 T \approx \hbar v_0 k / k_0 T \ll 1$,

we obtain

$$\bar{N}_q \approx \bar{N}_q + 1 \approx k_0 T / \hbar v_0 q. \quad (24)$$

Replacing the summation in Eq. (22) by an integration in polar coordinates, with the polar axis coinciding with \mathbf{k} , we get

$$\frac{1}{\tau} = - \frac{\pi k_0 T}{NM v_0^2 \hbar (2\pi)^3} \int \frac{\Delta k_x}{k_x} \Phi(q) \quad (25)$$

$$\times [\delta(\varepsilon_{\mathbf{k}'} - \varepsilon_{\mathbf{k}} - \hbar v_0 q)$$

$$+ \delta(\varepsilon_{\mathbf{k}'} - \varepsilon_{\mathbf{k}} + \hbar v_0 q)] q^2 dq \sin \theta d\theta d\phi.$$

Integrating over ϕ , on which only $\Delta k_x / k_x$ depends, gives

$$\int_0^{2\pi} \frac{\Delta k_x}{k_x} d\phi = -2\pi q^2 / 2k^2. \quad (26)$$

Integrating over θ eliminates the delta functions and gives a factor $\mu_{\text{exc}} / \hbar^2 k q$ in place of each of them. Thus the mean free path of an exciton $l = \tau v = \tau \hbar k / \mu_{\text{exc}}$ is given by

$$\frac{1}{l} = \frac{\Omega_0 \mu_{\text{exc}}^2 (C_1 - C_2)^2 k_0 T}{\pi M v_0^2 \hbar^4} \frac{1}{4k^4} \int_0^{2k} \frac{\Phi(q)}{(C_1 - C_2)^2} q^3 dq. \quad (27)$$

We examine first the particular case when $\mu_1 = \mu_2 = \mu^*$, then

¹² B. I. Davydov and I. M. Shmushkevich, Usp. Fiz. Nauk 24, 21 (1940)

¹³ H. Bethe and A. Sommerfeld, Electron Theory of Metals, Handbuch der Physik, vol. 24, p. 2

¹⁴ H. Fröhlich, Proc. Roy. Soc. 160A, 230 (1937)

$$\Phi(q) = (C_1 - C_2)^2 / [1 + \beta^2 q^2]^4, \quad (20a)$$

where

$$\beta = 1/4 a_{\text{exc}}.$$

Substituting this form of $\Phi(q)$ in Eq. (27) and carrying out the integration, we obtain

$$l = \frac{\pi M v_0^2 \hbar^4}{\Omega_0 \mu_{\text{exc}}^2 (C_1 - C_2)^2 k_0 T} \frac{(1 + b\epsilon)^3}{1 + 1/3 b\epsilon^3}, \quad (18a)$$

where $\epsilon = \hbar^2 k^2 / 2\mu_{\text{exc}}$ is the energy of the exciton and $b = [\mu^* e^4 / 4\kappa^2 \hbar^2]^{-1}$. It can be easily seen that for the criterion (7) to be justified it is necessary that $\epsilon \leq 0.75/b$. From Eq. (18a) it is seen that for the particular case considered here the mean free path of the exciton is a monotonic function of the energy. For small values of the energy ϵ the numerical value of l is given by Eq. (18). For the maximum energy $\epsilon_{\text{max}} = 0.75/b$ the expression for l is 4.3 times larger.

For the general case a simple calculation gives

$$\frac{1}{4\hbar^4} \int_0^{2\hbar} \Phi(q) q^3 dq = \left(\frac{C_1}{C_1 - C_2} \right)^2 \frac{1 + 1/3 b_1 \epsilon}{(1 + b_1 \epsilon)^3} + \left(\frac{C_2}{C_1 - C_2} \right)^2 \frac{1 + 1/3 b_2 \epsilon}{(1 + b_2 \epsilon)^3} - \frac{2C_1 C_2}{(C_1 - C_2)^2} \frac{2}{(b_1 - b_2)^2 \epsilon^3} \quad (28)$$

$$\times \left[\frac{b_1 + b_2}{b_1 - b_2} \ln \frac{1 + b_1 \epsilon}{1 + b_2 \epsilon} - \frac{b_1 \epsilon + b_2 \epsilon + 2b_1 b_2 \epsilon^2}{(1 + b_1 \epsilon)(1 + b_2 \epsilon)} \right],$$

where ϵ is the energy of the exciton and

$$b_1 = \left(\frac{\mu_1}{\mu_1 + \mu_2} \frac{\mu_1 e^4}{2\hbar^2 \kappa^2} \right)^{-1}, \quad b_2 = \left(\frac{\mu_2}{\mu_1 + \mu_2} \frac{\mu_2 e^4}{2\hbar^2 \kappa^2} \right)^{-1} \quad (29)$$

are coefficients, with dimensions of inverse energy and of the order of magnitude of the inverse of the internal energy of the exciton.

It seems expedient to write Eq. (27) in the form

$$l = \frac{\pi M v_0^2 \hbar^4}{\Omega_0 (\mu_1 + \mu_2)^2 (C_1 - C_2)^2 k_0 T} F(z; s, g) = l_0 F \quad (30)$$

where

$$z = b_2 \epsilon, \quad s = C_1 / (C_1 - C_2), \quad g = \mu_2 / \mu_1 \quad (30a)$$

and

$$\frac{1}{F(z; s, g)} = s^2 \frac{1 + 1/3 g^2 z}{(1 + g^2 z)^3} + (s - 1)^2 \frac{1 + 1/3 z}{(1 + z)^3} \quad (30b)$$

$$- 2s(s - 1) \frac{2}{(g^2 - 1)^2 z^2} \left[\frac{g^2 + 1}{g^2 - 1} \ln \frac{1 + g^2 z}{1 + z} \right.$$

$$\left. - \frac{(g^2 + 1)z + 2g^2 z^2}{(1 + z)(1 + g^2 z)} \right].$$

It should be noted that $z = b_2 \epsilon = 3/4 (\mu_1 / \mu_2) \gamma \approx \gamma/g$, but $\gamma \leq 1$, from which

$$0 \leq z \leq 1/g. \quad (30c)$$

It can be easily seen that for $z \rightarrow 0$, the function F converges to unity for all values of s , that is, Eq. (30) transforms into Eq. (18).

We see from Eq. (30) that the mean free path of excitons, just as that for electrons (holes), is inversely proportional to the absolute temperature. On the other hand the mean free path of an exciton, in contrast to that of an electron (hole), depends on its energy.

Since this problem is completely symmetrical with respect to the electron and the hole, let us consider only the case of $g > 1$, which corresponds physically to the more probable assumption that the effective mass of the hole μ_2 is larger than the effective mass of the electron μ_1 . It appears that $C_1 > C_2$, as it can be imagined that, for a given relative change in the volume of a crystal, the displacement of the lower edge of the conduction band is larger than the displacement of the upper edge of the valence band.

To give visually an idea of the behavior of the function $F(z; s, g)$ for various values of its arguments, graphs of $F(z)$ for several values of g and s have been constructed. In Fig. 1 the behavior of $F(z)$ is depicted, for $g = 3$, and several values of s , from unity ($C_2 = 0$) to infinity ($C_1 = C_2$). Figure 2 shows the same relationship, for $g = 9$.

In the case of $s = 1$ ($C_2 = 0$), the function is

$$F(z) = (1 + g^2 z)^3 / (1 + 1/3 g^2 z).$$

If $C_1 = C_2 = C$, and consequently, $s = \infty$, then

$$\frac{(C_1 - C_2)^2}{F(z)} = C^2 \left\{ \frac{1 + 1/3 g^2 z}{(1 + g^2 z)^3} + \frac{1 + 1/3 z}{(1 + z)^3} \right.$$

$$\left. - \frac{4}{(g^2 - 1)^2 z^2} \left[\frac{g^2 + 1}{g^2 - 1} \ln \frac{1 + g^2 z}{1 + z} \right. \right.$$

$$\left. - \frac{(g^2 + 1)z + 2g^2 z^2}{(1 + z)(1 + g^2 z)} \right\},$$

and in this case we shall designate as $F(z)$ the inverse of the quantity contained in the brackets on the right hand side.

In discussing the graphs shown it is necessary

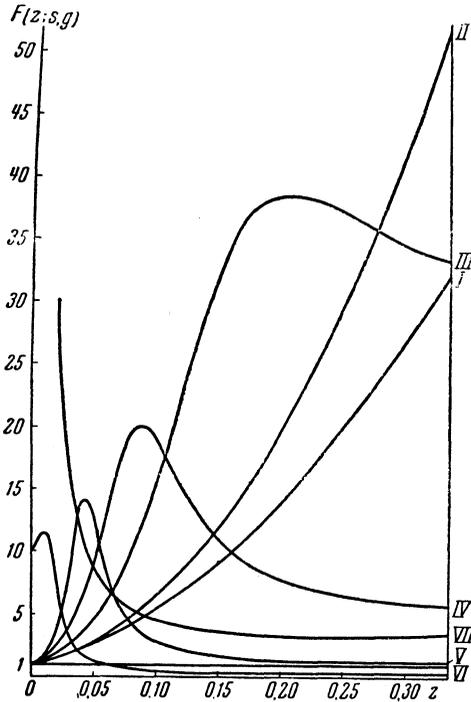


Fig. 1. $g = 3$. I: $s = 1$; $C_2 = 0$; II: $\phi s = 1.1$; $C_1 = 11C_2$; III: $s = 1.5$; $C_1 = 3C_2$; IV: $s = 2$; $C_1 = 2C_2$; V: $s = 3$; $C_1 = 1.5C_2$; VI: $s = 11$; $C_1 = 1.1C_2$; VII: $s = \infty$; $C_1 = C_2$. The ordinates of curve VI are magnified 10 times.

to keep in mind that the ordinates of the curves VI in Figs. 1 and 2 are magnified ten times, while the ordinates of the curves I and II in Fig. 2 are reduced ten times. Also, the curve VII for $s = \infty$ is not shown in Fig. 2, as it is similar to the curve VII in Fig. 1. The ordinates of the curve VI of Fig. 2 are of the order of 0.014 for values of $z > 0.02$.

Now if we regard l_0 as given (i.e., the difference $C_1 - C_2$ is given), then a number of conclusions can be drawn concerning the behavior of the dimensionless factor F , which, when multiplied by l_0 , determines the mean free path of the exciton. We see that in all cases, when C_1 is of the order C_2 , i.e., their difference is of the same order of magnitude (curves III, IV, and V), the function $F(z)$ has a maximum in the energy interval in which the excitons can exist, thus increasing the mean free path (with respect to l_0) by a factor of 10 - 40. The larger the value of C_1 as compared to C_2 , the

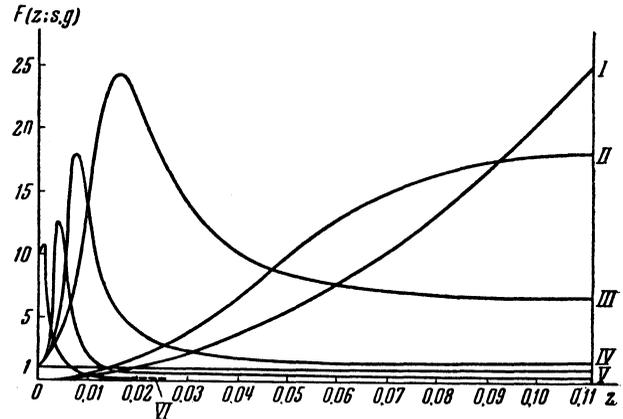


Fig. 2. $g = 9$. Curves I-VI are calculated for the same values of the parameter s , as in Fig. 1. The ordinates for curves I and II have been reduced 10 times, those for curve VI have been magnified 10 times.

higher will be the values of the exciton energy at which the length of the mean free path reaches its maximum. In the cases when C_1 differs only slightly from C_2 (curves VI), and the energy of the exciton is not overly small, its mean free path is several dozen times smaller than l_0 .

Let us determine the temperature T_m , which corresponds to the energy $\epsilon = k_0 T_m$ for which F has a maximum, for the case of $g = \mu_2/\mu_1 = 3$ and $s = 2$. Assuming, for example, $\kappa = 15$ and $\mu_2 = 2m_e$, we obtain $T_m = 96^\circ \text{K}$. It is easy to see that for $g = 9$, the maxima of F are located, generally speaking, at somewhat lower temperatures, of the order of 10-20°K.

We see that the dependence of the length of the mean free path of the exciton on energy is materially connected with the relative magnitude of the effective masses of the electron and the hole, and of the interaction constants C_1 and C_2 . Of course, no exact quantitative determinations of the mean free path of the exciton can be made unless the constants μ_1 , μ_2 , C_1 , C_2 are known. As far as that is concerned, the conditions are similar to those encountered in considering the theory of the mean free path of an electron (hole).

The corresponding calculations for an exciton in a polar crystal will be published in the very near future.