Binding of electrons and holes into excitons

V. N. Avakumov, V. I. Perel', and I. N. Yassievich

A. F. Ioffe Physicotechnical Institute, USSR Academy of Sciences
(Submitted 13 September 1979)
Zh. Eksp. Teor. Fiz. **78**, 1240–1252 (March 1980)

The cross section for the binding of electrons and holes into excitons is calculated for the case when the energy relaxation is due to the interaction with acoustic phonons. It is shown that the binding cross section exceeds the cross section for the capture of the carriers by attracting Coulomb centers and has a different temperature dependence. A comparison is made with the available experimental data.

PACS numbers: 71.35. + z

1. INTRODUCTION

The binding of electrons and holes into excitons in interactions with acoustic phonons can be naturally analyzed in analogy with the capture of carriers by attracting Coulomb centers.[1,2] The electron and hole are bound via highly excited states of the exciton, and then the bound pair loses energy by emitting acoustic phonons and diffuses in energy space into the region of negative values of the total energy. The electron-hole pair can be regarded as practically bound into an exciton if its total energy is negative and higher in absolute value than kT (T is the lattice temperature), inasmuch as in this case the probability of the thermal disintegration of the exciton is exponentially small. The pair binding is thus determined, just as capture of a carrier by a center, by the rate of energy diffusion. However, a direct application of Pitaevskii's method,[3] used in Refs. 1 and 2 to analyze capture by a center, is impossible in this case because there is no finite classical diffusion coefficient in the space of the total energy of the two particles. In fact, the "dynamic-friction coefficient" $B(E)$ in the space of the total energy E of the two particles is defined as

$$B(E) = \int d^3r \int \rho_1(\varepsilon_1) d\varepsilon_1 \int \rho_2(\varepsilon_2) d\varepsilon_2 \delta(E - \varepsilon_1 - \varepsilon_2 - u(r)) \varepsilon_1 / \tau_1(\varepsilon_1), \quad (1)$$

where $\varepsilon_1, \varepsilon_2, \rho_1, \rho_2$ are the kinetic energies and state densities of the two particles, $u(r) = -e^2/\varkappa r$ is the Coulomb energy of their interaction, and $\varkappa$ is the dielectric constant. We assume for simplicity that only the first particle interacts with the phonons [$\tau_1(\varepsilon_1)$ is the time of its energy relaxation. The ratio $\varepsilon_1/\tau_1(\varepsilon_1)$] is the average change of energy of the first particle (meaning also of the entire system) per unit time on account of acoustic-phonon emission.

Recognizing that

$$\rho_i(\varepsilon) = [8 \cdot 2^{1/2} \pi m_i^{3/2}/(2\pi\hbar)^3] \varepsilon^{1/2}, \quad \tau_1^{-1} = (2\varepsilon)^{1/2}/l_0 m_1^{1/2},$$

we can easily calculate the integrals with respect to ε_1 and ε_2 and reduce (1) to the form

$$B(E) = [8 \cdot 2^{1/2} \pi/(2\pi\hbar)^3]^2 \frac{m_1 m_2^{3/2}}{l_0} \cdot \frac{16}{105} \int\limits_{E-u>0} d^3r (E-u)^{7/2}. \quad (2)$$

The integral in (2) diverges at short distances. (The characteristic length l_0 in terms of which the time of energy relaxation on the phonons is expressed depends neither on the energy nor on the temperature:

$$l_0 = \pi\hbar^4 \rho_0/2m_1^3 E_{c1}^2,$$

where ρ_0 and E_{c1} are the density of the crystal and the deformation-potential constant.) To understand the physical cause of this difficulty, we consider an electron-hole pair with total energy $E(|E| \sim kT)$. At this total energy the pair has states with arbitrarily large particle kinetic energies ε_1 and ε_2. These states correspond to small distances between the electron and the hole, so that the large negative potential energy of the particle is almost offset by the large positive kinetic energy. These states are the most favorable for the energy losses, since the rate of energy transfer depends only on the particle kinetic energy and increases rapidly (like $\varepsilon^{3/2}$) with increase of the latter. The divergence in (2) indicates that it is precisely these states which play the principal role in the energy relaxation of the pair.

It is clear that the treatment of energy relaxation of diffusion in the total-energy space is meaningful when the pair distribution function depends only on its total energy, i.e., when all the other variables that characterize the state of the pair vary in the course of collision with the phonons much more rapidly than the total energy, and equipartition among them is established. At a low total energy and large kinetic energy of the particles (i.e., at short distances) this is not the case—the rate of exchange between the energies of the gravity center and the internal energy of the pair becomes less than the rate of loss of the total energy. In fact, if the first particle emits or absorbs a phonon with momentum q, then the total energy of the pair changes by an amount $\Delta E = sq$ (where s is the speed of sound). A redistribution between the internal energy and the energy of the center of gravity then takes place, and these energies change by an amount $\Delta\varepsilon = p_2 q/M$, where M is the total mass of the pair and p_2 is the momentum of the second particle.[1] The total-energy relaxation will be slower than the exchange between the internal and the translational energies of the pair if $kT/\Delta E \gg \varepsilon_c/\Delta\varepsilon$. This inequality compares the number of collisions after which the total energy changes by kT (the scale of the distribution function) with the number of collisions after which the energy ε_c of the center of gravity changes by an amount on the order of ε_c itself. Substituting ΔE and $\Delta\varepsilon$ in this inequality and putting $\varepsilon_c \sim |u|$ and $p_2 \sim (2m_2 |u|)^{1/2}$, we obtain an estimate of the distances at which equipartition still occurs with respect to all the variables except the energy E:

$$e^2/\varkappa r \ll (kT)^2 m_2/s^2 M^2. \quad (3)$$

If we compare this inequality with the restriction imposed by quantum mechanics

$$e^2/\varkappa r \ll E_B \qquad (4)$$

(E_B is the Bohr energy of the exciton), we see that at low temperatures the limitation (3) is more stringent than (4). Consequently the reasoning that leads to (2) is inapplicable even in the classical region.

Thus, the entire temperature scale can be divided into three regions. At high temperatures, when

$$kT \gg [(M^2/m_2)s^2 E_B]^{1/3}, \qquad kT \ll E_B, \qquad (5)$$

the most stringent is the inequality (4). It can be assumed in this case that the pair distribution function depends only on the total energy at all internal-motion energies (it will be shown below that this is actually the case). The process of binding into an exciton can be regarded as a continuous descent in the total-energy space. The principal role in the energy relaxation, however, is played by distances on the order of the Bohr radius, and therefore the quantum description of the pair motion must be used in the calculation of the energy losses.

In the low-temperature region

$$M^2 s^2/m_2 \ll kT \ll (M^2 s^2 E_B/m_2)^{1/3} \qquad (6)$$

the pair distribution function is a function of the total energy only at the distances bounded by the inequality (3), which in this case is stronger than (4). The principal role is played by distances that are still in the classical region but are such that the rate of relaxation of the total energy becomes comparable with the rate of exchange between the internal and translational energies of the exciton.

Finally, if the temperature is very low,

$$kT \ll M^2 s^2/m_2, \qquad (7)$$

then, as seen from (4), the mixing of the internal and translational energies does not manage to take place at all (even at distances such that $|u| \leq kT$). If the light particle interacts mainly with the phonons ($m_1 < m_2$), the binding into an exciton is completely analogous in this case to capture by an attracting Coulomb center. We can use for the cross section formula (5) of our review,[2] with m replaced by m_1.

The presence of scattering by the impurities increases the effectiveness of the mixing with respect to all the variables except the energy, and at sufficiently high frequency of the impurity collisions it may turn out that the exciton distribution function is a function of the total energy at all distances even at low temperature, when the inequality (5) does not hold.

2. ESTIMATE OF THE BINDING CROSS SECTION

We obtain in this section the binding cross section in the temperature intervals (5) and (6), accurate to numerical factors. For this purpose we express the binding cross section in terms of the dynamic friction coefficient $B(E)$ in the space of the total energy of the particle pair, and estimate $B(E)$ by using expression (2), in which the integration region is limited by the inequalities (4) and (3).

The flux j in the total-energy space of the electron-hole pair is determined in the Fokker-Planck approximation by the expression (the sign of j is chosen such that $j > 0$ on going towards lower energy)

$$j = B(E)\left[f(E) + kT \frac{df(E)}{dE}\right], \qquad (8)$$

where E is the total energy of the pair and includes the kinetic energies of both particles and the potential energy of their Coulomb interaction, and $f(E)$ is the distribution function. The flux j is connected with the effective cross section σ for binding into an exciton by the formula

$$j = np\sigma\langle v\rangle; \qquad (9)$$

here n and p are respectively the densities of the electrons and holes, $\langle v\rangle = (8kT/\pi\mu)^{1/2}$ is the average relative velocity of the electron and hole (μ is the reduced mass). The flux is calculated per unit volume. The normalization volume is assumed to be unity hereafter.

To calculate the flux j we employ the usual procedure (see Refs. 1-3). The solution of (8) at $E < 0$ is of the form

$$f(E) = (j/kT)\exp(-E/kT)\int_{-\infty}^{E}\exp(E'/kT)B^{-1}(E')\,dE'. \qquad (10)$$

This solution must be joined at $E = 0$ with the Boltzmann distribution at positive energies:

$$f(E) = Ae^{-E/kT}, \quad A = \frac{np}{4}\left(\frac{2\pi\hbar^2}{kT(\mu M)^{1/2}}\right)^3. \qquad (11)$$

In the determination of the normalization constant A we have neglected the Coulomb interaction of the electrons and holes.[2)] Joining the results and using (9), we obtain the effective cross section for binding into an exciton in the form

$$\sigma = \frac{\pi^2}{4}\left(\frac{2\pi\hbar^2}{kTM}\right)^{3/4}\frac{\hbar^3}{kT\mu}\left[\int_{-\infty}^{0}\frac{\exp(E/kT)}{B(E)}dE\right]^{-1}. \qquad (12)$$

To estimate $B(E)$ we use Eq. (2), in which the region of integration is cut off by the inequality $r > r_0$. The value of r_0 must be chosen in accord with inequalities (3) and (4). In both cases the integral (2) is determined by the value of $u(r)$ at the lower limit, where $|u(r_0)| \gg kT$, so that the quantity E under the integral sign can be neglected (since the significant values are $|E| \leq kT$). Then B does not depend on the energy E and is proportional to $r_0^{-1/2}$. Taking for r_0 the limiting values corresponding to inequalities (3) and (4), we write down the binding cross section in the form

$$\sigma = \frac{4\pi}{3}\frac{1}{l_0}\left(\frac{e^2}{\varkappa kT}\right)^3\left(\frac{kT}{Ms^2}\right)^{1/2}\eta\frac{m_2}{M}, \quad \frac{M^2 s^2}{m_2} \ll kT \ll \left(\frac{M^2}{m_2}s^2 E_B\right)^{1/3}, \qquad (13)$$

$$\sigma = \frac{4\pi}{3}\frac{1}{l_0}\left(\frac{e^2}{\varkappa kT}\right)^3\left(\frac{E_B}{kT}\right)^{1/2}\eta'\left(\frac{m_2}{M}\right)^{1/3}, \quad E_B \gg kT \gg \left(\frac{M^2}{m_2}s^2 E_B\right)^{1/3}, \qquad (14)$$

where η and η' are numerical factors of the order of unity. They are calculated for various mass ratios in Secs. 3 and 4 in the rigorous solution of the problem. The numerical factor $4\pi/3$ in (13) and (14) is chosen to facilitate the comparison with the expression for the cross section for carrier capture by an attracting Coulomb center[1,2]

$$\sigma = \frac{4\pi}{3}\frac{1}{l_0}\left(\frac{e^2}{\varkappa kT}\right)^3. \qquad (15)$$

3. CLASSICAL DIFFUSION IN TWO-DIMENSIONAL ENERGY SPACE

This section is devoted to the solution of the problem of pair binding in the low-temperature interval (6), when the motion of the particles in the essential binding-energy region can be treated classically. The integrals of motion for a pair coupled by Coulomb interaction are the interval angular momentum, the momentum of the center of gravity, and the internal (or total) energy. Since the problem is isotropic, we can assume that the distribution function does not depend on the direction of the center-of-gravity momentum and of the direction of the internal angular momentum. It is thus necessary to consider the change of three variables: the center-of-gravity energy, the internal angular momentum, and the total energy.

The problem simplifies if the electron and hole masses differ greatly. We assume for the sake of argument that only the light particle $(m_1 \ll m_2)$ interacts with the phonons. Then the angular momentum changes greatly in a single collision, but the center-of-gravity energy changes only in proportion to the mass ratio m_1/m_2. Since the collisions are quasielastic, the total energy also varies little. This allows us to assume that the distribution function depends only on two variables, ε_c and E, and the kinetic equation in terms of both variables can be written in the Fokker-Planck approximation:

$$\rho(\varepsilon_c, E) \frac{\partial f}{\partial t} = \frac{\partial j_E}{\partial E} + \frac{\partial j_{\varepsilon_c}}{\partial \varepsilon_c}. \tag{16}$$

The expressions for the flux components in two-dimensional energy space are of the form[3]

$$j_E = B(\varepsilon_c, E) \left[f(\varepsilon_c, E) + kT \frac{\partial f(\varepsilon_c, E)}{\partial E} \right],$$
$$j_{\varepsilon_c} = kTD(\varepsilon_c, E) \frac{\partial f(\varepsilon_c, E)}{\partial \varepsilon_c}. \tag{17}$$

(The fluxes are so defined that they are positive in the direction of decreasing energies E and ε_c.) The diffusion coefficients are connected with the mean squared losses of the total energy and of the mass-center energy by the formulas

$$B(\varepsilon_c, E) = \frac{\langle (\Delta E)^2 \rangle}{2kT}; \quad D(\varepsilon_c, E) = \frac{\langle (\Delta \varepsilon_c)^2 \rangle}{2kT}. \tag{18}$$

The expression for $B(\varepsilon_c, E)$ differs from the expression given by Eq. (1) for $B(E)$ only in that the particle momenta p_1 and p_2 should be connected by the condition that fixes the mass-center energy prior to the collision, $(p_1 + p_2)^2/2M = \varepsilon_c$. It is thus possible to insert under the integral sign in (1) the factor

$$\frac{1}{2} \int_0^\pi \delta[\varepsilon_c - (p_1 + p_2)^2/2M] \sin \vartheta \, d\vartheta,$$

where ϑ is the angle between the momenta p_1 and p_2. Calculating the corresponding integrals and recognizing that $m_1 \ll m_2$, we get

$$B(\varepsilon_c, E) = B_0 \frac{\varepsilon_c^{1/2}}{\varepsilon_c - E}, \quad B_0 = \frac{8 \cdot 2^{1/2}}{3\pi^3} \frac{m_1 m_2^{1/2}}{l_0 \hbar^6} \left(\frac{e^2}{\varkappa} \right)^3. \tag{19}$$

To calculate the coefficient D we recognize that $\Delta \varepsilon_c \approx p_2 \cdot q/M$, where q is the momentum of the phonon emitted or absorbed by the first particle. Therefore

$$(\Delta \varepsilon_c)^2 = \frac{2\varepsilon_c m_2}{M^2 s^2} (\Delta E)^2 \cos^2 \theta, \tag{20}$$

where θ is the angle between p_2 and q. Averaging and again putting $m_1 \ll m_2$, we get

$$D(\varepsilon_c, E) = \frac{2\varepsilon_c}{3m_2 s^2} B(\varepsilon_c, E). \tag{21}$$

We present also the formula for the two-dimensional state density:

$$\rho(\varepsilon_c, E) = \frac{(m_1 m_2)^{3/2}}{2\pi^2} \left(\frac{e^2}{\varkappa \hbar^2} \right)^3 \frac{\varepsilon_c^{1/2}}{(\varepsilon_c - E)^{5/2}}. \tag{22}$$

Formulas (19), (21), and (22) pertain to the states of bound electron-hole pairs (excitons). It was assumed in their derivation that $\varepsilon_c - E > 0$.

To find the distribution function $f(\varepsilon_c, E)$ under stationary conditions we must solve Eq. (16) with zero left-hand side:

$$\frac{2kT}{3m_2 s^2} \frac{\partial}{\partial \varepsilon_c} \frac{\varepsilon_c^{1/2}}{\varepsilon_c - E} \frac{\partial f}{\partial \varepsilon_c} + \frac{\partial}{\partial E} \frac{\varepsilon_c^{1/2}}{\varepsilon_c - E} \left(f + kT \frac{\partial f}{\partial E} \right) = 0 \tag{23}$$

and with boundary conditions

$$f(\varepsilon_c, E) \xrightarrow[\varepsilon_c \to \infty]{} 0, \quad f(\varepsilon_c, E) \xrightarrow[E \to -\infty]{} 0,$$
$$f(\varepsilon_c, E) |_{E = \varepsilon_c} = A e^{-E/kT}. \tag{24}$$

The boundary condition on the line $E = \varepsilon_c$ means that the highly excited states of the excitons are at equilibrium with the free carriers, which have a Boltzmann distribution [cf. (11)].

We introduce the dimensionless variables

$$x = E/kT, \quad y = (6\varepsilon_c m_2 s^2)^{1/2}/kT. \tag{25}$$

As will be shown later, for our analysis the important values of x and y are of the order of unity. We can therefore neglect E in the denominators of (23) compared with ε_c, assuming the condition $ms^2 \ll kT$ to be satisfied. Equation (23) then takes the form

$$\frac{\partial^2 f}{\partial y^2} + \frac{\partial}{\partial x} \left(f + \frac{\partial f}{\partial x} \right) = 0. \tag{26}$$

In the limit as $m_2 s^2/kT \to 0$ the line $E = \varepsilon_c$ changes into the line $y = 0, x > 0$, so that we can use as the boundary conditions for (26)

$$f \to 0 \text{ as } |x| \to \infty \text{ or } y \to \infty,$$
$$f|_{y=0, x>0} = A e^{-x}, \quad \frac{\partial f}{\partial y} \bigg|_{y=0, x<0} = 0. \tag{27}$$

The last condition is the consequence of the finite value of the derivative $\partial f/\partial \varepsilon_c$ at $\varepsilon_c = 0$.

The solution of the problem (26), (27) is

$$f(x, y) = \frac{A}{2\pi} e^{-x/2} \int_{-\infty}^{+\infty} \frac{\exp\{ixt - y(t^2 + 1/4)^{1/2}\}}{(1/2 + it)(1/2 - it)^{1/2}} dt. \tag{28}$$

It can be verified by direct substitution that the function (28) satisfies Eq. (26). The integrand in (28) has in the complex t plane a pole $t = i/2$ and branch points $t = \pm i/2$. At $y = 0$ and $x > 0$ we can close the integration contour in (28) in the upper half-plane and verify that the corresponding boundary condition is satisfied. At $y = 0$, $x > 0$ the integration contour in the expression that follows from (28) for $\partial f/\partial y$ can be closed in the lower half-plane and it can be verified that the latter of the boundary conditions (27) is satisfied.

With the aid of the function (28) we can calculate the total exciton flux in the region of negative energies E:

$$j = \int_0^\infty j_E d\varepsilon_c, \qquad (29)$$

where j_E is defined in (17). We note that the flux j does not depend on the value of E. It is convenient to calculate the flux through the zero level of the total energy ($E = 0$). Using (17), (19), and (25) we can write the expression for j in the form

$$j = B_0 \int_0^\infty dy \left[f + \frac{\partial f}{\partial x} \right]_{x=0} \left(\frac{2}{3m_2 s^2} \right)^{1/2} kT.$$

Using (28), we obtain $j = B_0 A [2(kT)^2/3m_2 s^2]^{1/2}$. Substituting the values of B_0 and A [Eqs. (19) and (11)] and taking into account the connection between j and the cross section σ [Eq. (9)], we obtain an expression for the cross section for binding into an exciton ($m_1 \ll m_2$):

$$\sigma = \frac{8 \cdot (2\pi)^{1/2}}{3 \cdot 3^{1/2} l_0} \left(\frac{kT}{m_2 s^2} \right)^{1/2} \left(\frac{e^2}{\varkappa kT} \right)^3. \qquad (30)$$

Expression (30) coincides with (13) at[4] $\eta = (8/3\pi)^{1/2}$ ($m_1 \ll m_2$).

To conclude this section, we discuss the form of the hot-exciton distribution function. Expression (28) for the exciton distribution function can be easily converted to a real form:

$$f(x,y) = Ae^{-x} \left\{ 1 - \frac{\sqrt{2}}{\pi} \int_1^\infty \frac{e^{-(z-1)x/2} \sin\{^{1}/_2 y (z^2-1)^{1/2}\}}{(z-1)(z+1)^{1/2}} dz \right\}, \quad x > 0, \qquad (31)$$

$$f(x,y) = A \frac{\sqrt{2}}{\pi} e^{-x/2} \int_1^\infty \frac{e^{xz/2} \cos\{^{1}/_2 y (z^2-1)^{1/2}\}}{(z+1)(z-1)^{1/2}} dz, \quad x < 0. \qquad (32)$$

We recall that x and y are connected with the total energy E and with energy of the center of gravity ε_c by formulas (25). Expression (31) and (32) [just as (28)] are valid at $E \ll \varepsilon_c$, i.e., at $x \ll y^2 (kT/6m_2 s^2)$. It is assumed here that the ratio $kT/m_2 s^2$ is large.

We consider first the behavior of the distribution function at $y \ll 1$, i.e., at $\varepsilon_c \ll (kT)^2/6m_2 s^2$. Then

$$f(x,y) = Ae^{-x}, \quad x > 0,$$

$$f(x,y) = A \frac{2}{\pi} e^{|x|} \int_{(|x|)^{1/2}}^\infty e^{-t^2} dt, \quad x < 0. \qquad (33)$$

It is seen that in this case f depends only on the total energy, i.e., equipartition over the states takes place at a given total energy.

At $y \gtrsim 1$ the distribution function becomes dependent on ε_c and decreases with increasing y. For $y \gg 1$ and $y > x^2$ we have [it is convenient to start out with Eq. (28)]

$$f(x,y) = A \left(\frac{2}{\pi y} \right)^{1/2} \exp\left\{ -\frac{x+y}{2} \right\}. \qquad (34)$$

The region in which (34) is valid exists only under the condition $(m_2 s^2 E_B)^{1/2} \gg kT$. In the opposite case the condition $y \gg 1$ cannot be satisfied if it is recognized that $\varepsilon_c < E_B$ (at $E \lesssim kT$). In this case equipartition over the states takes place at a given total energy in the entire range of allowed values of ε_c. The classical approach, however, is not valid here, since binding energies of the order of E_B become significant. This case

will be considered in Sec. 4.

We present, finally, the form of the distribution function in the energy of the center of gravity for excitons with fixed binding energy $\varepsilon_i = \varepsilon_c - E$. This distribution, which follows from (33), is shown schematically in the figure. It is seen that the hotter the exciton the deeper the level on which it is located. The distribution function in ε_c has a maximum at $\varepsilon_c = \varepsilon_i$ so long as $\varepsilon_i < (kT)^2/6m_2 s^2$.

4. QUANTUM CALCULATION OF THE DYNAMIC FRICTION COEFFICIENT

In the high-temperature interval (5) the distribution function of the electron-hole pair depends only on the total energy. This was demonstrated in Sec. 1 on the basis of the classical picture of the energy relaxation. In the interval (5), however, an important role is played by distances of the order of the Bohr radius, so that a quantum calculation is essential.

We determine first the condition for equipartition of the energy of the center of gravity in the quantum limit. We write down the quantum expression for the probability $w_{nn'}$ of the transition between the states with principal quantum numbers n and n', averaged over the initial degenerate state and summed over the final one at a given mass-center energy $\varepsilon_c = p_c^2/2M$:

$$w_{nn'} = \frac{2\pi}{\hbar} \int \frac{d^3 q}{(2\pi\hbar)^3} |c_q|^2 \delta \left(\frac{p_c^2}{2M} + \varepsilon_n - \frac{(p_c - q)^2}{2M} - \varepsilon_{n'} \right) \frac{1}{n^2} I_{nn'} (2N_q + 1). \qquad (35)$$

Here q is the momentum of the emitted phonon, ε_n is the internal energy, $|c_q|^2 = E_{c1}^2 q/2\rho_0 s$ is the square of the modulus of the matrix element of the interaction of the first particle with the acoustic phonons, and N_q is the number of phonons with momentum q. We have neglected in (35) the phonon energy in the argument of the function,

$$I_{nn'} = \sum_{l,m,l',m'} \left| \left\langle n,l,m \left| \exp\left(i \frac{m_2}{M\hbar} \mathbf{qr} \right) \right| n'l'm' \right\rangle \right|^2. \qquad (36)$$

The summation in (36) can be carried out by changing to the momentum representation[4]:

$$I_{nn'}(u) = \int d^3 p_1 d^3 p_2 G_n(\mathbf{p}_1, \mathbf{p}_2) G_{n'}(\mathbf{p}_1 + \mathbf{u}, \mathbf{p}_2 + \mathbf{u}),$$

$$G_n(\mathbf{p}_1, \mathbf{p}_2) = \frac{8n^4}{\pi^2} [n^2 p_1^2 + 1]^{-2} [n^2 p_2^2 + 1]^{-2} \frac{\sin n\varphi}{\sin \varphi},$$

$$\cos \varphi = 1 - 2n^2 |\mathbf{p}_1 - \mathbf{p}_2|^2/[n^2 p_1^2 + 1][n^2 p_2^2 + 1];$$

$$u = \left(\frac{m_2}{m_1} \right)^{1/2} \frac{q}{(2ME_B)^{1/2}}. \qquad (37)$$

Substituting $N_q = kT/sq \gg 1$ in (35) and integrating over
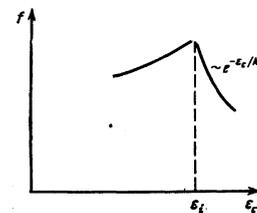
FIG. 1. Schematic form of the distribution (33) at fixed exciton binding energy $\varepsilon_i = \varepsilon_c - E$ (explanation in text).

the angles, we get

$$w_{nn'} = \nu \frac{1}{n^2} \int_{u_-}^{u_+} I_{nn'}(u) u\, du, \qquad (38)$$

where

$$\nu = \frac{1}{l_0} \left(\frac{2E_B}{M} \right)^{1/2} \frac{kT}{Ms^2} \left(\frac{E_B}{\varepsilon_c} \right)^{1/2} \left(\frac{M}{2m_1} \right)^3 \frac{m_1}{m_2}, \qquad (39)$$

$$u_\pm = \left(\frac{m_2}{m_1 E_B} \right)^{1/2} \{ (\varepsilon_c + \varepsilon_n - \varepsilon_{n'})^{1/2} \pm \varepsilon_c^{1/2} \}.$$

We are interested in the transition probability at low total energy ($E \sim kT$) and large internal energy ($|\varepsilon_n| \sim \varepsilon_c \sim E_B$). If m_1 and m_2 are of the same order, then $w_{nn'} \sim \nu$; if $m_1 \gg m_2$, then $u \ll 1$ and $I_{nn'}(u) \sim u^2$ ($n \neq n'$) [this is easiest to see from Eq. (36)] and $w_{nn'} \sim \nu(m_2/m_1)^2$. Finally, if $m_1 \ll m_2$, then $u \gg 1$, as seen from (37), $I_{nn'} \sim u^{-8}$ and $w_{nn'} \sim \nu(m_1/m_2)^3$. The quantity $w_{nn'}$ gives the frequency of the energy exchange between the inner motion of the exciton and the motion of its center of gravity. We compare now this quantity with the rate of energy loss, which can be obtained by substituting under the integral sign in (35) the energy lost in the emission of the phonon sq, replacing the factor $2N_q + 1$ by unity and summing over $n' < n$. We then obtain

$$\dot{E} = \nu \frac{2Ms^2}{kT} \frac{m_1}{m_2} E_B \frac{1}{n^2} \sum_{n'} \int_{u_-}^{u_+} I_{nn'}(u) u^3\, du. \qquad (40)$$

The criterion for the equipartition is the condition $\dot{E}/(kTw_{nn'}) \ll 1$. It is seen that if m_1 and m_2 are of the same order, then this criterion coincides with inequality (5) obtained from classical mechanics. If the masses differ greatly, then the main contribution to the sum in (40) is made by transition without a change of the internal state ($n = n'$). If $m_1 \gg m_2$, then $I_{nn'} \sim 1$ and the obtained equipartition criterion is again the inequality (5). On the other hand if $m_1 \ll m_2$ then we obtain in lieu of (5) a more stringent condition[5]: an additional factor m_2/m_1 must be inserted in the right-hand side of the inequality (5).

We write down now the quantum expression for the dynamic-friction coefficient:

$$B(E) = 2 \sum_n n^2 \int \rho_c(\varepsilon_c) d\varepsilon_c \delta(E - \varepsilon_c - \varepsilon_n) \dot{E}, \qquad (41)$$

where $\dot{E}$ is defined by (40) (the factor 2 takes into account the spin degeneracy[6]). Since $E \sim kT$, and the main contribution to the sum (40) is made by the lower levels of the exciton, we can put $E = 0$ in (41). Substituting (41) in (12), we obtain Eq. (14) and an explicit expression for the numerical factor η':

$$\eta' = \frac{3\sqrt{\pi}}{16} \left(\frac{M}{m_2} \right)^2 \left(\frac{M}{m_1} \right)^{1/2} \sum_{nn'} \int_{u_-}^{u_+} I_{nn'}(u) u^3\, du,$$

$$u_\pm = \left(\frac{m_2}{m_1} \right)^{1/2} \left(\frac{1}{n'} \pm \frac{1}{n} \right), \quad n' < n. \qquad (42)$$

If $m_2 \ll m_1$, then we can take $I_{nn'}$ in (42) outside the integral sign at $u = 0$. It is seen from (36) that $I_{nn'}(0) = \delta_{mn} n^2$. From (42) we then obtain $\eta' = \pi^{5/2}_2/8$ (we use the fact that $\sum n^{-2} = \pi^2/6$). We note that in this case the energy relaxation takes place mainly for transitions within one quantum state of the exciton. (The contribution made to the energy relaxation by the hot excitons in the

ground state is 60%.) This does not mean that the transitions between the quantum states are insignificant and that the relaxation processes take place independently in individual states. When the inequality (5) is satisfied the situation is just the reverse, but the energy is lost just to transitions within one and the same state. Although the transitions between levels are less probable than transitions within a level, the fact that the energy loss takes place in small batches, $\Delta E \sim (E_B m_1 s^2)^{1/2}$, complete intermixing of the quantum states can take place within the time required for the energy to change by kT.

We consider now the opposite limiting case $m_2 \gg m_1$ (the light particle interacts with the phonons). Then the region of integration in (42) shifts at $n \neq n'$ into the region of large u, therefore the corresponding terms in the sum are small. On the other hand, in terms the sum with $n = n' - n$ can be integrated from zero to infinity. We have thus

$$\eta' = \sum_n \eta_{n'}, \quad \eta_{n'} = \frac{3\sqrt{\pi}}{16} \left(\frac{m_2}{m_1} \right)^{1/2} \int_0^\infty u^3 I_{nn}(u)\, du.$$

Calculation of the first two terms yields $\eta_1' = (\sqrt{\pi}/4)$ $(m_2/m_1)^{1/2}$, $\eta_2' = (\sqrt{\pi}/32) \times (m_2/m_1)^{1/2}$, so that $\eta' \approx 0.3\pi^{1/2}$ $(m_2/m_1)^{1/2}$. The contribution of the ground state in this case is ~80%.

5. EFFECT OF SCATTERING BY IMPURITIES

As already noted in the Introduction, if the scattering by the impurities is the predominant momentum-relaxation mechanism, then a situation can arise wherein the distribution function, at binding energies up to $\varepsilon_i = E_B$, depends only on the total energy, even at low temperatures. At $E > 0$ the distribution function is the Boltzmann function (11). In states with higher binding energies ε_i the exciton emits strong phonons with energy ~$(\varepsilon_i ms^2)^{1/2}$. At low temperatures [the criterion (6)] this energy loss suffices for the exciton to go over, in a single emission act, into a state with negative total energy $|E| > kT$, from which backward ejection is unlikely.

Under these conditions the exciton flux from the region of positive energies into bound states can be written in the form

$$j = \int d^3r \int d\varepsilon_1 \int d\varepsilon_2 \int d\varepsilon_1' A e^{-E/kT} \rho_1(\varepsilon_1) \rho_2(\varepsilon_2) w(\varepsilon_1, \varepsilon_1'), \qquad (43)$$

where ε_1 and ε_2 are the kinetic energies of the particles prior to the phonon emission, ε_1^1 is the kinetic energy of the first particle after the phonon emission, $E = \varepsilon_1 + \varepsilon_2 + u(r), u(r) = -e^2/\varkappa r$, and $w(\varepsilon_1, \varepsilon_1')$ is the probability of the transition with emission of a phonon by the first particle (see, e.g., Ref. 2). The integration in (43) is over the region defined by the inequalities $E > 0$ and $E' = \varepsilon_1' + \varepsilon_2 + u(r) < 0$. The integral (43) diverges logarithmically at small r. The reason for this divergence is that the classical analysis is not valid at distances smaller than the Bohr radius. The divergence can therefore be eliminated by restricting the integration by the condition $r > r_{min} = e^2/\varkappa E_B$. Since direct captures can take place only from states such that $(8\varepsilon_1 m_1 s^2)^{1/2} > kT$, the energy ε_1 must be high enough, i.e., the par-

ticles must travel close enough to one another. Then $\varepsilon_1 \sim |u(r)|$, and when account is taken of the foregoing inequality we get $r < r_{max} = (8e^2/\varkappa) [m_1 s^2/(kT)^2]$. Calculating the integral (43) subject to the indicated limitations of the integration region, we obtain with logarithmic accuracy

$$j = \frac{2\pi}{3} \frac{nps}{l_0} \frac{kT}{m_1 s^2} \left(\frac{e^2}{\varkappa kT}\right)^3 \ln \frac{8E_B m_1 s^2}{(kT)^2}. \tag{44}$$

From this we get, according to (9), for the binding cross section in the case of strong impurity scattering

$$\sigma = \frac{\pi^{1/2}}{3 \cdot 2^{1/2} l_0} \left(\frac{kT}{\mu s^2}\right)^{1/2} \frac{\mu}{m_1} \left(\frac{e^2}{\varkappa kT}\right)^3 \ln \frac{8E_B m_1 s^2}{(kT)^2}. \tag{45}$$

This expression is valid if the argument of the logarithm is large, i.e., if the criterion (6) is satisfied. Comparison of formulas (45) and (50) shows that the impurity scattering increases somewhat the binding cross section.

6. COMPARISON WITH OTHER CALCULATIONS AND WITH EXPERIMENT

The first to consider the binding of an electron and a hole into an exciton was Linnik.[6] He calculated the probability of the transition of a free electron-hole pair into the ground state of an exciton with emission of one acoustic phonon. In such a process, owing to the almost elastic interaction with the phonon, the total energy of the electron-hole pair remains practically unchanged, so that the produced exciton is hot. The kinetic energy of its center of gravity is equal to the sum of the binding energies of the exciton and the initial energy of the pair. The transition into such a state does not yet constitute binding, since the hot electron can be easily ionized in one collision with the phonon.

Barrau et al.[6] calculated numerically the probability of pair binding into an exciton, using two methods. The first consisted of solving the balance equations, in which account is taken of the transitions between the states of the continuous spectrum of the exciton and the four lowest quantum states, as well as transitions between these two four states. It is assumed here that in each state the excitons have a Maxwellian mass-center energy distribution, i.e., that the transition between the quantum states is slower than the thermalization in a given state. Barrau et al.[6] suggest that this calculation is valid at low temperatures. At low temperatures, however, transitions from the continuous spectrum go mainly to highly excited states of the exciton, and not to low-lying ones, and the mixing between these highly excited states is faster than thermalization in each of them. The second method, which Barrau et al.[6] regard as valid for calculations at high temperatures, uses the Lax semiclassical approach.[7] The sticking-probability approximation assumed in Ref. 6 means that, to become bound into an exciton, the electron and the hole must give up to the lattice an energy not less than kT in one collision with the phonon. In fact, however, at high temperatures the pair descends continuously in the total-energy space. In addition, at temperatures $kT > (ms^2 E_B)^{1/2}$ it is important that the principal energy losses take place in hot-exciton states with total energy $\sim kT$ and with a binding energy corresponding of the

lowest quantum states (see Sec. 4).

We mention also a paper by Nolle,[8] who estimated numerically the probability of pair binding into an exciton for Si and CdTe.

We know of only one experimental study[9] devoted to a direct investigation of the cross section of the binding of an electron and a hole into an exciton. The value obtained for the binding coefficient is $\sigma\langle v\rangle = 0.9 \cdot 10^{-3} T^{-2}$ cm^3/sec (where T is in degrees Kelvin), in the temperature interval 4–13 K.

In this temperature interval the binding of electrons and holes into excitons is due to classical diffusion in energy space [low-temperature interval of type (5)]. The numerical coefficients in Eq. (5) cannot be used directly for silicon, because the masses of the electrons and holes, as well as the effectivness of their interaction with the phonons, are comparable. Supposing, however, that the binding into exciton is due to the interaction of the holes with phonons, then Eq. (13) yields $\sigma\langle v\rangle = 5 \cdot 10^{-3} T^{-2}$ cm^3/sec and the same result is obtained from (13) if it is assumed that the principal role is played by the electrons.

Thus, the theory leads to a correct temperature dependence, but overestimates the binding coefficient. We note that the constants of the deformation potential, which enter in the characteristic length l_0 [see Eq. (13)], were taken by us from data on the acoustic mobility of the free holes and electrons (see Ref. 2). It is possible that the discrepancy in the values of the theoretical and experimental binding coefficients are due to the fact that the interaction of the free electrons (holes) with the phonons differs from the interaction of the carriers bound into an exciton.[10]

[1] The change of the energy of the center of gravity is $\Delta\varepsilon_c = [(p_1 + p_2)^2 - (p_1 + p_2 + q)^2]/2M$, and when the first particle collides with the phonon its momentum only rotates and hardly changes in magnitude, $(p_1 + q)^2 \approx p_1^2$. Therefore $\Delta\varepsilon_c = p_2 q/M$.

[2] This neglect is valid if the condition $n(e^2/\varkappa kT)^3 \ll 1$ is satisfied.

[3] The cross terms can be shown to be of higher order of smallness.

[4] It can be shown analogously that at $m_1 \gg m_2$ we have $\eta = (3\pi/32)^{1/2}$ and the distribution function retains the same form, but now $y^2 = \varepsilon_c m_1^2 s^2/m_2(kT)^2$.

[5] This difference is due to the fact that in the quasiclassical region, where $\varepsilon_n - \varepsilon_{n'} \ll E_B$, the momentum q of the emitted phonon is of the order of p_1, so that the energy is $sq \sim (m_1 s^2 \varepsilon)^{1/2}$. On the other hand, in the region where the distances between the levels are of the order of E_B, the phonon momentum is of the order of the momentum $p_1 + p_2$ of the center of gravity, and the energy of the obtained phonon is of the order of $(Ms^2\varepsilon)^{1/2}$ (ε is the energy of the mass center). At $m_1 \gtrsim m_2$ these energies are of the same order, but at $m_1 \ll m_2$ they differ substantially.

[6] The result for the binding cross section is, of course, independent of whether the electron has a spin or not. However, since we include the spin factor of two in the state density, it must be taken into account also in the quantum formula (41).

[1] V. N. Abakumov and I. N. Yassievich, Zh. Eksp. Teor. Fiz.

71, 657 (1976) [Sov. Phys. JETP **44**, 345 (1976)].

[2]V. N. Abakumov, V. I. Perel', and I. N. Yassievich, Fiz. Tekh. Poluprovod. **12**, 3 (1978) [Sov. Phys. Semicond. **12**, 1 (1978)].

[3]L. P. Pitaevskiĭ, Zh. Eksp. Teor. Fiz. **42**, 1326 (1962) [Sov. Phys. JETP **15**, 919 (1962)].

[4]W. A. Fok, Zs. für Physik **98**, 145 (1935).

[5]A. A. Linnik, Fiz. Tverd. Tela (Leningrad) **2**, 2044 (1960); **3**, 2322 (1961) [Sov. Phys. Solid State **2**, 1835 (1961); **3**, 1683 (1962)].

[6]J. Barrau, M. Heckmann, J. Collet, and M. Brousseau, J.

Phys. Chem. So. **34**, 1567 (1973).

[7]M. Lax, Phys. Rev. **119**, 1502 (1960).

[8]E. L. Nolle, Fiz. Tverd. Tela (Leningrad) **9**, 122 (1967) [Sov. Phys. Solid State **9**, 90 (1967)].

[9]J. Barrau, M. Heckmann, M. Brousseau, J. Phys. Chem. Sol. **34**, 381 (1973).

[10]G. L. Bir and G. E. Pikus, Simmetriya i deformatsionnye éffekty v poluprovodnikakh (Symmetries and Deformation Effects in Semiconductors), Nauka, 1972.

Translated by J. G. Adashko

Velocity dependence of the density of the normal component, and hydrodynamics of superfluid flow at high velocities

L. V. Kiknadze and Yu. G. Mamaladze

Physics Institute, Georgian Academy of Sciences
(Submitted 20 September 1979)
Zh. Eksp. Teor. Fiz. **78**, 1253–1260 (March 1980)

It is shown that the dependence of the densities of the normal and superfluid components of helium II on their relative flow velocity gives rise to a velocity dependence of the type of the equation to which the hydrodynamics of the superfluid flow reduces. As a result, hyperbolicity regions enclosed in the ellipticity region of the equation for the velocity potential (similar to "supersonic zones in subsonic flow") can arise in nonuniform flow around corners and roughnesses. The critical velocity of the transition from the elliptic type to the hyperbolic type is determined and its temperature dependence is calculated.

PACS numbers: 67.40.Bz, 67.40.Hf

We discuss in this article the circumstances that reveal certain singularities of supersonic-flow hydrodynamics, which escape attention when an analogy is drawn with the flow of an ideal classical incompressible liquid. For example, it must be assumed that when a superfluid flows around sharp corners or convexities on a solid surface there exist in the vicinities of the latter regions where the continuity equation changes from elliptic to hyperbolic. These regions are similar to the supersonic inclusions in superfluid flow, which are know from gasdynamics (see, e.g., Refs. 1 and 2), and whose presence is accompanied usually by formation of discontinuity surfaces (shock waves[3]). It seems to us that these circumstances are of importance for the hydrodynamics of helium II in general, and when vortex formation is considered in particular. Their physical basis is the dependence of the density of the normal component on the relative velocity of the components, as determined by Khalatnikov.[4]

1. To demonstrate the hydrodynamically important consequences of the velocity dependence of the components of helium II, we confine ourselves to the relativly simple case of stationary isothermal flow of the superfluid component while the normal component is at rest ($v_n = 0$) and in the absence of an external-force field. The system of equations of two-velocity hydrodynamics[4,5] reduces in this case to the equations that specify the potential character and the continuity of the

flow:

$$\operatorname{rot} \mathbf{v}_s = 0, \tag{1}$$

$$\operatorname{div} \mathbf{j}_s = 0, \tag{2}$$

where $\mathbf{j}_s = \rho_s \mathbf{v}_s$. The continuity equation for the entropy is satisfied identically. The continuity equation for the momentum and the equation of motion of the superfluid component yield one and the same equation, which determines the pressure gradient[1].

$$\operatorname{grad} P = -\rho_s \operatorname{grad} (\tfrac{1}{2} v_s^2). \tag{3}$$

The system of hydrodynamic equations is supplemented by the dependence of ρ_s on v_s, the concrete form of which is immaterial for the time being (see Sec. 4 below).

2. Equation (2) can be transformed in the following manner:

$$\rho_s \operatorname{div} \mathbf{v}_s + \mathbf{v}_s \operatorname{grad} \rho_s = 0, \tag{2a}$$

or

$$\rho_s \operatorname{div} \mathbf{v}_s + \frac{d\rho_s}{dv_s} v_s \operatorname{grad} v_s = 0, \tag{2b}$$

where $v_s \equiv |\mathbf{v}_s|$ and $d\rho_s/dv_s = \partial \rho_s/\partial v_s + (\partial \rho_s/\partial P)(dP/dv_s)$, and according to (3) we have $dP/dv_s = -\rho_s v_s$. It follows from the last two equations that the solutions of the Laplace equation that holds for an incompressible fluid

$$\Delta \varphi = 0, \tag{4}$$