

$$\Delta E = \pm \frac{4\pi V}{15} H_0^2 \chi^2 e^4, \quad (11)$$

where the + and - signs correspond to ellipsoids prolate and oblate along  $H_0$ , while  $\chi$  is the diamagnetic or paramagnetic susceptibility. It is seen from (11) that a drop of diamagnetic or paramagnetic liquid finds it energy-wise more convenient to become stretched along the magnetic field, whereas recombination magnetization leads to ablation of the EHD.

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<sup>1</sup>M. N. Gurnee, M. Glicksman, and P. W. Yu, *Solid State Commun.* **11**, 11 (1972).

<sup>2</sup>M. Glicksman, M. N. Gurnee, and J. R. Meyer, *Lecture Note in Physics* **57**, Physics of Highly Excited States in Solids, Springer, Berlin-New York, 1976, p. 219.

<sup>3</sup>V. M. Asinin and A. A. Pogachev, *Pis'ma Zh. Eksp. Teor. Fiz.* **7**, 464 (1968) [*JETP Lett.* **7**, 360 (1968)].

<sup>4</sup>V. M. Asinin and A. A. Pogachev, *Pis'ma Zh. Eksp. Teor. Fiz.* **14**, 494 (1971) [*JETP Lett.* **14**, 338 (1971)].

<sup>5</sup>A. S. Kaminskiĭ and Ya. E. Pokrovskii, *Pis'ma Zh. Eksp. Teor. Fiz.* **24**, 332 (1976) [*JETP Lett.* **24**, 300 (1976)].

<sup>6</sup>C. D. Jeffries, J. P. Wolfe, and R. S. Markiewicz, *Proc. Thirteenth Intern. Conf. on Physics of Semiconductors*, Marves, Rome, 1976, p. 879.

<sup>7</sup>A. C. Kaminskiĭ, Ya. E. Pokrovskii, and S. V. Poteshin, *Prib. Tekh. Eksp.* No. 3, 87 (1977).

<sup>8</sup>L. D. Landau and E. M. Lifshitz, *Electrodinamika sploshnykh sred* (Electrodynamics of Continuous Media), Gostekhizdat, 1957 [Pergamon, 1958].

<sup>9</sup>H. Baber, *Proc. R. Soc. London Ser. A* **158**, 383 (1937).

<sup>10</sup>R. Smith, *Semiconductors*, Cambridge Univ. Press.

<sup>11</sup>J. C. Hensel, T. G. Phillips, and T. M. Rice, *Phys. Rev. Lett.* **30**, 227 (1973).

<sup>12</sup>R. S. Markiewicz, J. E. Furneaux, and J. P. Wolfe, *Bull. Am. Phys. Soc.* **21**, 223 (1976).

<sup>13</sup>J. P. Wolfe, J. E. Furneaux, and R. S. Markiewicz, *Proc. Thirteenth Intern. Conf. on Physics of Semiconductors*, Marves, Rome, 1976, p. 954.

<sup>14</sup>A. S. Kaminskiĭ and Ya. E. Pokrovskii, *Pis'ma Zh. Eksp. Teor. Fiz.* **21**, 434 (1975) [*JETP Lett.* **21**, 198 (1975)].

<sup>15</sup>V. L. Kononenko and V. N. Murzin, *Pis'ma Zh. Eksp. Teor. Fiz.* **24**, 590 (1976) [*JETP Lett.* **24**, 548 (1976)].

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## Screening and localized impurity states in "optical" and exciton insulators

A. S. Aleksandrov and V. F. Elesin

*Moscow Engineering Physical Institute*

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We show that when a semiconductor (due to electron and hole pairing through a strong electromagnetic wave) or a semimetal (due to electron-hole Coulomb attraction) change into a dielectric state the nature of the charge screening changes considerably: in the ground state the screening radius becomes infinite, the static permittivity starts to depend on the intensity of the electromagnetic wave in a semiconductor and on the magnitude of the dielectric gap in a semimetal, and the point charge retains a Coulomb potential but with a smaller effective charge. The set of Bogolyubov equations which describes the impurity states in a semiconductor in a strong electromagnetic field and in a metal is reduced to the relativistic Dirac equations. We find as a result the wavefunctions and energies of the localized impurity states.

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In the field of a strong electromagnetic wave with a frequency in the region of the intrinsic absorption ( $\omega_0 > E_g$ ) a semiconductor goes as the result of the appearance of an energy gap<sup>[1]</sup> over into a dielectric state<sup>[2-4]</sup> ("optical" insulator). It is natural to expect that at low temperatures the screening due to the transition into a new phase is changed considerably: electrons and holes bound by the electromagnetic wave into neutral pairs cannot move in the field of a test charge so that the screening radius becomes infinite. The calculations given below confirm this qualitative statement: the long-wavelength limit of the static permittivity turns out to be finite in the ground state and dependent on the magnitude of the "optical" gap  $2\lambda = E_d$ :

$$\epsilon = \epsilon_0 \left( 1 + \frac{2}{3} \left( \frac{\omega_p}{2\lambda} \right)^2 \right),$$

where  $\omega_p$  is the plasma frequency of the free carriers,  $\epsilon_0$  takes into account the interband polarizability,  $E$  is the wave amplitude, and  $d$  the dipole moment of the interband transition.

In the short-wavelength region ( $q\xi_0 \gg 1$ ,  $\xi_0 = v_F/\lambda$  is the coherence length) the dielectric permittivity has the usual metallic character:

$$\epsilon(0, q) = \epsilon_0 (1 + (r_0 q)^{-2}),$$

where  $r_0 = (8\pi N e^2 / \epsilon_0)^{-1/2}$  is the usual Debye radius;  $v_F$

and  $N$  are the velocity and density of states near the resonance transition. The effect of the field of the electromagnetic wave on the charge screening in a semiconductor thus turns out to be very considerable.

It has been noted earlier<sup>[3]</sup> that the electric properties of an "optical" insulator are the same as those of an exciton insulator,<sup>[5]</sup> if we replace the "optical" gap  $2\lambda$  by the dielectric one  $2\Delta$  which is caused by the Coulomb attraction between electrons and holes. This is also completely confirmed by evaluating the static dielectric permittivity. In particular, the long-wavelength limit of the static permittivity in the ground state is the same as the dielectric constant of a semimetal found in Ref. 6 by calculating the vertex part.

The infinite screening radius in "optical" and exciton insulators in the ground state leads to the fact that at distances  $r < r_0$  the short-range screened potential of a point charge  $V(r) \propto e^{-r/r_0}/r$  changes to a pure Coulomb one  $1/r$ . When the temperature is raised the screening radius becomes finite as a result of the appearance of excitations, but exceeds the coherence length up to temperatures  $T \sim 0.4 T_c$  ( $T_c$  is the temperature of the transition into an exciton insulator). This character of the screening is, in the first place, reflected in the bound impurity states in an exciton insulator considered by Kopaev and Rusinov<sup>[7]</sup> who assumed that one could use as impurity potential a screened Coulomb potential with the usual Debye radius which in the case of strong screening was assumed to have the  $\delta$ -function shape.

We show in the present paper that in the weak coupling limit ( $\Delta \ll \mu$ ,  $\mu$  is the Fermi level of the semimetal) the set of Bogolyubov equations which describes bound impurity states<sup>[7]</sup> reduces to the relativistic Dirac equations which enables us to study localized states with a Coulomb potential. This possibility is not a chance one, as Keldysh<sup>[8]</sup> has shown that the two-band problem of deep impurity levels in semiconductors has an analog with the relativistic equations and in an exciton insulator the impurity state problem will always be a two-band one. The solution of the relativistic equations gives a set of discrete levels in the gap which, however, are not hydrogen-like. The existence of such a set of levels itself reflects the similarity of the general properties of an exciton insulator and of a normal semiconductor.

As to impurity states in a semiconductor in a strong electromagnetic field, one should note that an electromagnetic wave delocalizes the normal acceptor and donor states so that under well-defined conditions<sup>[9]</sup> an impurity band can be formed.<sup>[10]</sup> The problem of localized impurity states in a semiconductor in the field of an electromagnetic wave must be solved, starting from new equations in which simultaneously the conduction band, the valence band, and the interaction with a strong wave which couples them are taken into account. In view of the above-mentioned analogy between "optical" and exciton insulators those equations will be Bogolyubov equations and the set of discrete levels will arise within the limits of the "optical" gap.

## 1. PERMITTIVITY

In the self-consistent field approximation the longitudinal permittivity is as usual defined as the ratio of the potential of external sources  $V_0(\omega, \mathbf{q})$  to the sum of that potential and the potential of the induced charges  $V_s(\omega, \mathbf{q})$ :

$$\epsilon(\omega, \mathbf{q}) = V_0/V, \quad V = V_0 + V_s. \quad (1)$$

One can find the density of the induced charges using perturbation theory and choosing as the unperturbed Hamiltonian  $H$  the Hamiltonian of the electron and holes of the semimetal with a pairing potential.<sup>[5]</sup> It is convenient for a spatially non-uniform problem to write  $H$  in terms of spinor field operators:

$$H = \int d\mathbf{r} \Psi^\dagger(\mathbf{r}) (\hat{H}_0 + \Delta \hat{\sigma}_1) \Psi(\mathbf{r}), \quad (2)$$

where

$$\Psi(\mathbf{r}) = \begin{pmatrix} \Psi_c(\mathbf{r}) \\ \Psi_v(\mathbf{r}) \end{pmatrix}$$

$\Psi_{c,v}$  are the annihilation operators for an electron in the conduction and the valence band,  $\hat{\sigma}_{1,2,3}$  are the Pauli matrices,

$$H_0 = \begin{pmatrix} \epsilon_c(-i\nabla) - \mu & 0 \\ 0 & \epsilon_v(-i\nabla) - \mu \end{pmatrix},$$

$\epsilon_{c,v}(\mathbf{p})$  are the dispersion laws in the bands.

As  $H$  is a single-particle operator it can be diagonalized by going over to quasi-particle operators  $\gamma_n$ :

$$\Psi(\mathbf{r}) = \sum_n \psi_n(\mathbf{r}) \gamma_n, \quad \psi_n = \begin{pmatrix} u_n(\mathbf{r}) \\ v_n(\mathbf{r}) \end{pmatrix},$$

where the single-particle wavefunctions  $\psi_n$  satisfy a set of Bogolyubov equations

$$(\hat{H}_0 + \Delta \hat{\sigma}_1) \psi = \epsilon \psi,$$

or, in expanded form

$$\begin{aligned} (\epsilon_c(-i\nabla) - \mu) u + \Delta v &= \epsilon u, \\ (\epsilon_v(-i\nabla) - \mu) v + \Delta u &= \epsilon v. \end{aligned} \quad (3)$$

In the simple band model<sup>[1,5]</sup> with equal effective masses for the electrons and holes ( $\epsilon_c = \hbar^2/2m$ ,  $\epsilon_v = -\hbar^2/2m + 2\mu$ ) the solution of (3) has the form

$$\psi_\alpha(\mathbf{r}) = e^{i\mathbf{p}\mathbf{r}} \begin{pmatrix} u_p \\ v_p \end{pmatrix}, \quad \psi_\beta(\mathbf{r}) = e^{i\mathbf{p}\mathbf{r}} \begin{pmatrix} v_p \\ -u_p \end{pmatrix}, \quad (4)$$

$$u_p^2, v_p^2 = 1/2(1 \pm \xi_p/\epsilon_p), \quad \epsilon_{\alpha,\beta}(\mathbf{p}) = \pm \epsilon_p = \pm (\xi_p^2 + \Delta^2)^{1/2},$$

$$\xi_p = (\hbar^2 p^2 - p_F^2)/2m, \quad p_F = (2m\mu)^{1/2}$$

(two kinds of quasi-particles).

We can write the Hamiltonian of a semiconductor in the field of an electromagnetic wave in the form (2) by means of the unitary transformation<sup>[11]</sup>

$$U(t) = \exp(-1/2 i \omega_0 t (\hat{N}_c - \hat{N}_v))$$

with  $\mu = \frac{1}{2}\omega_0$  for the conduction band and  $\mu = -\frac{1}{2}\omega_0$  for the valence band. The further calculations are therefore equally valid for a semiconductor in the field of an electromagnetic wave, if we put  $\Delta = \lambda$ ,

$$p_F = [m(\omega_0 - E_g)]^{1/2}.$$

The interaction with the field of the external and the induced charges is the sum of an intraband  $H_1$  and an interband  $H_2$ :

$$H_{int} = H_1 + H_2, \quad (5)$$

$$H_1 = e \int d\mathbf{r} V(\mathbf{r}, t) \Psi^\dagger \Psi = eV(\omega, \mathbf{q}) e^{-i\omega t} \sum_{n, n'} m_{nn'}(\mathbf{q}) \gamma_n^\dagger \gamma_{n'},$$

$$H_2 = e \int d\mathbf{r} V(\mathbf{r}, t) (\Psi_c^\dagger \Psi_v + \Psi_v^\dagger \Psi_c),$$

where the "coherence factor"

$$m_{nn'}(\mathbf{q}) = \int d\mathbf{r} e^{i\mathbf{q}\cdot\mathbf{r}} \psi_{n'}(\mathbf{r}) \psi_n(\mathbf{r}).$$

Considering  $H_{1,2}$  as a perturbation one can in the standard way determine the Fourier component of the induced charge density

$$\rho_s(\omega, \mathbf{q}) = e \sum_{n, n'} m_{nn'}(\mathbf{q}) \int dt e^{i\omega t} \langle \gamma_n^\dagger \gamma_{n'} \rangle, \quad (6)$$

and, hence, also  $\varepsilon(\omega, \mathbf{q})$ .

It then turns out that the contribution to  $\varepsilon$  from the interband polarizability (the interaction  $H_2$ ) is practically independent of the wavevector and in the case of the "optical" insulator also of the intensity of the strong electromagnetic wave. This is explained by the fact that the corresponding contribution is determined, as in an ordinary dielectric,<sup>[11]</sup> by all states of the valence and conduction bands so that the change in the energy spectrum near the band edges as the result of Coulomb pairing (or the interaction with a strong electromagnetic field in a semiconductor) does not affect it. On the other hand, the polarizability of the free carriers (the interaction  $H_1$ ) changes appreciably in the phase transition.

Noting that Eqs. (5), (6) for  $H_1$  and the charge density  $\rho$  differ from the corresponding expressions for free electrons by the substitution of the electron creation and annihilation operators by quasi-particle operators and the electron charge by  $em_{nn}$ , we can use the well known formula for the longitudinal permittivity of free electrons (see, e.g., Ref. 11) replacing in it the electron energies and distribution function by the quasi-particle ones and the electron charge by  $em_{nn}$ . As a result the dielectric permittivity of an exciton or "optical" insulator takes the form

$$\varepsilon(\omega, \mathbf{q}) = \varepsilon_0 + \frac{4\pi e^2}{q^2} \sum_{n, n'} |m_{nn'}(\mathbf{q})|^2 \frac{f_{n'} - f_n}{\varepsilon_n - \varepsilon_{n'} - \omega}, \quad (7)$$

where  $f_n = \langle \gamma_n^\dagger \gamma_n \rangle$  is the number of quasi-particles in the state  $n$  and  $\varepsilon_0$  the contribution from the interband polarizability.

## 2. SCREENING IN THE GROUND AND WEAKLY EXCITED STATES

We consider the electrostatic screening  $\varepsilon(0, \mathbf{q})$  and for the sake of simplicity we restrict ourselves to the band model (4) with equal effective masses. Due to the symmetry of the bands the quasi-particle distribution can be expressed in terms of a single function  $f_p$ :

$$f_{\alpha p} = f_p, \quad f_{\beta p} = 1 - f_p.$$

In equilibrium

$$f_p = (\exp(\varepsilon_p/T) + 1)^{-1},$$

so that in the ground state ( $T=0$ )  $f_p = 0$ .

It is convenient to split off the contribution from the excitations and contribution from the polarizability of the electron-hole condensate, by writing (7) in the form

$$\varepsilon(0, \mathbf{q}) = \varepsilon_0 + \frac{8\pi e^2}{q^2} \sum_p \frac{(u_p u_{p+\mathbf{q}} + v_p v_{p+\mathbf{q}})^2 (f_{p+\mathbf{q}} - f_p)}{\varepsilon_p - \varepsilon_{p+\mathbf{q}}} + \frac{8\pi e^2}{q^2} \sum_p \frac{(u_p v_{p+\mathbf{q}} - v_p u_{p+\mathbf{q}})^2 (1 - f_p - f_{p+\mathbf{q}})}{\varepsilon_{p+\mathbf{q}} + \varepsilon_p}. \quad (8)$$

In the ground or weakly excited states the second term in (8) is small and in the last one one can put  $f_p = 0$ . Substituting  $u_p, v_p$  from (4) we get

$$\varepsilon(0, \mathbf{q}) = \varepsilon_0 + \frac{4\pi e^2}{q^2} \sum_p \frac{\varepsilon_p \varepsilon_{p+\mathbf{q}} - \xi_p \xi_{p+\mathbf{q}} - \Delta^2}{\varepsilon_p \varepsilon_{p+\mathbf{q}} (\varepsilon_{p+\mathbf{q}} + \varepsilon_p)}. \quad (9)$$

The integral in (9) has the same structure as when one calculates the Meissner effect in superconductors.<sup>[12]</sup> We can, through the substitution  $\xi_p = \sinh\theta$ ,  $\xi_{p+\mathbf{q}} = \sinh\theta'$  reduce it for  $q \ll p_F$  to the following form:

$$\frac{\varepsilon(0, \mathbf{q})}{\varepsilon_0} = 1 + (r_0 q)^{-2} \left( 1 - \frac{2}{q \xi_0} \int_0^{\frac{1}{2}} dx \frac{\arctg(q \xi_0 x / 2)}{(1-x^2)^{1/2}} \right). \quad (10)$$

In the long-wavelength limit ( $q \xi_0 \ll 1$ ) we find by expanding  $\arctan x$  in powers of  $x$

$$\frac{\varepsilon}{\varepsilon_0} = 1 + \frac{2}{3} \left( \frac{\omega_p}{2\Delta} \right)^2, \quad (11)$$

which is the same as the low-frequency polarizability found earlier in Ref. 6. Here

$$\omega_p^2 = \frac{v_F^2}{3r_0^2} = \frac{8\pi n e^2}{m \varepsilon_0},$$

$n = p_F^3 / 6\pi^2$  is the free electron or hole density (neglecting spin).

Equation (11) is analogous to the expression for the permittivity of a semiconductor<sup>[11]</sup> if we understand by the forbidden band the magnitude of the dielectric gap  $2\Delta$  and take for the plasma frequency the plasma frequency of the free carriers. As the quantity  $\varepsilon$  is independent of  $q$  as  $q \rightarrow 0$ , the screening radius in exciton and "optical" insulators becomes infinite in the ground state.

In the short-wavelength limit ( $q\xi_0 \gg 1$ ) the integral in (10) is small so that pairing does not affect the screening:

$$\varepsilon(0, q)/\varepsilon_0 = 1 + (r_0 q)^{-2}. \quad (12)$$

We show in Fig. 1 the function  $\varepsilon(0, q)$  for different coherence lengths for intermediate values of  $q$ . In the weak coupling case ( $\Delta \ll \omega_p$ ) the value of  $\varepsilon$  is much larger than  $\varepsilon_0$ . In the opposite case ( $\Delta \sim \omega_p$ )  $\varepsilon \approx \varepsilon_0$ .

The screened potential of a point charge has the form

$$V(r) = \frac{2e}{\pi r} \int_0^\infty dq \frac{\sin(qr)}{q\varepsilon(0, q)}. \quad (13)$$

Substituting Eq. (10) into (13) we find for  $r \geq \xi_0$  ( $q\xi_0 < 1$ ):

$$V(r) = e/\varepsilon_0 r \left( 1 + \frac{2}{3} \left( \frac{\omega_p}{2\Delta} \right)^2 \right), \quad (14)$$

i.e., a Coulomb potential remains at distances large compared with  $\xi_0$ , but with a smaller effective charge. At small distances  $r < r_0$  ( $q r_0 > 1$ )  $\varepsilon = \varepsilon_0$  so that

$$V(r) = e/\varepsilon_0 r. \quad (15)$$

It can be seen in Fig. 2 which shows the results of a numerical calculation that at intermediate distances ( $r_0 \lesssim r < \xi_0$ ) the potential drops monotonically from the value (15) to the magnitude (14).

When the temperature is non-vanishing or a state of equilibrium is not reached it is necessary to take into account also a contribution to  $\varepsilon$  from excitations (second term in (8)) which leads to a finite screening radius. Indeed, letting  $q$  in that term tend to zero we get

$$\varepsilon(0, q) = \varepsilon_0 \left( 1 + \frac{2}{3} \left( \frac{\omega_p}{2\Delta} \right)^2 \right) (1 + (\tilde{r}_0 q)^{-2}), \quad (16)$$

where the new screening radius is

$$\tilde{r}_0 = r_0 \left[ \left( 1 + \frac{2}{3} \left( \frac{\omega_p}{2\Delta} \right)^2 \right) / \delta n \right]^{1/2}, \quad \delta n = - \int d\xi \frac{\partial f}{\partial \varepsilon},$$

$\delta n$  is a dimensionless parameter which characterizes the degree of excitation. When obtaining (16) we assumed for the sake of simplicity that  $f \ll 1$  in order not to have to change the last term in (8).

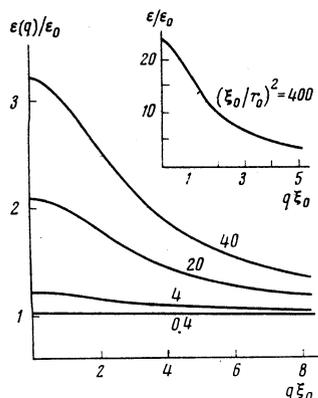


FIG. 1. Spatial dispersion of the dielectric permittivity of "optical" and exciton insulators for different coherence lengths.

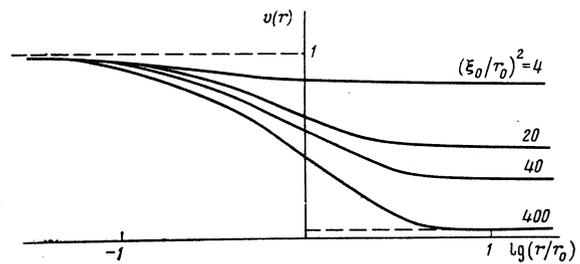


FIG. 2. Point charge potential  $v(r) = V(r) (e/\varepsilon_0 r)^{-1}$  in "optical" and exciton insulators for various coherence lengths. The dotted line corresponds to a model potential for calculating impurity levels.

As long as  $\tilde{r}_0 > \xi_0$  the presence of excitations does not affect the function  $V(r)$  in the region of most interest  $r \lesssim \xi_0$ . The screening will thus have a dielectric nature under the conditions:

$$\delta n < \frac{\Delta^2}{3\omega_p^2} \left( 1 + \frac{2}{3} \left( \frac{\omega_p}{2\Delta} \right)^2 \right). \quad (17)$$

In particular, when  $\Delta \ll \omega_p$ ,  $\delta n < \frac{1}{18}$ . We note that in equilibrium

$$\delta n = 2 \left( \frac{\pi \Delta}{T} \right)^{1/2} e^{-\Delta/T} \quad (T \ll \Delta)$$

and condition (17) is satisfied up to  $T \lesssim 0.4 T_c$  where  $T_c$  is the transition temperature.

### 3. IMPURITY STATES

For the solution of the problem of the presence of localized impurity states in an exciton or "optical" insulator it is necessary to consider the set (3) of Bogolyubov equations with an impurity potential  $V_{c,v}(r)$ :

$$\begin{aligned} \left( -\frac{\nabla^2 + p_F^2}{2m} + V_c(r) \right) u(r) + \Delta v(r) &= \varepsilon u(r), \\ \left( \frac{\nabla^2 + p_F^2}{2m} + V_v(r) \right) v(r) + \Delta u(r) &= \varepsilon v(r). \end{aligned} \quad (18)$$

We have noted above that the dielectric character of the screening does not enable us to consider the potential to be short-range so that we consider the solution of (18) with the potential of Fig. 2.

First of all we show in the general form that for a neutral impurity acting in the same way on an electron and on a hole ( $V_c = -V_v$ ) there are no bound states (this result was obtained in Ref. 7 for a  $\delta$ -function potential). The absence of bound states for a neutral impurity is caused by the fact that in the case of a neutral impurity the whole energy spectrum lies in the region  $|\varepsilon| \geq \Delta$  while the bound states must correspond to energies  $|\varepsilon| < \Delta$ . Indeed, at large distances from the impurity  $u = ae^{-kr}$ ,  $v = be^{-kr}$ , where the constants  $a$  and  $b$  are determined from (18) with  $V_{c,v} = 0$ :

$$\begin{aligned} \left( \varepsilon + \frac{k^2 + p_F^2}{2m} \right) a - \Delta b &= 0, \\ \left( \varepsilon - \frac{k^2 + p_F^2}{2m} \right) b - \Delta a &= 0. \end{aligned}$$

Hence we find

$$k^2 = -p_r^2 \pm 2m(\varepsilon^2 - \Delta^2)^{1/2}.$$

It is clear from this expression that an exponentially decreasing solution can exist only for energies  $|\varepsilon| < \Delta$  and for  $|\varepsilon^2 - \Delta^2| > \mu$ , when  $k$  has a real part. However, in the second case there is not only a solution decreasing at infinity (upper sign) but also a solution with imaginary  $k$  (lower sign) corresponding to infinite motion. Levels with  $|\varepsilon^2 - \Delta^2| > \mu$  will thus be quasi-stationary and electrons and holes will "leave" into a complex spectrum. In the case of a semiconductor in the field of an electromagnetic wave these states correspond to the usual acceptor or donor levels, delocalized by the field of the wave. Hence, bound states can exist only when  $|\varepsilon| < \Delta$ .

However, if  $V_c = -V_v$ , the whole of the spectrum of (18) lies in the region  $|\varepsilon| \geq \Delta$ . One can verify this by expanding  $u$  and  $v$  in terms of the single-electron functions  $\Phi_n$  which are solutions of the equation

$$\left(-\frac{\nabla^2 + p_r^2}{2m} + V_c(r)\right) \Phi_n = \xi_n \Phi_n,$$

$$u = \sum_n a_n \Phi_n, \quad v = \sum_n b_n \Phi_n.$$

For the expansion coefficients we get the set of equations

$$(\varepsilon - \xi_n) a_n - \Delta b_n = 0,$$

$$(\varepsilon + \xi_n) b_n - \Delta a_n = 0,$$

from which it follows that  $|\varepsilon| = (\xi_n^2 + \Delta^2)^{1/2} \geq \Delta$ .

To determine the levels in the case of a charged impurity ( $V_c = V_v = V$ ) we note that a large energy  $\mu \gg \Delta$  occurs in Eq. (18) which can be cancelled only due to fast oscillations of the wavefunction. It is therefore convenient to look for the wavefunction in the form of a product of a fast oscillating function of period  $\sim 1/p_F$  and a more slowly varying function with a characteristic length  $\xi_0$ :

$$u(r) = (f \cos(p_F r) + g \sin(p_F r)) Y_{lm}(\theta, \varphi),$$

$$v(r) = (\tilde{f} \cos(p_F r) - \tilde{g} \sin(p_F r)) Y_{lm}(\theta, \varphi),$$
(19)

where  $Y_{lm}(\theta, \varphi)$  are the angular momentum eigenfunctions.

If we take the coherence length  $\xi_0$  as the unit length and the potential  $\Delta$  as the unit energy, we get the following equations for the functions  $f, g, \tilde{f}$ , and  $\tilde{g}$ :

$$f' + \frac{f}{r} - (\varepsilon - V)g - \tilde{g} - \frac{\eta}{4} \left( g'' + \frac{2}{r} g' - \frac{l(l+1)}{r^2} g \right) = 0,$$

$$g' + \frac{g}{r} + (\varepsilon - V)f - \tilde{f} + \frac{\eta}{4} \left( f'' + \frac{2}{r} f' - \frac{l(l+1)}{r^2} f \right) = 0,$$

$$f' + \frac{\tilde{f}}{r} - (\varepsilon - V)\tilde{g} - g + \frac{\eta}{4} \left( \tilde{g}'' + \frac{2}{r} \tilde{g}' - \frac{l(l+1)}{r^2} \tilde{g} \right) = 0,$$

$$\tilde{g}' + \frac{\tilde{g}}{r} + (\varepsilon - V)\tilde{f} - f - \frac{\eta}{4} \left( \tilde{f}'' + \frac{2}{r} \tilde{f}' - \frac{l(l+1)}{r^2} \tilde{f} \right) = 0,$$
(20)

where  $\eta = \Delta/\mu$  is a small parameter, primes denote differentiation with respect to the dimensionless variables  $r$ , and all energies relate to  $\Delta$ .

Apart from small terms of order  $\eta$  we can put  $\tilde{f} = f$ ,  $\tilde{g} = g$ , and the equations for  $f$  and  $g$  become

$$(rf)' - (\varepsilon - V + 1)(rg) = 0,$$

$$(rg)' + (\varepsilon - V - 1)(rf) = 0.$$
(21)

The set (21) is the same as the Dirac equations for an electron in a spherically symmetric field,<sup>[13]</sup> if in the latter we put  $j + \frac{1}{2} = 0$  ( $j$  is the total angular momentum of the electron). We note that Eqs. (21) cannot be reduced to the one-dimensional Schrödinger equation so that the conclusion about the one-dimensional motion at large distances from the impurity which was reached in Ref. 14 is erroneous.

Apart from the solutions of (21) there are also solutions with  $\tilde{f} = -f$ ,  $\tilde{g} = -g$ , the equations for which differ from (21) through the substitutions of  $V, \varepsilon, f$  by  $-V, -\varepsilon, -f$ :

$$(rf)' - (\varepsilon - V - 1)(rg) = 0,$$

$$(rg)' + (\varepsilon - V + 1)(rf) = 0.$$
(21')

The existence of such solutions reflects the symmetry of the initial Eqs. (18) with respect to replacing a repulsive potential by an attractive potential with the simultaneous replacement of  $u$  by  $-v$ ,  $v$  by  $u$ , and  $\varepsilon$  by  $-\varepsilon$ . We shall in what follows therefore, to fix the ideas, consider only a repulsive potential ( $V > 0$ ).

To begin with we find the localized ( $|\varepsilon| < 1$ ) solutions of (21) and (21') for a potential well:

$$V(r) = V_0, \quad r < a; \quad V(r) = 0, \quad r > a.$$

In order that  $u$  and  $v$  remain finite it is necessary that  $rf \rightarrow 0$ , as  $r \rightarrow 0$  while  $rg$  remains finite. The solution of the set (21) which satisfies this condition has the form

$$f = A \frac{\sin(kr)}{r}, \quad g = A(\varepsilon - V_0 - 1) \frac{\cos(kr)}{kr} \quad \text{if } r < a,$$

$$f = B \frac{e^{-\kappa r}}{r}, \quad g = B(\varepsilon - 1) \frac{e^{-\kappa r}}{\kappa r} \quad \text{if } r > a,$$
(22)

Here  $\kappa = (1 - \varepsilon^2)^{1/2}$ ,  $k = ((V_0 - \varepsilon)^2 - 1)^{1/2}$ ,  $A$  and  $B$  are arbitrary constants.

The condition that  $f$  and  $g$  are continuous at  $r = a$  gives the equation for the energy:

$$\left(\frac{V_0 - \varepsilon - 1}{V_0 - \varepsilon + 1}\right)^{1/2} \operatorname{tg}(ka) = \left(\frac{1 + \varepsilon}{1 - \varepsilon}\right)^{1/2}.$$
(23)

In particular, for a  $\delta$ -function potential ( $a \rightarrow 0$ ,  $V_0 a = J = \text{const}$ ) we get from (23) the result of Ref. 7:

$$\varepsilon = (J^2 - 1)/(J^2 + 1),$$
(24)

i. e., a single localized level in the gap  $2\Delta$ .

The set (21') has no solutions with  $|\varepsilon| < 1$ . For a  $\delta$ -function attractive potential the localized level is obtained from the set (21').

We turn to the solution of the equations with the potential  $V(r)$  shown in Fig. 2. It is clear from Fig. 2

that at small and large  $r$  ( $r \ll r_0$ ,  $r \gg r_0$ ) we can assume the potential to be Coulombic. However, for such a potential, which diverges at the origin, Eqs. (21) and (21') give solutions which oscillate as  $r \rightarrow 0$  without tending to any definite limit. There thus arises the well known situation of the "collapse" into the center.<sup>[13]</sup> Notwithstanding this there exist also in this case stationary localized solutions with  $|\epsilon| < 1$ . It was shown in Refs. 15, 16 that the "collapse" into the center in the Dirac equations leads to the levels depending on the cut-off of the Coulomb potential at small distances. In the case considered the potential remains Coulombic, but it is clear from (20) that Eqs. (21), (21') themselves are inapplicable at small distances  $r \lesssim \eta$ . In order to take the essential dependence of the energy on the behavior of the wavefunction at the origin which arises due to the "collapse" into the center into account it is therefore necessary to find from the initial set (18) the solution for  $r \ll 1$  which is regular at the origin and to join it to the solutions of the sets (21), (21') for  $\eta \ll r \ll 1$ .

As we can for  $r \ll 1$  neglect in the Bogolyubov equations the pairing potential  $\Delta$ <sup>[14]</sup> the functions  $u$ , and hence,  $f$  and  $g$  will satisfy the normal Schrödinger equation which in dimensional form has the form

$$\left(-\frac{\nabla^2}{2m} + V(r)\right)u(r) = \frac{Pr^2}{2m}u(r). \quad (25)$$

For  $r < r_0$  we can put  $V(r) = \alpha/r$  and for  $r > r_0$ ,  $V(r) = \tilde{\alpha}/r$ , where  $\alpha = e^2/\epsilon v_F$  is the coupling constant,  $\tilde{\alpha} = \epsilon_0 \alpha / \epsilon$ , while  $\epsilon$  is given by Eq. (11). In the weak coupling case the inequality  $\eta \ll r_0 \ll 1$  is satisfied so that we can use for  $r > r_0$  the solution of (21) or (21') with the solution  $V(r) = \tilde{\alpha}/r$  and join it at the point  $r = r_0$  to the asymptotic solution of Eq. (25) with the potential  $V(r) = \alpha/r$  for large  $r$  (in dimensional form  $r_0 \gg 1/p_F$ )<sup>[17]</sup>:

$$u(r) = \frac{A}{r} \sin\left(2\frac{r}{\eta} - \alpha \ln \frac{4r}{\eta} + \delta_l\right) Y_{lm}(\theta, \varphi), \quad (26)$$

where  $\delta_l = -\frac{1}{2}\pi l + \arg \Gamma(l+1+i\alpha)$ .

Using (19) we get from (26):

$$f = -\frac{A}{r} \sin\left(\alpha \ln \frac{4r}{\eta} - \delta_l\right), \quad (27)$$

$$g = \frac{A}{r} \cos\left(\alpha \ln \frac{4r}{\eta} - \delta_l\right), \quad \eta \ll r < r_0.$$

The solution of the Dirac Eqs. (21) with the potential  $V(r) = \tilde{\alpha}/r$  which converges at infinity can be expressed in terms of Whittaker functions or the second hypergeometric functions  $\Psi(a, c, z)$ <sup>[13, 16, 18]</sup>:

$$\begin{aligned} f(r) = & B(1+\epsilon)^{1/2} e^{-\kappa r} r^{-i\tilde{\alpha}-1} \left[ \Psi\left(-i\tilde{\alpha} + \frac{\tilde{\alpha}\epsilon}{\kappa}, -2i\tilde{\alpha}+1, 2\kappa r\right) \right. \\ & \left. - \frac{\tilde{\alpha}}{\kappa} \Psi\left(-i\tilde{\alpha}+1 + \frac{\tilde{\alpha}\epsilon}{\kappa}, -2i\tilde{\alpha}+1, 2\kappa r\right) \right], \\ g(r) = & -B(1-\epsilon)^{1/2} e^{-\kappa r} r^{-i\tilde{\alpha}-1} \left[ \Psi\left(-i\tilde{\alpha} + \frac{\tilde{\alpha}\epsilon}{\kappa}, -2i\tilde{\alpha}+1, 2\kappa r\right) \right. \\ & \left. + \frac{\tilde{\alpha}}{\kappa} \Psi\left(-i\tilde{\alpha}+1 + \frac{\tilde{\alpha}\epsilon}{\kappa}, -2i\tilde{\alpha}+1, 2\kappa r\right) \right]. \end{aligned} \quad (28)$$

For small distances ( $z \ll 1$ )<sup>[18]</sup>

$$\Psi(a, c, z) \approx \frac{\Gamma(1-c)}{\Gamma(a-c+1)} + \frac{\Gamma(c-1)}{\Gamma(a)} z^{1-c}. \quad (29)$$

Using (28), (29) we find for  $r_0 < r \ll 1$

$$f = -B \frac{\sin(\tilde{\alpha} \ln(2\kappa r) - \delta(\epsilon))}{r}, \quad (30)$$

$$g = B \frac{\cos(\tilde{\alpha} \ln(2\kappa r) - \delta(\epsilon))}{r},$$

where

$$\delta(\epsilon) = \frac{\pi}{2} + \arg \frac{\Gamma(1+2i\tilde{\alpha})(\kappa+i(1-\epsilon))}{\Gamma(1+i\tilde{\alpha}+\tilde{\alpha}\epsilon/\kappa)}.$$

Equating (30) and (27) for  $r = r_0$  we get the following equation for the energy:

$$\begin{aligned} \mp \arctg\left(\frac{1\mp\epsilon}{1\pm\epsilon}\right)^{1/2} = & \arg \Gamma(1+2i\tilde{\alpha}) - \arg \Gamma\left(1+i\tilde{\alpha} + \frac{\tilde{\alpha}\epsilon}{\kappa}\right) \\ - \tilde{\alpha} \ln(2\kappa r_0) + \frac{\pi}{2} (l-2n\pm 1) + \alpha \ln \frac{4r_0}{\eta} - & \arg \Gamma(l+1+i\alpha), \end{aligned} \quad (31)$$

where the  $n$  are integers and the upper sign correspond to the solution of the set (21) and the lower sign to that of the set (21').

For an exciton insulator in the weak coupling case the inequality  $\Delta \ll \omega_p$  is satisfied as well as the condition  $\Delta \ll \mu$ . Therefore  $\tilde{\alpha} \sim \eta \ll \alpha$  and we can in Eq. (31) for not too shallow levels neglect all terms  $\propto \tilde{\alpha}$  and expand the last term in  $\alpha$ :

$$\mp \arctg\left(\frac{1\mp\epsilon}{1\pm\epsilon}\right)^{1/2} = \frac{\pi}{2} (l-2n\pm 1) + \frac{\alpha}{2} \ln \frac{\pi}{\alpha} - \alpha \psi(l+1), \quad (32)$$

where  $\psi(x)$  is the logarithmic derivative of the  $\Gamma$  function.

In an "optical" insulator the magnitude of the gap is determined by the external field and may be comparable to  $\omega_p$ , even when  $\lambda \ll \mu$ . In that case it is necessary to solve Eq. (31).

The solution (32) exists only for  $n = (l+1)/2$  (upper sign) or for  $n = (l-1)/2$  (lower sign). Because  $\alpha$  is small all levels turn out to be shallow, lying close to the lower edge of the gap ( $1 + \epsilon \ll 1$ ). Expanding  $\arctan x$  in a series for large (upper sign) or small (lower sign)  $x$  we get the following expression for the ionization energy of the levels:

$$E_{l=1+\epsilon} = \frac{\alpha^2}{2} \left( \ln \frac{\pi}{\alpha} - 2\psi(l+1) \right)^2, \quad (33)$$

$$l=0, 1, 2, 3, \dots$$

Using the series expansion for the  $\psi$  function<sup>[18]</sup>:

$$\psi(l+1) = -C + \sum_{k=1}^l \frac{1}{k}$$

we find for the lowest s-state ( $l=0$ ):

$$E_0 = \frac{\alpha^2}{2} \ln^2 \left( \frac{e^{2C}\pi}{\alpha} \right), \quad C = 0.577. \quad (34)$$

The distance between the first excited level ( $p$  state) and the ground state will be equal to

$$E_0 - E_1 = 2\alpha^2 \left( \ln \left( \frac{e^{2C}\pi}{\alpha} \right) - 1 \right). \quad (35)$$

We note that using the Bohr formula with a quasi-particle effective mass

$$\frac{1}{m^*} = \frac{d^2 \epsilon}{dp^2} \Big|_{p=p_F} = \frac{2\mu}{m\Delta}$$

to estimate the ionization energy gives  $E_0 = \frac{1}{2}\alpha^2$  which differs from (33) by the absence of the square of a large logarithm.

In conclusion we elucidate the cause of the lifting of the "accidental" degeneracy in  $l$  which is specific for the Coulomb field. The lifting of that degeneracy is not connected with the approximations used in solving the Bogolyubov Eqs. (18) but is caused because the pairing potential does not commute with the matrix analogue of the operator

$$A^* = [pl] \pm r/r,$$

which is conserved in a repulsive (attractive) Coulomb field<sup>[17]</sup>:

$$[\hat{A}\hat{\Delta}] = 2i\Delta \frac{\mathbf{r}}{r} \hat{\sigma}_z, \quad (36)$$

where

$$\hat{A} = \begin{pmatrix} A^+ & 0 \\ 0 & A^- \end{pmatrix}, \quad \hat{\Delta} = \Delta \hat{\sigma}_1.$$

The pairing potential thus lifts the "accidental" degeneracy in the Coulomb field.

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- <sup>1</sup>V. M. Galitskii, S. P. Goreslavskii, and V. F. Elesin, Zh. Eksp. Teor. Fiz. **57**, 207 (1969) [Sov. Phys. JETP **30**, 117 (1970)].
- <sup>2</sup>S. P. Goreslavskii and V. F. Elesin, Pis'ma Zh. Eksp. Teor. Fiz. **10**, 491 (1969) [JETP Lett. **10**, 316 (1969)].
- <sup>3</sup>A. S. Aleksandrov, V. F. Elesin, and P. L. Nevskii, Kvantovaya Elektron. (Moscow) No. **6**, 74 (1972) [Sov. J. Quantum Electron. **2**, 574 (1972)].
- <sup>4</sup>A. S. Aleksandrov and V. F. Elesin, Fiz. Tekh. Poluprovodn. **10**, 1154 (1976) [Sov. Phys. Semicond. **10**, 685 (1976)].
- <sup>5</sup>L. V. Keldysh and Yu. V. Kopaev, Fiz. Tverd. Tela (Leningrad) **6**, 2791 (1964) [Sov. Phys. Solid State **6**, 2219 (1965)].
- <sup>6</sup>E. V. Baklanov and A. V. Chaplik, Fiz. Tverd. Tela (Leningrad) **7**, 2768 (1965) [Sov. Phys. Solid State **7**, 2240 (1966)].
- <sup>7</sup>Yu. V. Kopaev and A. I. Rusinov, Fiz. Tverd. Tela (Leningrad) **11**, 1306 (1969) [Sov. Phys. Solid State **11**, 1059 (1969)].
- <sup>8</sup>L. V. Keldysh, Zh. Eksp. Teor. Fiz. **45**, 364 (1963) [Sov. Phys. JETP **18**, 253 (1964)].
- <sup>9</sup>A. S. Aleksandrov and V. F. Elesin, Zh. Eksp. Teor. Fiz. **62**, 762 (1973) [Sov. Phys. JETP **35**, 403 (1973)].
- <sup>10</sup>V. F. Elesin, Fiz. Tverd. Tela (Leningrad) **12**, 1133 (1970) [Sov. Phys. Solid State **12**, 885 (1970)].
- <sup>11</sup>J. M. Ziman, Principles of the Theory of Solids, Cambridge Univ. Press, 1964.
- <sup>12</sup>P. G. de Gennes, Superconductivity of Metals and Alloys, Benjamin, New York, 1966.
- <sup>13</sup>V. B. Berestetskii, E. M. Lifshitz, and L. P. Pitaevskii, Relyativistskaya kvantovaya teoriya (Relativistic quantum theory) Vol. 1, Nauka, 1968 [translation published by Pergamon, Oxford].
- <sup>14</sup>Yu. M. Kuz'min, Fiz. Tverd. Tela (Leningrad) **14**, 1883 (1972) [Sov. Phys. Solid State **14**, 1634 (1973)].
- <sup>15</sup>I. Pomeranchuk and Ya. Smorodinsky, J. Phys. USSR **9**, 97 (1945).
- <sup>16</sup>V. S. Popov, Yad. Fiz. **12**, 429 (1970) [Sov. J. Nucl. Phys. **12**, 235 (1971)].
- <sup>17</sup>L. D. Landau and E. M. Lifshitz, Kvantovaya mekhanika (Quantum mechanics) Fizmatgiz, 1963 [translation published by Pergamon, Oxford].
- <sup>18</sup>E. Jahnke, F. Emde, and F. Lösch, Tables of Higher Functions, Stuttgart, 1966.

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