Theory of the Excitonic Insulator in the Presence of Normal Impurities*

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Recently several papers have discussed the possibility of a new kind of insulating phase in semimetals or semiconductors with small band gap. This phase can be described as a condensate of electron-hole pairs (excitons) due to an effective interaction between valence and conduction electrons. This paper extends the analysis of the excitonic phase in the semimetallic region in the presence of randomly distributed normal (i.e., nonmagnetic) impurities. It is shown that the impurities have a pair-breaking effect similar to the case of magnetic impurities in superconductors. The Abrikosov-Gorkov theory developed for the latter case is applied with minor modifications to the excitonic phase. It is shown that beyond a critical impurity concentration the excitonic phase cannot exist. Changes in the transition temperature and in the order parameter are calculated, as well as the density of states. It is found that in a region close to the critical concentration the excitation spectrum of the system has no energy gap.

I. INTRODUCTION

RECENTLY several papers[1–7] have discussed the possibility of a new kind of phase in solids with small energy-band gaps. The underlying model is the usual two-band model of valence and conduction electrons with exchange interaction between the two bands. In the normal state we consider either the conventional semiconductor (positive band gap) or the conventional semimetal (negative band gap or overlap). It has been realized in both cases that for low temperatures the normal state under certain circumstances becomes unstable against the formation of electron-hole pairs or excitons on a macroscopic scale, as there is an effective attractive interaction between electrons and holes due to the exchange interaction. The resulting new phase which has been called the "excitonic insulator"[2] is stable in the semiconductor region (positive band gap) as long as the exciton binding energy is larger than the band gap. In the semimetallic region (band overlap) the occurrence of the excitonic phase is only limited by an anisotropic band structure.[4,7] In the case of isotropic bands the new phase exists for any negative band gap (overlap) though the transition temperature decreases exponentially for larger overlap due to screening effects.[3,5]

Properties of the phase have been investigated in several papers.[2–5] Especially, Jerome, Rice, and Kohn[2] have discussed the experimental observability in certain divalent metals and Group V semimetals. Though no clear experimental evidence has yet been given, recent measurements of the resistivity in strontium under high pressure[8] indicate a transition to an insulating state at about 35 kbar. This fact might be explained as the transition to the new excitonic phase, as strontium was proposed earlier as the most promising material to observe the new phase.[2]

The main property of the new phase is its insulating behavior. On the other hand, Kozlov and Maksimov[5] have pointed out that the excitonic phase is an antiferromagnet, if the excitonic pair is in a spin triplet state. This question is in any particular case decided by subsidiary interactions which are not responsible for the condensation process.[5] It is interesting to note that in the case of triplet excitons the above model is similar to the two-band model proposed by Martin-Fedders[9] and Lomer[10] to explain the itinerant antiferromagnetism in chromium. In fact, with certain simplifications Martin and Fedders arrive at essentially the same model. As pointed out in Ref. 9, this model is much too simple to apply specifically to a metal like chromium. There are contributions from other bands to the properties of chromium; "unpaired" electrons and holes, especially, lead to metallic conductivity.

In this paper we investigate the effect of normal, i.e. nonmagnetic, impurities on the excitonic phase. We confine our discussion to the semimetallic region and assume for simplicity that the valence band has a single maximum at $\mathbf{p}=0$ such that the single-particle energy is given by an isotropic dispersion

$$\epsilon_a(\mathbf{p}) = (p_0^2 - p^2)/2m_a. \quad (1)$$

We also assume a single conduction-band minimum at

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[6] E. V. Baklanov and A. V. Chaplik, Fiz. Tverd. Tela **7**, 2768 (1965) [English transl.: Soviet Phys.—Solid State **7**, 2240 (1966)].
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$\mathbf{p}=\mathbf{w}$ such that the band energy is

$$\epsilon_b(\mathbf{p})=(p^2-p_0^2)/2m_b, \tag{2}$$

where the momentum is measured relative to the minimum momentum $\mathbf{w}$.[2] The chemical potential μ is set equal to zero and the density of (conduction) electrons and holes (in the valence band) is related in the usual way to the Fermi momentum p_0 by

$$\rho=p_0^3/3\pi^2. \tag{3}$$

The impurities are assumed to be randomly distributed. If the mean free path l is larger than the inverse Fermi momentum, i.e., $lp_0\gg1$, the impurities will have a negligible effect on the single-particle spectrum, but will mainly give rise to finite lifetimes.[11] As the thermodynamic description of the excitonic phase[2-7] is very similar to the theory of superconductivity, we can treat the impurity effects in our case using well-known methods from superconductivity.[11] There is one important difference, however. Normal impurities in a superconductor have no effect on the superconducting pairs, whereas in the excitonic phase normal impurities tend to destroy the electron-hole pairs.[12] Thus the present case turns out to be similar to the case of magnetic impurities in superconductors.[13] The analogy stems from the fact that in both cases the impurity potential acts with opposite sign on the two constituents of the pairs which make up the condensate. In superconductivity the spin-dependent force of magnetic impurities acts on a pair of electrons with opposite spin; in the excitonic phase normal impurities representing an electric potential act on an electron-hole pair, i.e., oppositely charged particles.

Therefore it is not surprising that we can apply the well-known Abrikosov-Gorkov theory[13] to our problem with only minor modifications. We shall see that the impurities tend to destroy the ordered phase of electron-hole pairs and that there exists a critical concentration where the transition temperature T_c and the order parameter go to zero. Secondly, there exists a gapless region close to the transition temperature, i.e., a region in which the excitation spectrum does not exhibit a gap. From this, it follows that the transition to the excitonic state is of second order.

[11] A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinski, *Quantum Field Theory in Statistical Physics* (Prentice-Hall, Inc., Englewood Cliffs, New Jersey, 1963). As discussed in Sec. 39 of this book, we have to restrict ourselves to impurities, i.e., foreign atoms or other lattice defects, which on the whole would have a negligible effect on the electronic spectrum of the substance in the normal state. This can be roughly expressed by demanding $lp_0\gg1$. The condition implies both that the concentration of impurities is not too high and the impurity scattering not too strong, as in both cases changes in the band structure would have to be taken into account.

[12] Kopaev (Ref. 4) has briefly considered impurity effects. Due to several errors in his calculations he derives wrong conclusions about the influence of impurities on the excitonic state.

[13] A. A. Abrikosov and L. P. Gorkov, Zh. Eksperim. i Teor. Fiz. **39**, 1781 (1960) [English transl.: Soviet Phys.—JETP **12**, 1243 (1961)]. S. Skalski, O. Betbeder-Matibet, and P. R. Weiss, Phys. Rev. **136**, A1500 (1964).

Section II contains the basic formulation in terms of Greens functions. In Sec. III we consider the transition temperature T_c and the order parameter at abolute zero. In Sec. IV we investigate the density of states and the gapless region as well as the order parameter close to T_c. Section V contains a discussion of the results.

II. GREEN'S-FUNCTION FORMULATION OF THE IMPURITY PROBLEM

We consider the following Hamiltonian for the electron system[14]:

$$H=\sum_{\mathbf{p}}[\epsilon_a(\mathbf{p})a_{\mathbf{p}}^{\dagger}a_{\mathbf{p}}+\epsilon_b(\mathbf{p})b_{\mathbf{p}}^{\dagger}b_{\mathbf{p}}]+\tfrac{1}{2}\sum_{\mathbf{q}\neq0}v(\mathbf{q})\rho(\mathbf{q})\rho(-\mathbf{q})+\sum_{\mathbf{q}\neq0}u(\mathbf{q})\rho(\mathbf{q}). \tag{4}$$

Here, we have introduced $a_{\mathbf{p}}$, $a_{\mathbf{p}}^{\dagger}$ as annihilation and creation operators for valence-band electrons with momentum $\mathbf{p}$, whereas the operators $b_{\mathbf{p}}$ and $b_{\mathbf{p}}^{\dagger}$ destroy and create conduction electrons with momentum $\mathbf{p}+\mathbf{w}$.[2,7] The electron density operator is given by[15]

$$\rho(\mathbf{q})=\sum_{\mathbf{p}}[a_{\mathbf{p}+\mathbf{q}}^{\dagger}a_{\mathbf{p}}+b_{\mathbf{p}+\mathbf{q}}^{\dagger}b_{\mathbf{p}}]. \tag{5}$$

The second term in (4) represents the mutual interaction with an interaction potential

$$v(\mathbf{q})=4\pi e^2/q^2\epsilon(\mathbf{q}), \tag{6}$$

where $\epsilon(\mathbf{q})$ is an effective dielectric constant.[2] The last term in (4) describes the interaction with impurities, and $u(\mathbf{q})$ is the Fourier transform of

$$u(\mathbf{r})=\sum_i u(\mathbf{r}-\mathbf{r}_i), \tag{7}$$

the summation going over all impurities at positions $\mathbf{r}_i$. We further remark that the $\mathbf{q}=0$ terms in (4) have been left out. Both are assumed to be incorporated in the single-particle energies, one representing the Hartree energy, the other a shift of the chemical potential due to the averaged impurity potential.

It is convenient to use a two-component Nambu notation. If we write

$$\Psi(\mathbf{p})=\begin{pmatrix}b_{\mathbf{p}}\\ a_{\mathbf{p}}\end{pmatrix},\qquad \Psi^{\dagger}(\mathbf{p})=(b_{\mathbf{p}}^{\dagger},\,a_{\mathbf{p}}^{\dagger}), \tag{8}$$

the density operator (5) is given by

$$\rho(\mathbf{q})=\sum_{\mathbf{p}}\Psi^{\dagger}(\mathbf{p}+\mathbf{q})\Psi(\mathbf{p}). \tag{9}$$

We define the temperature-dependent matrix Green's

[14] We use units in which $\hbar=1$.

[15] As discussed in Ref. 2, the total density operator contains some Bloch matrix elements. The operator in Eq. (5) has the appropriate form, if we approximate the Bloch matrix elements in the limit $\mathbf{q}\to0$. We also have left out spin indices, as the electron spin is unimportant in the present problem.

function:

$$G(\mathbf{p};t,t')=-\langle T\Psi(\mathbf{p}t)\bar{\Psi}(\mathbf{p}t')\rangle, \tag{10}$$

where T is Wick's time ordering symbol, and the imaginary times t, t' are confined to: $0<t,\ t'<\beta$. The brackets $\langle\cdots\rangle$ denote a thermal average as well as a spatial average over the positions of impurities, and the Heisenberg field operators are

$$\begin{Bmatrix}\Psi(\mathbf{p}t)\\ \bar{\Psi}(\mathbf{p}t)\end{Bmatrix}=e^{tH}\begin{Bmatrix}\Psi(\mathbf{p})\\ \Psi^{+}(\mathbf{p})\end{Bmatrix}e^{-tH}. \tag{11}$$

As the Green's function (10) only depends on the time difference $t-t'$, we introduce the Fourier transform as usual:

$$G(\mathbf{p},t-t')=\beta^{-1}\sum_{\omega}G(\mathbf{p},i\omega_n)\ \exp[-i\omega_n(t-t')],$$
$$\omega_n=(\pi/\beta)(2n+1) \tag{12}$$

and the summation runs over all integers n.

The next step is to introduce the self-energy Σ through the Dyson equation

$$G^{-1}(\mathbf{p},i\omega_n)=G_0^{-1}(\mathbf{p},i\omega_n)-\Sigma(\mathbf{p},i\omega_n), \tag{13}$$

where G_0^{-1} is the Green's function in absence of any interaction,

$$G_0^{-1}=\begin{pmatrix}G_{0b}^{-1} & 0\\ 0 & G_{0a}^{-1}\end{pmatrix}=\begin{pmatrix}i\omega_n-\epsilon_b & 0\\ 0 & i\omega_n-\epsilon_a\end{pmatrix}. \tag{14}$$

We confine ourselves to the lowest-order contributions to the self-energy which are represented diagrammatically in Fig. 1.[16] The contribution from the mutual interaction is given by

$$\Sigma_1(\mathbf{p})=-\beta^{-1}\sum_{\mathbf{q}\omega}v(\mathbf{q})G(\mathbf{p}-\mathbf{q},i\omega_n). \tag{15}$$

Using

$$G=\begin{pmatrix}G_b & F\\ F^{+} & G_a\end{pmatrix}, \tag{16}$$

where F and F^{+} are Gorkov F functions

$$F(\mathbf{p},t-t')=-\langle Tb_{\mathbf{p}}(t)\bar{a}_{\mathbf{p}}(t')\rangle,$$
$$F^{\dagger}(\mathbf{p},t-t')=-\langle Ta_{\mathbf{p}}(t)\bar{b}_{\mathbf{p}}(t')\rangle, \tag{17}$$

we get, neglecting diagonal terms,

$$\Sigma_1(\mathbf{p})=\begin{pmatrix}0 & \Delta(\mathbf{p})\\ \Delta^{*}(\mathbf{p}) & 0\end{pmatrix}, \tag{18}$$

where the order parameter Δ is defined by

$$\Delta(\mathbf{p})=-\beta^{-1}\sum_{\mathbf{q}\omega}v(\mathbf{q})F(\mathbf{p}-\mathbf{q},i\omega_n). \tag{19}$$

[16] The approximation is justified for the mutual interaction, as we assume the coupling constant to be sufficiently weak. Higher-order contributions from the impurity interaction also can be neglected because $l/p_0\gg 1$ (see Ref. 11 for a discussion).

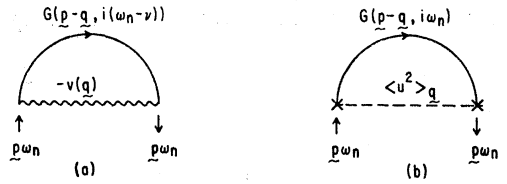

FIG. 1. Lowest-order contributions to the self-energy from (a) the mutual interaction, and (b) the interaction with impurities.

The diagonal terms left out in (18) are the usual Hartree-Fock terms which are assumed to be included in the single-particle energies ϵ_a and ϵ_b. Turning now to the lowest-order contribution from the impurity interaction, we first note that $\langle u^2\rangle_{\mathbf{q}}$ in Fig. 1 is given explicitly by

$$\langle u^2\rangle_{\mathbf{q}}$$
$$=\int d\mathbf{r}\ \exp[-i\mathbf{q}(\mathbf{r}-\mathbf{r}')]\langle u(\mathbf{r})u(\mathbf{r}')\rangle_{\text{average over impurities}}$$
$$=\rho_{sc}\mid u(\mathbf{q})\mid^2, \tag{20}$$

where ρ_{sc} is the density of scatterers. Σ_2 can therefore be written as

$$\Sigma_2(\mathbf{p},i\omega_n)=\rho_{sc}\sum_{\mathbf{p}'}\mid u(\mathbf{p}-\mathbf{p}')\mid^2 G(\mathbf{p}',i\omega_n)\equiv\bar{G}(i\omega_n). \tag{21}$$

We shall see later on that the Green's function $G(\mathbf{p},i\omega_n)$ is strongly peaked at the Fermi surface. Thus it is justified to approximate $\mid u(\mathbf{p}-\mathbf{p}')\mid^2$ assumed to be slowly varying by $\mid u(\Theta)\mid^2$, where Θ is the angle between $\mathbf{p}$ and $\mathbf{p}'$, both on the Fermi surface. As indicated in Eq. (21) the resulting $\bar{G}$ therefore depends on ω_n only.

Combining the expressions (13), (14), (18), and (21) we get the inverse matrix Green's function

$$G^{-1}(\mathbf{p},i\omega_n)=\begin{pmatrix}i\tilde{\omega}_{n,b}-\epsilon_b & -\tilde{\Delta}_n(\mathbf{p})\\ -\tilde{\Delta}_n^{+}(\mathbf{p}) & i\tilde{\omega}_{n,a}-\epsilon_a\end{pmatrix}, \tag{22}$$

where we have introduced the notation

$$i\tilde{\omega}_{n,b}=i\omega_n-\bar{G}_b(i\omega_n),$$
$$i\tilde{\omega}_{n,a}=i\omega_n-\bar{G}_a(i\omega_n),$$
$$\tilde{\Delta}_n(\mathbf{p})=\Delta(\mathbf{p})+\bar{F}(i\omega_n). \tag{23}$$

From now on we choose the phase of the order parameter $\Delta(\mathbf{p})$ equal to zero. Thus $\Delta(\mathbf{p})$ is real and positive and the same holds true for $\tilde{\Delta}_n$. Inverting Eq. (22) we obtain finally

$$G(\mathbf{p},i\omega_n)=-\frac{1}{D}\begin{pmatrix}i\tilde{\omega}_{n,a}-\epsilon_a & \tilde{\Delta}_n(\mathbf{p})\\ \tilde{\Delta}_n(\mathbf{p}) & i\tilde{\omega}_{n,b}-\epsilon_b\end{pmatrix}, \tag{24}$$

where the denominator D is given by

$$D=\tilde{\Delta}_n^2+\tilde{\omega}_{n,a}\tilde{\omega}_{n,b}-\epsilon_a\epsilon_b+i(\epsilon_b\tilde{\omega}_{n,a}+\epsilon_a\tilde{\omega}_{n,b}). \tag{25}$$

Equations (19), (21), and (24) form a closed system of

equations which can be solved for all relevant quantities involved.

First, we consider (21) for the off-diagonal component $\bar{F}(i\omega_n)$:

$$\bar{F}(i\omega_n)=\frac{\rho_{sc}}{4\pi^3}\int d\Omega\,|\,u(\Theta)\,|^2\int_0^\infty p^2dp\,F(\mathbf{p},i\omega_n). \quad (26)$$

Using (1) and (2) the integral is evaluated at the Fermi surface. With

$$z=(p^2-p_0^2)/2(m_am_b)^{1/2} \qquad (-\infty<z<\infty) \quad (27)$$

as integration variable we immediately obtain

$$\bar{F}(i\omega_n)=-\tfrac{1}{2}\Gamma[\tilde{\Delta}_n/(\tilde{\omega}_n^2+\tilde{\Delta}_n^2)^{1/2}]. \quad (28)$$

Here $\tilde{\omega}_n$ is defined as the mass average

$$\tilde{\omega}_n=(m_a\tilde{\omega}_{n,a}+m_b\tilde{\omega}_{n,b})/2(m_am_b)^{1/2}, \quad (29)$$

$\tilde{\Delta}_n$ is the value at the Fermi surface, and

$$\Gamma=(\Gamma_a\Gamma_b)^{1/2}, \quad (30)$$

where

$$\Gamma_{a,b}=(\tau_{a,b})^{-1}=\frac{\rho_{sc}p_0m_{a,b}}{2\pi^2}\int d\Omega\,|\,u(\Theta)\,|^2; \quad (31)$$

τ_a and τ_b are the scattering lifetimes for a and b electrons at the Fermi surface.[11] Inserting (28) into (23) we get the relation

$$\tilde{\Delta}_n=\Delta-\tfrac{1}{2}\Gamma\tilde{\Delta}_n/(\tilde{\omega}_n^2+\tilde{\Delta}_n^2)^{1/2}. \quad (32)$$

In the calculation of the diagonal components $\tilde{G}_a$ and $\tilde{G}_b$ we have to take into account a contribution to the z-integral from regions far away from the Fermi surface where the integral behaves like[11]

$$\int\frac{dz}{z}\,|\,u(\mathbf{p}-\mathbf{p}')\,|^2. \quad (33)$$

This gives a small shift $\delta\mu$ of the chemical potential.[11] Assuming that this has been included in the single-particle energies ϵ_a and ϵ_b, we can remove the spurious contribution by a Pauli-Villars renormalization of the integral. The integral is evaluated with a factor $M^2/(M^2+z^2)$ and the limit $M\to\infty$ taken afterwards. A simple calculation leads to

$$\tilde{G}_a(i\omega_n)=-i\tfrac{1}{2}\Gamma_a\tilde{\omega}_n/(\tilde{\omega}_n^2+\tilde{\Delta}_n^2)^{1/2},$$
$$\tilde{G}_b(i\omega_n)=-i\tfrac{1}{2}\Gamma_b\tilde{\omega}_n/(\tilde{\omega}_n^2+\tilde{\Delta}_n^2)^{1/2}, \quad (34)$$

with $\Gamma_{a,b}$ given by (31). Inserting (34) into (28) we have two relations complimentary to the relation (32):

$$\tilde{\omega}_{n,a}=\omega_n+\tfrac{1}{2}\Gamma_a\tilde{\omega}_n/(\tilde{\omega}_n^2+\tilde{\Delta}_n^2)^{1/2},$$
$$\tilde{\omega}_{n,b}=\omega_n+\tfrac{1}{2}\Gamma_b\tilde{\omega}_n/(\tilde{\omega}_n^2+\tilde{\Delta}_n^2)^{1/2}. \quad (35)$$

The relations (32) and (35) determine $\tilde{\omega}_{n,a}$, $\tilde{\omega}_{n,b}$, and $\tilde{\Delta}_n$ in terms of ω_n and Δ. It is remarkable that these relations are just the same as those obtained by Abrikosov and Gorkov in their investigation of the influence of paramagnetic impurities on the superconducting state.[13] The only difference in our case comes from the fact that two different band masses are involved which leads to the two relations (35) instead of one. As mentioned in the Introduction the analogy stems from the fact that in both cases the impurity potential acts with opposite sign on the two partners of the bound pair. In superconductivity the magnetic interaction acts on a pair of electrons with opposite spin; in our case the electric potential of normal impurities acts on an excitonic pair, i.e., oppositely charged particles. We conclude that the impurities in the excitonic phase have a pair-breaking effect, too. This will be investigated in subsequent sections. It is convenient, however, to rewrite the relations (32) and (35) in somewhat different form. Using (29) and (30) we derive a relation for $\tilde{\omega}_n$ from the two relations (35):

$$\tilde{\omega}_n=\tfrac{1}{2}(M/\mu)^{1/2}\omega_n+(M/2\mu-1)\tfrac{1}{2}\Gamma\tilde{\omega}_n/(\tilde{\omega}_n^2+\tilde{\Delta}_n^2)^{1/2}, \quad (36)$$

where M and μ are the total mass and the reduced mass, respectively:

$$M=m_a+m_b, \qquad \mu^{-1}=m_a^{-1}+m_b^{-1}. \quad (37)$$

Then introducing

$$u_n=\tilde{\omega}_n/\tilde{\Delta}_n, \quad (38)$$

one gets by combining (32) and (36)

$$\tfrac{1}{2}(M/\mu)^{1/2}(\omega_n/\Delta)=u_n(1-\alpha/(1+u_n^2)^{1/2}), \quad (39)$$

where

$$\alpha=(M/4\mu)\,(\Gamma/\Delta). \quad (40)$$

We should mention that for equal masses, $m_a=m_b$, all of the above results reduce to the analogous results of Abrikosov and Gorkov.[13]

III. TRANSITION TEMPERATURE AND ORDER PARAMETER

We study the Eq. (19) determining the order parameter Δ:

$$\Delta(\mathbf{p})=-\beta^{-1}\sum_{\omega\mathbf{p}'}v(\mathbf{p}-\mathbf{p}')\,F(\mathbf{p}',i\omega_n). \quad (41)$$

In this equation we use the screened Coulomb potential

$$v(\mathbf{q})=4\pi e^2/(q^2+\kappa^2), \quad (42)$$

where

$$\kappa^2=(e^2/\pi)\,p_0M \quad (43)$$

gives the screening due to both electrons and holes. The "normal" dielectric constant $\epsilon(q)=1+\kappa^2/q^2$, used in (42), is certainly not correct at $\mathbf{q}=0$ as we no longer have metallic screening in the excitonic phase. But

Baklanov and Chaplik have shown in detail[6] that in the semimetallic limit (large p_0) the range in which this formula breaks down is very small, namely

$$q^2<\Delta^2/v_f^2, \qquad v_f=p_0/m_{a,b} \tag{44}$$

and that this has practically no effect in the calculation of the order parameter in Eq. (41). As the integrand on the right-hand side of (41) is strongly peaked at the Fermi surface, we can set $|\mathbf{p}'|=p_0$ in $v(\mathbf{p}-\mathbf{p}')$. The angular average over $v(\mathbf{p}-\mathbf{p}')$ then gives an effective interaction for large Fermi momentum p_0:

$$\int \frac{d\Omega}{4\pi} v(\mathbf{p}-\mathbf{p}') \Big|_{|\mathbf{p}'|=p_0} \approx \bar{V} \qquad |p_0-p|<\kappa$$
$$\approx 0 \qquad \text{otherwise}, \tag{45}$$

where

$$\bar{V}=(\pi e^2/p_0^2)\ln(4p_0^2+\kappa^2)/\kappa^2. \tag{46}$$

Using (27) and inserting F from Eq. (24) we simplify the equation for the order parameter,

$$1=\left(\frac{M}{\mu}\right)^{1/2}\frac{C}{\beta}\sum_\omega\int_{-\epsilon_0}^{\epsilon_0} dz\,\frac{\tilde{\Delta}_n/\Delta}{\tilde{\Delta}_n^2+\tilde{\omega}_{n,a}\tilde{\omega}_{n,b}+z^2+iz[(m_a/m_b)^{1/2}\tilde{\omega}_{n,a}-(m_b/m_a)^{1/2}\tilde{\omega}_{n,b}]}, \tag{47}$$

with

$$C=\mu p_0\bar{V}/\pi^2, \qquad \epsilon_0=p_0\kappa/(m_a m_b)^{1/2}; \tag{48}$$

the factor $\mu p_0/\pi^2$ in the constant C can be interpreted as the density of states at the Fermi surface for a particle with reduced mass μ.

A. Transition Temperature Region

In the region $T\lesssim T_c$ we subtract from both sides of Eq. (47) the expression corresponding to the right-hand side in the pure material with $\Delta=0$. This leads to the equation

$$1-C\int_0^{\epsilon_0}\frac{dz}{z}\left\{\tanh\left[\tfrac{1}{2}\beta\left(\frac{m_a}{m_b}\right)^{1/2}z\right]+\tanh\left[\tfrac{1}{2}\beta\left(\frac{m_b}{m_a}\right)^{1/2}z\right]\right\}$$
$$=\left(\frac{M}{\mu}\right)^{1/2}\frac{\pi C}{\beta}\sum_\omega\left\{\frac{\tilde{\Delta}_n/\Delta}{(\tilde{\omega}_n^2+\tilde{\Delta}_n^2)^{1/2}}-2\left(\frac{\mu}{M}\right)^{1/2}|\omega_n|^{-1}\right\}, \tag{49}$$

where we have performed the ω summation in the subtracted term on the left-hand side and also the z integral on the right-hand side; the latter was extended to infinity as $\beta\epsilon_0\gg 1$. The left-hand side L gives the standard result known from superconductivity[11]

$$L=1-2C\ln((2\gamma/\pi)\beta\epsilon_0), \qquad \beta\epsilon_0\gg 1, \tag{50}$$

where

$$\ln\gamma=0.577 \tag{51}$$

is the Euler-Mascheroni constant. As the right-hand side of (49) vanishes at the transition temperature T_{c0} of the pure material ($\Gamma=0$), T_{c0} is given by equating (50) to zero:

$$K_B T_{c0}=(2\gamma/\pi)\epsilon_0\exp(-1/2C), \tag{52}$$

and we can express the Eq. (49) through the ratio T/T_{c0} by using (50) and (52). Canceling constants we get

$$\ln T_{c0}/T=(\pi/\beta)\sum_\omega\left\{|\omega_n|^{-1}-\frac{1}{2}\left(\frac{M}{\mu}\right)^{1/2}\Delta^{-1}(1+u_n^2)^{-1/2}\right\}, \tag{53}$$

making use of (38). Near the transition temperature T_c we expand Eq. (53) in terms of the order parameter Δ. Expanding Eq. (39) in terms of Δ and defining an average collision time τ from (31),

$$\tau^{-1}=\tfrac{1}{2}(\tau_a^{-1}+\tau_b^{-1})=\tfrac{1}{2}(\Gamma_a+\Gamma_b), \tag{54}$$

we get after some algebra up to terms of the order Δ^2

$$\ln\frac{T_{c0}}{T}=\frac{2\pi}{\beta}\sum_{\omega>0}\left\{\omega_n^{-1}-(\omega_n+1/\tau)^{-1}+\frac{2\mu}{M}\Delta^2\frac{\omega_n}{(\omega_n+1/\tau)^4}\right\}. \tag{55}$$

The transition temperature T_c is determined by $\Delta=0$. The sum over the first expression in (55) leads to[13]

$$\ln T_{c0}/T_c=\Psi(\tfrac{1}{2}+\beta_c/2\pi\tau)-\Psi(\tfrac{1}{2}), \tag{56}$$

where $\Psi(x)$ is the digamma function, $\Psi(x)=(d/dx)\log\Gamma(x)$. Expanding (56) for large τ, i.e., small impurity density, we get the first-order shift of the transition temperature

$$K_B T_c=K_B T_{c0}-\pi/4\tau. \tag{57}$$

On the other hand we find a critical collision time τ_{cr}:

$$\tau_{cr}^{-1}=(\pi/2\gamma)K_B T_{c0}, \tag{58}$$

where the transition temperature vanishes. Therefore, as in the case of magnetic impurities in superconductors, a critical impurity concentration destroys the excitonic phase completely. Assuming T_{c0} of the order of a few degrees and an average Fermi velocity of 10^6 cm/sec, we can roughly estimate a critical mean free path,

$$l_{cr}=v_f\tau_{cr}\approx 10^{-5}\text{ cm}, \tag{59}$$

which corresponds to a very low concentration of impurities.

From this we conclude that the presence of impurities puts severe limitations on the observability of the excitonic phase in those materials discussed by Jerome, Rice, and Kohn.[2] This is especially true in the case of

high-pressure experiments, as it is very doubtful whether under these experimental conditions one could control impurity effects resulting from dislocations. As mentioned in the Introduction, Martin and Fedders[9] have proposed essentially the same two-band model we have treated here as a possible explanation for the antiferromagnetism in chromium. The application of the above analysis to their model would likewise predict drastic changes of the Néel temperature when impurities are added, though a quantitative analysis might not be possible due to the crudeness of the model.

The order parameter near T_c can be obtained from Eq. (55) by expanding the left-hand side and the first term on the right. Collecting terms we get

$$\Delta^2(T)=\frac{M}{\mu}\frac{2\pi^2}{\beta_c^2}\frac{1-(\beta_c/2\pi\tau)\sum_{n=0}(n+\frac{1}{2}+\beta_c/2\pi\tau)^{-2}}{\sum_{n=0}^{\infty}[(n+\frac{1}{2})/(n+\frac{1}{2}+\beta_c/2\pi\tau)^4]}\frac{T_c-T}{T_c},\qquad T_c\gtrsim T. \tag{60}$$

B. Order Parameter at Absolute Zero

At absolute zero we denote the order parameter by

$$\Delta_0=\Delta(T=0,\Gamma),\qquad \Delta_{00}=\Delta(T=0,\Gamma=0), \tag{61}$$

and we replace the ω_n summation by an integration,

$$\beta^{-1}\sum_{\omega}\rightarrow\int\frac{d\omega}{2\pi}.$$

Subtracting from both sides of Eq. (47) the expression corresponding to the right-hand side with the replacements, $\tilde{\Delta}_n\rightarrow\Delta_0$, $\tilde{\omega}_{a,b}\rightarrow\omega$, we get

$$1-\left(\frac{M}{\mu}\right)^{1/2}C\int_0^{\epsilon_0}\frac{dz}{[\Delta_0^2+(M/4\mu)z^2]^{1/2}}=\tfrac{1}{2}C\left(\frac{M}{\mu}\right)^{1/2}\int_{-\infty}^{\infty}d\omega\left\{\frac{\tilde{\Delta}_\omega/\Delta_0}{(\tilde{\Delta}_\omega^2+\tilde{\omega}^2)^{1/2}}-[\Delta_0^2+(M/4\mu)\omega^2]^{-1/2}\right\}, \tag{62}$$

where we have performed the ω integral in the subtracted term on the left-hand side and also the z integral on the right-hand side, the latter extended to infinity. On the left we obtain at once

$$1-2C\ln\left(\left(\frac{M}{\mu}\right)^{1/2}\frac{\epsilon_0}{\Delta_0}\right),\qquad \epsilon_0\gg\Delta_0. \tag{63}$$

This can be expressed in terms of the order parameter in the pure material Δ_{00} when the right-hand side of (62) vanishes:

$$\Delta_{00}=\left(\frac{M}{\mu}\right)^{1/2}\epsilon_0\exp(-1/2C)=\frac{\pi}{\gamma}\frac{1}{2}\left(\frac{M}{\mu}\right)^{1/2}K_BT_{c0}, \tag{64}$$

which aside from the factor $\frac{1}{2}$ $(M/\mu)^{1/2}$ is the well-known relation from superconductivity.[11]

Using (64) in (63) and inserting into (62) we obtain

$$\ln\frac{\Delta_0}{\Delta_{00}}=\tfrac{1}{4}\left(\frac{M}{\mu}\right)^{1/2}\int_{-\infty}^{\infty}d\omega\,\{\Delta_0^{-1}(1+u_\omega^2)^{-1/2}-[\Delta_0^2+(M/4\mu)\omega^2]^{-1/2}\}. \tag{65}$$

Introducing $x=\frac{1}{2}(M/\mu)^{1/2}(\omega/\Delta_0)$, this can be rewritten as

$$\ln\frac{\Delta_0}{\Delta_{00}}=\int_0^{\infty}dx\,\{[1+u^2(x)]^{-1/2}-(1+x^2)^{-1/2}\}, \tag{66}$$

where from (39)

$$x=u[1-\alpha/(1+u^2)^{1/2}]. \tag{67}$$

Transforming the x integration in the first part of (66) into an integration over u, and choosing the proper lower limits from (67),

$$\begin{aligned} x_0=0&\rightarrow u_0=0, && \alpha\leq 1\\ x_0=0&\rightarrow u_0=(\alpha^2-1)^{1/2}, && \alpha\geq 1 \end{aligned} \tag{68}$$

one gets the Abrikosov-Gorkov result[13]

$$\begin{aligned} \ln\Delta_0/\Delta_{00}&=-\tfrac{1}{4}\pi\alpha && \alpha\leq 1\\ &=-\tfrac{1}{2}\alpha\arctan(\alpha^2-1)^{-1/2}+\tfrac{1}{2}\alpha^{-1}(\alpha^2-1)^{1/2}-\ln[\alpha+(\alpha^2-1)^{1/2}] && \alpha\geq 1. \end{aligned} \tag{69}$$

One may check that Δ_0 vanishes at the critical collision time (58), too. Numerical solutions for intermediate values can be found in the paper by Skalski, Betbeder-Matibet, and Weiss.[13]

IV. DENSITY OF STATES AND THE GAPLESS REGION

As a final application of the Abrikosov-Gorkov theory to the excitonic insulator we now show that there is a region just below the critical concentration of impurities in which the excitation spectrum of the system does not exhibit a gap.

We consider the density of states defined by

$$N(\omega) = -\pi^{-1} \sum_{\mathbf{p}} \operatorname{Im} \operatorname{Tr} G(\mathbf{p}, \omega + i\delta). \tag{70}$$

Using (24) and replacing $i\omega_n \to \omega + i\delta$, $iu_n \to u(\omega + i\delta)$ the integrations in (70) are similar to those leading to the relations (34). The result is

$$N(\omega)/N_0 = \operatorname{Im}[u/(1-u^2)^{1/2}], \tag{71}$$

where

$$N_0 = (p_0/\pi^2)(m_a + m_b) \tag{72}$$

is the density of states of the normal system at the Fermi surface. u is here determined by the modified relation (39):

$$\tfrac{1}{2}(M/\mu)^{1/2}(\omega/\Delta) = u[1-\alpha/(1-u^2)^{1/2}], \tag{73}$$

the radical here and in (71) defined as the analytical continuation of the positive square root for real u, $|u|<1$, into the upper half plane of the complex variable u. In the pure material ($\alpha=\Gamma=0$) Eq. (71) reduces to

$$\frac{N(\omega, \Gamma=0)}{N_0} = 0 \qquad 0<\omega<2(\mu/M)^{1/2}\Delta$$

$$= \frac{\omega}{[\omega^2 - (4\mu/M)\Delta^2(\Gamma=0)]^{1/2}} \qquad 2(\mu/M)^{1/2}\Delta<\omega, \tag{74}$$

where the gap is

$$\omega_g = 2\left(\frac{\mu}{M}\right)^{1/2} \Delta(\Gamma=0). \tag{75}$$

In the impure system, the gap ω_g is given by the highest value of ω for which the relation (73) exhibits a real solution for $u=u(\omega)$ with $|u|<1$. Maximizing the right-hand side of (73) we find

$$u_g = (1-\alpha^{2/3})^{1/2}, \qquad \alpha \leq 1, \tag{76}$$

which leads to

$$\begin{aligned} \omega_g &= 0 && \alpha \geq 1 \\ &= 2(\mu/M)^{1/2}\Delta(1-\alpha^{2/3})^{3/2} && \alpha \leq 1. \end{aligned} \tag{77}$$

Thus there is no gap in the excitation spectrum, if $\alpha \geq 1$. In the region $\alpha \leq 1$, the gap is smaller by the factor $(1-\alpha^{2/3})^{3/2}$ as compared to the pure case [Eq. (75)]. Near T_c we are always in the gapless region, as $\Delta \to 0$ and $\alpha \geq 1$. The gapless region extends over all temperatures, if at $T=0$ we have $\alpha \geq 1$. The corresponding value for Δ_0 follows from (69),

$$\Delta_0 = \exp(-\pi/4)\Delta_{00}, \tag{78}$$

and $\alpha=1$ leads to a scattering time

$$1/\tau' = 2\exp(-\tfrac{1}{4}\pi)\tau_{cr}^{-1} \approx 0.91\tau_{cr}^{-1}. \tag{79}$$

For concentrations such that $\tau_{cr}<\tau<\tau'$, the gapless region extends over all temperatures.

Other thermodynamic quantities such as the free energy, specific heat, etc. could be equally well calculated within the framework of the Abrikosov-Gorkov theory. As these quantities would be very similar to those in superconductivity,[13] we do not go into further details here. The application of the foregoing analysis to transport problems, i.e., electrical and thermal conductivity, is reserved for a later publication.

V. SUMMARY

In this paper, we have discussed the effect of normal impurities on the excitonic insulator in the semimetallic region. Due to the fact that the impurity potential acts with opposite sign on the constituents of the excitonic pair, the impurities have a pair-breaking effect. We have seen that the situation is very similar to the case of magnetic impurities in superconductors. Thus the Abrikosov-Gorkov theory[13] could be taken over with only minor modifications to describe the present situation. Several predictions of the Abrikosov-Gorkov theory, especially, also hold in this case, as discussed in the last two sections.

The most important of these predictions is the fact that there exists a critical concentration of impurities beyond which the excitonic phase is destroyed at all temperatures. As the critical density, according to our estimates, is very low, the presence of impurities puts severe limitations on the occurrence of the excitonic phase. Furthermore, as was shown in Ref. 7, an anisotropic band structure also would be unfavorable to the excitonic state in the semimetallic region.

In spite of this, impurities might prove to be a very useful tool in identifying the transition to the excitonic phase in contrast to transitions to other insulating

"normal" phases, i.e., polymorphic transitions, etc. This could be done by varying the density of impurities in doubtful cases and studying changes in the transition temperature. In the same way, a careful study of antiferromagnetism in chromium alloys could help to decide on the applicability of the Lomer two-band model to chromium.[9,10] Due to the crudeness of the model in contrast to the real band structure in the latter case, quantitative estimates might be very difficult, however.

Though we have investigated the effect of impurities on the excitonic phase only in the semimetallic limit, it is clear that qualitatively the results of this paper should hold true also in the semiconductor region (positive or zero band gap in the underlying two-band model). The quantitative description would be different, however. There are two important differences from the former situation. First, the modifications of the single-particle energies due to impurities could not be neglected; in the semimetallic case we only have a small negligible shift of the Fermi energies. Secondly, the collision times $\tau_{a,b}$ will become energy- (or temperature-) dependent. It remains to be seen whether and how the Abrikosov-Gorkov theory has to be modified in order to deal with this situation.

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Dielectric Constant of a Dense Electron Gas Containing a Fixed Point Charge

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An expression for the dielectric constant of a dense electron gas containing a positive point charge Ze with a neutralizing positive background is obtained by employing the diagram technique of quantum field theory. The present derivation leads to some more terms in addition to those obtained in the self-consistent-field approximation. Besides, our derivation rigorously takes into account the Pauli exclusion principle. The simplest evaluation of the dielectric constant is made in the region where collective effect dominates, and the results are compared with those obtained in the self-consistent-field approximation.

1. INTRODUCTION

SINGLE-PARTICLE Green's functions $G(x, x')$ for a homogeneous system consisting of an interacting electron gas are widely used to obtain information regarding its ground-state properties and the nature of its elementary excitations. But most systems which one finds in nature are inhomogeneous. An inhomogeneity in a system arises from any external field acting on it. The type of inhomogeneity considered here is that due to a point charge Ze fixed inside an electron gas. This is of great physical interest for the study of the discrete single-particle excitation spectrum. Recently, Layzer[1] has investigated the quasiparticle excitation of such a system. He has shown that for a positive point charge, there exists a discrete spectrum of bound holes, finite in number, which disappears beyond a certain limiting value of the electron density. A similar investigation has been made by Sziklas[2] on the collective oscillations of a dense electron gas containing a fixed point charge. He finds two distinct types of collective excitations of this system. The first one, called a free plasmon, has the same excitation spectrum as found for the homogeneous system; and the other, called a bound plasmon, belongs to a discrete type of spectrum, and has no counterpart in the homogeneous gas. It exists only if the impurity charge is negative. Layzer's investigation of the quasiparticle excitations is based on the one-particle Green's function $G^{(w)}(x, x')$ for the nonuniform many-fermion systems. Besides Layzer, Sham and Kohn[3] have recently studied the inhomogeneous system consisting of an interacting electron gas using its one-particle Green's function. In this paper, we shall, however, use the one-particle Green's function $G^{(w)}(x, x')$ for the inhomogeneous system to derive an expression for its dielectric constant.

In Sec. 2, a brief review of the Green's-function approach to a many-fermion system is presented. A perturbation expansion is obtained for the one-particle Green's function of the inhomogeneous system in terms of the corresponding Green's function of the homogeneous case.

In Sec. 3, an expression for the dielectric constant of the inhomogeneous system is obtained by using the perturbation expansion of its one-particle Green's function. It is found that the expression for the dielectric

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