

and by using the thermodynamic relation⁷

$$\chi_T = \chi_0 + \frac{T(\partial M/\partial T)_h^2}{C_h},$$

where C_h is the specific heat at fixed field.

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⁷J. H. Van Vleck, *Z. Physik. Chem. (Frankfurt)* **16**, 358 (1958).

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Transport Properties of the "Excitonic Insulator": Electrical Conductivity*

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The dc conductivity of the "excitonic insulator" recently discussed in the literature is calculated in the semimetallic region. The calculations are based on recent work on the description of the excitonic phase in the presence of impurities. It is shown that the conductivity decreases below the transition temperature to the excitonic state. For low impurity concentrations the system acquires insulating properties. For higher impurity concentrations the conductivity is still nonzero at $T=0$. Thus, metallic properties prevail in the excitonic phase. It is pointed out that this behavior depends essentially on the form of the excitation spectrum of the system, i.e., the presence or absence of a gap. At the transition temperature the conductivity-versus-temperature curve has a finite slope.

I. INTRODUCTION

RECENTLY, several papers have discussed the properties of an excitonic phase which is expected to occur in solids with small energy band gap.^{1,2} The phase can be described as a condensate of bound pairs of electrons and holes due to an effective attractive interaction between conduction-band and valence-band states. In the normal state one considers both a positive band gap (semiconductor) and a negative band gap (semimetals). The most extensive study of the properties of this phase has been given by Jerome, Rice, and Kohn.¹ Besides the question of experimental observability, they have discussed in detail the ordering phenomenon which takes place in the new state.

While the thermodynamic properties of the excitonic phase are similar to those of a superconductor, the electromagnetic properties are perhaps more interesting from an experimental point of view. According to the work of Jerome, Rice, and Kohn¹ the excitonic phase turns out to be an insulator. This is especially interesting in the case where the underlying two-band model has a negative band gap (semimetallic region) and therefore would conventionally have metallic properties.

This paper deals with the electrical conductivity of the excitonic phase at low temperatures where the main scattering mechanism is due to impurities and imperfections. Jerome, Rice, and Kohn¹ have calculated the frequency-dependent complex conductivity for the pure system and have derived the dc conductivity by using Kramers-Kronig relations and a simple ansatz for taking scattering into account. The more rigorous calculation in this paper does not confirm their results. The reason for this is that the impurities play a rather intricate role. In a former paper³ we have considered the influence of randomly distributed impurities on the excitonic phase. We found that the situation is very similar to the case of magnetic impurities in superconductors, i.e., the impurities have a pair-breaking

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¹D. Jerome, T. M. Rice, and W. Kohn, *Phys. Rev.* **158**, 462 (1967).

²L. V. Keldysh and Yu. V. Kopaev, *Fiz. Tverd. Tela* **6**, 2791 (1964) [English transl.: *Soviet Phys.—Solid State* **6**, 2219 (1965)]; Yu. V. Kopaev, *Fiz. Tverd. Tela* **8**, 223 (1966) [English transl.: *Soviet Phys.—Solid State* **8**, 175 (1966)]; A. N. Kozlov and L. A. Maksimov, *Zh. Eksperim. i Teor. Fiz.* **48**, 1184 (1965); **49**, 1284 (1965) [English transl.: *Soviet Phys.—JETP* **21**, 790 (1965); **22**, 889 (1966)]; J. Zittartz, *Phys. Rev.* **162**, 752 (1967). Other references can be found in Ref. 1.

³J. Zittartz, *Phys. Rev.* **164**, 575 (1967). This paper will be referred to as I.

effect. In I we have applied the theory of Abrikosov and Gorkov⁴ to our case with only minor modifications. The main property is the fact that there exists a critical concentration of impurities beyond which the excitonic phase cannot exist. Secondly, there is a region close to the critical concentration where the excitation spectrum of the system does not have a gap.

In the present paper we apply the theory of I to the calculation of the electrical conductivity. We shall see that the formalism is rather similar to calculations of transport properties in superconductors with magnetic impurities. Therefore, we can take advantage of the work of Ambegaokar and Griffin⁵ and Kadanoff and Falcko⁶ on thermal conductivity and ultrasonic attenuation in superconductors, respectively.

In Sec. II A we discuss briefly the model and the results of Paper I necessary for our calculations. In Sec. II B we set up basic formulas for the electrical conductivity. Sections III and IV contain the main calculations. We derive a final formula for the conductivity which is evaluated in several limiting cases in Sec. V. We shall see that the behavior of the dc conductivity is mainly determined by the excitation spectrum of the system and not by the order parameter. Thus, the dc conductivity goes to zero at $T=0$ only for small impurity concentrations where there is a gap in the excitation spectrum. At higher concentrations the gap vanishes, and the conductivity remains finite at $T=0$, though smaller than the corresponding conductivity of the normal state. Near T_c the system is always in the gapless region. From this fact it follows that the slope of the conductivity-versus-temperature curve is finite at T_c in contrast to the infinite slope reported in Ref. 1. The results are summarized and discussed in Sec. VI.

II. BASIC FORMULATION

A. Discussion of the Model

In I we have considered the following two-band model in the semimetallic region. The noninteracting part of the Hamiltonian is

$$H_0 = \sum_{\mathbf{p}} \{ \epsilon_b(\mathbf{p}) b_{\mathbf{p}}^\dagger b_{\mathbf{p}} + \epsilon_a(\mathbf{p}) a_{\mathbf{p}}^\dagger a_{\mathbf{p}} \}, \quad (1)$$

where the summation goes over the first Brillouin zone. For simplicity we assume that the conduction band (b) has a single minimum and the valence band (a) a single maximum. Furthermore, we assume a spherical shape for both bands near their extrema and measure momenta relative to the extremal momenta in both cases. Thus near the extrema we have

$$\begin{aligned} \epsilon_b(\mathbf{p}) &= (p^2 - p_0^2)/2m_b, \\ \epsilon_a(\mathbf{p}) &= (p_0^2 - p^2)/2m_a, \end{aligned} \quad (2)$$

⁴ A. A. Abrikosov and L. P. Gorkov, Zh. Eksperim. i Teor. Fiz. **39**, 1781 (1960) [English transl.: Soviet Phys.—JETP **12**, 1243 (1961)].

⁵ V. Ambegaokar and A. Griffin, Phys. Rev. **137**, 1151 (1965).

⁶ L. P. Kadanoff and I. I. Falcko, Phys. Rev. **136**, 1170 (1964).

while the density of (conduction) electrons or (valence band) holes is related to the Fermi momentum p_0 in the usual way: $\rho = p_0^3/3\pi^2$. Using a Nambu notation

$$\psi(\mathbf{p}) = \begin{pmatrix} b_{\mathbf{p}} \\ a_{\mathbf{p}} \end{pmatrix}, \quad (3)$$

we write the electronic density operator as

$$\rho(\mathbf{q}) = \sum_{\mathbf{p}} \psi^\dagger(\mathbf{p}+\mathbf{q})\psi(\mathbf{p}). \quad (4)$$

The interaction part of the Hamiltonian is then given by

$$H' = \frac{1}{2} \sum_{\mathbf{q}} v(\mathbf{q}) \rho(\mathbf{q}) \rho(-\mathbf{q}) + \sum_{\mathbf{q}} U(\mathbf{q}) \rho(\mathbf{q}), \quad (5)$$

where the first term describes the mutual interaction via screened Coulomb forces. As discussed in I and also in Ref. 1, the effective potential $V(\mathbf{r})$ becomes more and more short range in the semimetallic limit (large p_0); thus its Fourier transform $v(\mathbf{q})$ may finally be replaced by a constant \bar{V} . The second term in (5) describes the interaction with random impurities at sites \mathbf{r}_i such that

$$U(\mathbf{r}) = \sum_i u(\mathbf{r}-\mathbf{r}_i), \quad (6)$$

the summation going over all impurities.

The thermodynamic properties of the model follow from the matrix Green's function

$$G \equiv \begin{pmatrix} G_b & F \\ F & G_a \end{pmatrix} = - \langle T \psi(\mathbf{p}t) \bar{\psi}(\mathbf{p}t') \rangle, \quad (7)$$

where t, t' are imaginary times, $0 \leq t, t' \leq \beta$, the brackets indicate a thermal average as well as an average over impurity sites, and

$$\begin{Bmatrix} \psi(\mathbf{p}t) \\ \bar{\psi}(\mathbf{p}t) \end{Bmatrix} = e^{iHt} \begin{Bmatrix} \psi(\mathbf{p}) \\ \psi^\dagger(\mathbf{p}) \end{Bmatrix} e^{-iHt}. \quad (8)$$

The Green's function G has been derived in I and discussed extensively. We shall confine ourselves to the simple case of equal masses $m_a = m_b = m$ in the explicit calculations in the next sections.⁷ Therefore, it is sufficient here to give the result for G only in this simple case:

$$G(\mathbf{p}, i\omega_n) = - \frac{1}{\tilde{\omega}_n^2 + \tilde{\Delta}_n^2 + \epsilon^2} \begin{pmatrix} i\tilde{\omega}_n + \epsilon & \tilde{\Delta}_n \\ \tilde{\Delta}_n & i\tilde{\omega}_n - \epsilon \end{pmatrix}, \quad (9)$$

where $\epsilon = \epsilon_b = -\epsilon_a$, $\omega_n = (2n+1)\pi\beta^{-1}$. Furthermore, we have the relations defining $\tilde{\Delta}_n$ and $\tilde{\omega}_n$ through the order parameter Δ and ω_n :

$$\begin{aligned} \tilde{\omega}_n &= \omega_n + \frac{1}{2} \Gamma [\tilde{\omega}_n / (\tilde{\omega}_n^2 + \tilde{\Delta}_n^2)^{1/2}], \\ \tilde{\Delta}_n &= \Delta - \frac{1}{2} \Gamma [\tilde{\Delta}_n / (\tilde{\omega}_n^2 + \tilde{\Delta}_n^2)^{1/2}], \end{aligned} \quad (10)$$

⁷ This is only done for mathematical convenience. As there has been no indication in former calculations that any property depends essentially on the mass difference $m_a - m_b$, we feel that the simplification is not important.

where Γ is the inverse collision time (see I)

$$\Gamma = 1/\tau = (2\pi^2)^{-1} \rho_{sc} m p_0 \int d\Omega |u(\Theta)|^2. \quad (11)$$

The analytic properties of G and the functions defined in (10) are further explored in the Appendix.

B. Electromagnetic Response

In order to calculate the current generated by an electric field, we introduce a time-dependent vector potential

$$\mathbf{A}(t) = \int_{-\infty}^{\infty} d\omega \mathbf{A}(\omega) \exp(-i\omega t). \quad (12)$$

For general band structure this means we have to replace the band energies $\epsilon_{a,b}$ by

$$\epsilon_{a,b}(\mathbf{p}) \rightarrow \epsilon_{a,b}(\mathbf{p} - e\mathbf{A}), \quad (13)$$

where e is the electron charge. The linear response current may then be written as

$$\mathbf{j}(\omega) = K(\omega + i\delta) \mathbf{A}(\omega), \quad (14)$$

where we have anticipated spherical symmetry. The infinitesimal δ indicates that the response is "retarded." Finally, we have the frequency-dependent complex conductivity

$$\sigma(\omega) = (1/i\omega) K(\omega + i\delta). \quad (15)$$

There are two contributions to K . First we have the paramagnetic part $K^P(\omega + i\delta)$, which is most easily calculated in the following way: We consider the causal correlation function

$$K^P(t-t') = \frac{1}{3} \langle T \mathbf{J}(t) \mathbf{J}(t') \rangle, \quad (16)$$

where t, t' are imaginary times and $\mathbf{J}(t)$ is the electric current operator. Fourier transforming $K^P(t-t')$ in the usual way,

$$K^P(t-t') = \beta^{-1} \sum_{\nu} K^P(i\nu) \exp[-i\nu(t-t')],$$

$$\nu = 2n\pi\beta^{-1}, \quad (17)$$

we continue analytically into the complex energy plane: $i\nu \rightarrow z$. The retarded response function $K^P(\omega + i\delta)$ is then given by $K^P(z = \omega + i\delta)$.

The diamagnetic contribution to $K(\omega + i\delta)$ is simply a constant which is given for general band structure by

$$K^D = -\frac{1}{3} e^2 \sum_{\mathbf{p}} \{ [\nabla_{\mathbf{p}}^2 \epsilon_a(\mathbf{p})] n_a(\mathbf{p}) + [\nabla_{\mathbf{p}}^2 \epsilon_b(\mathbf{p})] n_b(\mathbf{p}) \}, \quad (18)$$

where $n_a(\mathbf{p})$ and $n_b(\mathbf{p})$ are the occupation numbers of a and b electrons in momentum space.⁸

Turning now to the calculation of the current-current correlation function (16), we first note that the spatially uniform current operator $\mathbf{J}(t)$ is given by

$$\mathbf{J}(t) = e \sum_{\mathbf{p}} \bar{\psi}(\mathbf{p}t) \mathbf{v}(\mathbf{p}) \psi(\mathbf{p}t), \quad 0 \leq t \leq \beta, \quad (19)$$

where the velocity matrix \mathbf{v} is explicitly

$$\mathbf{v}(\mathbf{p}) = \begin{pmatrix} \mathbf{v}_b(\mathbf{p}) & 0 \\ 0 & \mathbf{v}_a(\mathbf{p}) \end{pmatrix}, \quad \mathbf{v}_{a,b}(\mathbf{p}) = (\partial/\partial \mathbf{p}) \epsilon_{a,b}(\mathbf{p}). \quad (20)$$

Introducing (19) into (16) we can easily express the total expectation value through the Green's functions and an appropriate vertex function.⁹ Fourier transforming according to (17), we finally get

$$K^P(i\nu) = -\frac{1}{3} e^2 \beta^{-1} \sum_{\mathbf{p}\omega} \text{Tr}[\mathbf{v}(\mathbf{p}) G(\mathbf{p}, i\omega_n) \mathbf{W}(\mathbf{p}; i\omega_n, i\omega_n - i\nu) G(\mathbf{p}, i\omega_n - i\nu)], \quad (21)$$

where the summation over frequencies ω_n has to be performed first; the "Tr" in this expression comes in because the Green's functions and velocities are given in matrix form. \mathbf{W} is the vertex-corrected velocity matrix which replaces the zeroth-order velocity \mathbf{v} and will be considered in the next section.

Finally, we rewrite the diamagnetic contribution K^D (18) in a form similar to expression (21). We perform a partial integration over the Brillouin zone. This gives for one of the terms in (18), for example,¹⁰

$$\begin{aligned} \sum_{\mathbf{p}} [\nabla_{\mathbf{p}}^2 \epsilon_a(\mathbf{p})] n_a(\mathbf{p}) &= - \sum_{\mathbf{p}} [\partial \epsilon_a(\mathbf{p}) / \partial \mathbf{p}] \cdot (\partial / \partial \mathbf{p}) n_a(\mathbf{p}) \\ &= - \sum_{\mathbf{p}} \mathbf{v}_a(\mathbf{p}) \beta^{-1} \sum_{\omega} (\partial / \partial \mathbf{p}) G_a(\mathbf{p}, i\omega_n), \end{aligned} \quad (22)$$

where in the second line we have introduced the Green's-function representation for $n_a(\mathbf{p})$. Using (9) we get, combining both terms in (18),

$$\begin{aligned} K^D &= (e^2/3\beta) \sum_{\mathbf{p}\omega} [\mathbf{v}_b^2(\mathbf{p}) G_b^2(\mathbf{p}, i\omega_n) + \mathbf{v}_a^2(\mathbf{p}) G_a^2(\mathbf{p}, i\omega_n) + 2\mathbf{v}_a(\mathbf{p}) \mathbf{v}_b(\mathbf{p}) F^2(\mathbf{p}, i\omega_n)] \\ &= (e^2/3\beta) \sum_{\mathbf{p}\omega} \text{Tr}[\mathbf{v}(\mathbf{p}) G(\mathbf{p}, i\omega_n) \mathbf{v}(\mathbf{p}) G(\mathbf{p}, i\omega_n)], \end{aligned} \quad (23)$$

which is the desired form.

⁸ For free electrons, $\epsilon = (p^2 - p_0^2)/2m$, expression (18) reduces to the familiar result, $K^D = -(e^2/m)\rho$, where ρ is the density.

⁹ J. R. Schrieffer, *Theory of Superconductivity* (W. A. Benjamin, Inc., New York, 1964), Chap. 8.

¹⁰ The integrated term vanishes because of the periodicity of band energies over the Brillouin zone.

III. VERTEX CORRECTION

In I we have calculated the self-energy Σ to the lowest order in the interaction, i.e., mutual and impurity interaction. To be consistent with this approximation⁹ we have to sum all ladder diagrams in the calculation of the vertex function \mathbf{W} introduced in the last section. Thus \mathbf{W} satisfies the integral equation

$$\mathbf{W}(\mathbf{p}; i\omega_n, i\omega_{n-}) = \mathbf{v}(\mathbf{p}) - \beta^{-1} \sum_{\mathbf{p}'\omega'} v(\mathbf{p}-\mathbf{p}') G(\mathbf{p}', i\omega_n') \mathbf{W}(\mathbf{p}'; i\omega_n', i\omega_{n-}') G(\mathbf{p}', i\omega_{n-}') + \sum_{\mathbf{p}'} \rho_{sc} |u(\mathbf{p}-\mathbf{p}')|^2 G(\mathbf{p}', i\omega_n) \mathbf{W}(\mathbf{p}'; i\omega_n, i\omega_{n-}) G(\mathbf{p}', i\omega_{n-}), \quad (24)$$

where we have used the abbreviation $\omega_{n-} = \omega_n - \nu$. The second term on the left-hand side is due to the mutual interaction whereas the third term describes the scattering from impurities; ρ_{sc} is the density of scatterers.

Restricting ourselves to the semimetallic limit where the Fermi momentum p_0 becomes very large, we replace $v(\mathbf{p}-\mathbf{p}')$ by a constant \bar{V} as mentioned before. In this case the second term in (24) does not contribute to the vertex function, as $\mathbf{W}(\mathbf{p})$, like the inhomogeneous term $\mathbf{v}(\mathbf{p})$, is proportional to the momentum vector \mathbf{p} , and the angular integration gives a zero result. Using (2) and (20) with $\epsilon = \epsilon_0 = -\epsilon_a$ we may write

$$\mathbf{v}(\mathbf{p}) = (\partial\epsilon/\partial\mathbf{p})\sigma_3 = (\mathbf{p}/m)\sigma_3, \quad (25)$$

where σ_3 is the third Pauli matrix in the usual notation. We also make the ansatz

$$\mathbf{W}(\mathbf{p}; i\omega_n, i\omega_{n-}) = (\mathbf{p}/m) \Lambda(i\omega_n, i\omega_{n-}). \quad (26)$$

Multiplying expression (24) across with \mathbf{p}/p^2 and performing the angular integration we get the equation

$$\Lambda(i\omega_n, i\omega_{n-}) = \sigma_3 + \frac{\Gamma'}{2\pi} \int_{-\infty}^{\infty} d\epsilon G(\epsilon, i\omega_n) \Lambda(i\omega_n, i\omega_{n-}) G(\epsilon, i\omega_{n-}), \quad (27)$$

where

$$\Gamma' = (2\pi^2)^{-1} \rho_{sc} m p_0 \int d\Omega |u(\theta)|^2 \cos\theta, \quad (28)$$

assuming that $|u(\mathbf{p}-\mathbf{p}')|^2$ depends on the angle θ between \mathbf{p} and \mathbf{p}' only (see I). The remaining integrals in (27) are easily done by residue techniques. Inserting

the Green's functions from (9), we obtain after some algebra

$$\Lambda(i\omega_n, i\omega_{n-}) = \Lambda_1(i\omega_n, i\omega_{n-})\sigma_3 + \Lambda_2(i\omega_n, i\omega_{n-})\sigma_2, \quad (29)$$

where σ_2 is the second Pauli matrix and the scalar quantities $\Lambda_{1,2}$ are given explicitly by

$$\Lambda_1(i\omega_n, i\omega_{n-}) = 1 + \frac{1}{2}\Gamma' \frac{(\tilde{\omega}_n^2 + \tilde{\Delta}_n^2)^{1/2} \cdot (\tilde{\omega}_{n-}^2 + \tilde{\Delta}_{n-}^2)^{1/2} - \tilde{\omega}_n \tilde{\omega}_{n-} - \tilde{\Delta}_n \tilde{\Delta}_{n-}}{L + \Gamma'(\tilde{\omega}_n \tilde{\omega}_{n-} + \tilde{\Delta}_n \tilde{\Delta}_{n-})}, \quad (30a)$$

$$\Lambda_2(i\omega_n, i\omega_{n-}) = \frac{1}{2}\Gamma' \frac{\tilde{\Delta}_n \tilde{\omega}_{n-} - \tilde{\Delta}_{n-} \tilde{\omega}_n}{L + \Gamma'(\tilde{\omega}_n \tilde{\omega}_{n-} + \tilde{\Delta}_n \tilde{\Delta}_{n-})}, \quad (30b)$$

where

$$L = (\tilde{\omega}_n^2 + \tilde{\Delta}_n^2)^{1/2} \cdot (\tilde{\omega}_{n-}^2 + \tilde{\Delta}_{n-}^2)^{1/2} \times \{(\tilde{\omega}_n^2 + \tilde{\Delta}_n^2)^{1/2} + (\tilde{\omega}_{n-}^2 + \tilde{\Delta}_{n-}^2)^{1/2}\}. \quad (31)$$

In order to proceed with the calculation of expression (21), we have to insert \mathbf{W} from (26) and (29). At this stage we encounter the well-known difficulty that we are not allowed to interchange the momentum integration and the ω_n summation in (21),¹¹ as the double integral converges only conditionally. The difficulty is resolved by adding the paramagnetic and the diamagnetic parts [(21) and (23)]. The problematic terms just cancel out in the combined expression, as may be checked directly by an expansion of the integrands for large ω_n . Thus, adding (21) and (23), we first perform the momentum integral evaluating the total expression at the Fermi surface as usual. This leads to

$$K(i\nu) = -\frac{e^2 \rho}{\beta m} \sum_{\omega} \int_{-\infty}^{\infty} d\epsilon \text{Tr}[\sigma_3 G(\epsilon, i\omega_n) \Lambda(i\omega_n, i\omega_{n-}) G(\epsilon, i\omega_{n-}) - \sigma_3 G(\epsilon, i\omega_n) \sigma_3 G(\epsilon, i\omega_n)], \quad (32)$$

where we have used (25) and (26); ρ is the density of electrons or holes, respectively. Using expression (9) for the Green's functions and taking the trace in (32), we obtain after simple integrations and after rearranging terms

$$K(i\nu) = -(2e^2 \rho/m) (\pi/\beta) \sum_{\omega} \mathcal{F}(i\omega_n, i\omega_{n-}), \quad (33)$$

where

$$\mathcal{F}(i\omega_n, i\omega_{n-}) = \frac{1 - (\tilde{\omega}_n \tilde{\omega}_{n-} + \tilde{\Delta}_n \tilde{\Delta}_{n-}) / (\tilde{\omega}_n^2 + \tilde{\Delta}_n^2)^{1/2} (\tilde{\omega}_{n-}^2 + \tilde{\Delta}_{n-}^2)^{1/2}}{(\tilde{\omega}_n^2 + \tilde{\Delta}_n^2)^{1/2} + (\tilde{\omega}_{n-}^2 + \tilde{\Delta}_{n-}^2)^{1/2} + \Gamma' [(\tilde{\omega}_n \tilde{\omega}_{n-} + \tilde{\Delta}_n \tilde{\Delta}_{n-}) / (\tilde{\omega}_n^2 + \tilde{\Delta}_n^2)^{1/2} \cdot (\tilde{\omega}_{n-}^2 + \tilde{\Delta}_{n-}^2)^{1/2}]}. \quad (34)$$

¹¹ A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinski, *Quantum Field Theory in Statistical Physics* (Prentice-Hall, Inc., Englewood Cliffs, N.J., 1963), Chap. 7, Sec. 37.

The evaluation of expression (33) will be studied in the next section.

IV. EVALUATION OF THE CONDUCTIVITY FORMULA

The frequency summation in expression (33) can be written as a contour integral in the complex plane:

$$\begin{aligned} & (\pi/\beta) \sum_{\omega} \mathcal{F}(i\omega_n, i\omega_n - i\nu) \\ &= (4i)^{-1} \int_{C_0} dz \tanh \frac{1}{2}(\beta z) \mathcal{F}(z, z - i\nu), \end{aligned} \quad (35)$$

where the path C_0 runs up the imaginary axis on the right-hand side and down on the left, just embracing the poles of $\tanh \frac{1}{2}(\beta z)$ at $z = i\omega_n$. Using the relations (A1, 4, 5, 7) of the Appendix, the function \mathcal{F} can be expressed for general complex z and z' as

$$\begin{aligned} & \mathcal{F}(z, z') \\ &= \frac{1 - (uu' - 1)/(u^2 - 1)^{1/2}(u'^2 - 1)^{1/2}}{-i(\bar{\epsilon} + \bar{\epsilon}') + \Gamma'[(uu' - 1)/(u^2 - 1)^{1/2}(u'^2 - 1)^{1/2}]}, \end{aligned} \quad (36)$$

where primed and unprimed quantities refer to z' and z , respectively. The integral along the path C_0 in (35) is further transformed into an integral over the discontinuities of the function $\mathcal{F}(z, z - i\nu)$ across its cuts. These cuts are

- C_1 : extending from ω_0 to ∞ ,
- C_2 : extending from $-\omega_0$ to $-\infty$,
- C_3 : extending from $\omega_0 + i\nu$ to $\infty + i\nu$,
- C_4 : extending from $-\omega_0 + i\nu$ to $-\infty + i\nu$, (37)

where ω_0 is the gap in the excitation spectrum (A10). The two cuts $C_{1,2}$ are due to the discontinuity of the functions $u(z)$ and $\bar{\epsilon}(z)$ in (36), whereas $C_{3,4}$ are due to the discontinuity of $u' = u(z - i\nu)$ and $\bar{\epsilon}' = \bar{\epsilon}(z - i\nu)$. Using the fact that

$$\begin{aligned} & \mathcal{F}(z, z') = \mathcal{F}(-z, -z'), \quad \tanh \frac{1}{2}[\beta(z \pm i\nu)] = \tanh \frac{1}{2}(\beta z) \\ & \quad (\nu = 2n\pi\beta^{-1}), \end{aligned} \quad (38)$$

one can easily show that the integral over C_4 is identical to the integral over C_1 :

$$\begin{aligned} & \int_{-\infty + i\nu}^{-\omega_0 + i\nu} dz \tanh \frac{1}{2}(\beta z) [\mathcal{F}(z, z - i\nu + i\delta) - \mathcal{F}(z, z - i\nu - i\delta)] \\ &= \int_{\omega_0}^{\infty} dz \tanh \frac{1}{2}(\beta z) [\mathcal{F}(z - i\nu, z + i\delta) - \mathcal{F}(z - i\nu, z - i\delta)], \\ & \quad z \rightarrow -z + i\nu. \end{aligned} \quad (39)$$

Similarly one shows that the two integrals over C_2 and C_3 are identical. Now we combine both remaining integrals and continue $i\nu$ analytically to $z = \omega + i\delta$. Collecting

together we get, using (15) and (33), the frequency-dependent complex conductivity

$$\sigma(\omega) = (2e^2\rho/m)R(\omega), \quad (40a)$$

$$\begin{aligned} & R(\omega) = (2\omega)^{-1} \int_{\omega_0}^{\infty} dx \tanh \frac{1}{2}(\beta x) \\ & \quad \times [\mathcal{F}(x + i\delta, x - \omega - i\delta) - \mathcal{F}(x - i\delta, x - \omega - i\delta) \\ & \quad + \mathcal{F}(x + i\delta, x + \omega + i\delta) - \mathcal{F}(x - i\delta, x + \omega + i\delta)]. \end{aligned} \quad (40b)$$

In the following we are interested only in the dc conductivity which is obtained from (40) by expanding the whole expression for small ω . First we note that the integrand vanishes at $\omega = 0$ as the function \mathcal{F} (36) vanishes for identical arguments $z = z'$:

$$\mathcal{F}(z, z) \equiv 0. \quad (41)$$

Expanding the third integrand in (40b) for small ω , we get in the numerator with $u = u(x + i\delta)$, $u' =$

$$u(x + \omega + i\delta) = u + a\omega + O(\omega^2),$$

$$1 - \frac{u^2 - 1 + au\omega + O(\omega^2)}{[(u^2 - 1)(u^2 - 1 + 2au\omega + O(\omega^2))]^{1/2}} = O(\omega^2). \quad (42)$$

Therefore, the contribution of the third integrand in (40b) vanishes for small ω , and similarly, the second integrand does not contribute. The integral over the first term in (40b) is transformed to ($x \rightarrow x + \omega$):

$$\begin{aligned} & (2\omega)^{-1} \left(\int_{\omega_0 - \omega}^{\omega_0} + \int_{\omega_0}^{\infty} \right) dx \tanh \frac{1}{2}[\beta(x + \omega)] \\ & \quad \times \mathcal{F}(x + \omega + i\delta, x - i\delta). \end{aligned} \quad (43)$$

The first part of this expression vanishes for small ω , too:

$$\sim \frac{1}{2} \tanh \frac{1}{2}(\beta\omega_0) \mathcal{F}(\omega_0 + i\delta, \omega_0 - i\delta) \equiv 0. \quad (44)$$

This is obvious in the gapless region ($\omega_0 = 0$). If $\omega_0 \neq 0$, we obtain for the numerator of \mathcal{F} from (36), using the relations (A8) and (A10) of the Appendix,

$$1 + (|u_0|^2 - 1)/|u_0^2 - 1| \equiv 0. \quad (45)$$

Therefore, we are left with the second part of (43) and the last integrand in (40b) which at $\omega = 0$ combine to give

$$R = \frac{1}{2}\beta \int_{\omega_0}^{\infty} dx (\operatorname{sech}^2 \frac{1}{2}(\beta x)) \times \frac{1}{2} \mathcal{F}(x + i\delta, x - i\delta). \quad (46)$$

The dc conductivity

$$\sigma = (2e^2\rho/m)R \quad (47)$$

is studied in several limiting cases in the next section.

V. EXPLICIT CALCULATIONS

We rewrite the function $\frac{1}{2}\mathcal{F}(x+i\delta, x-i\delta)$ in expression (46) in a more convenient form,

$$\frac{1}{2}\mathcal{F}(x+i\delta, x-i\delta) = \frac{h(x)}{2[\Delta \operatorname{Im}(u^2-1)^{1/2}-\Gamma]+2\Gamma'(1-h)+\Gamma_{\text{tr}}}. \quad (48)$$

Here we used the relations (A8) of the Appendix to define the function

$$h(x) = \frac{1}{2}[1 + (|u|^2 - 1)/|u^2 - 1|], \quad (49)$$

which has been introduced by Ambegaokar and Griffin.⁵ The denominator in (48) has been obtained from (36) by using (49) and (A3) and (A8). Furthermore, we have introduced the inverse transport collision time

$$\Gamma_{\text{tr}} = \Gamma - \Gamma' = 1/\tau_{\text{tr}}. \quad (50)$$

At or above T_c , which depends on Γ (see I), the system is in the normal state, i.e., $\Delta=0$. As in this case $u = [(x+i\Gamma)/\Delta]$ (see A6), we get immediately

$$h \equiv 1, \quad \Delta \operatorname{Im}(u^2-1)^{1/2} \equiv \Gamma. \quad (51)$$

The remaining integral in (46) is unity ($\omega_0=0$), and we obtain the correct "normal" conductivity

$$\sigma_n = 2e^2 \rho \tau_{\text{tr}} / m, \quad (52)$$

where the factor 2 accounts for the two types of carriers in the system. We now write

$$\sigma/\sigma_n = \Gamma_{\text{tr}} \frac{1}{2} \beta \int_{\omega_0}^{\infty} dx \operatorname{sech}^2 \frac{1}{2} (\beta x) \times \frac{h(x)}{2[\Delta \operatorname{Im}(u^2-1)^{1/2}-\Gamma]+2\Gamma'(1-h)+\Gamma_{\text{tr}}}. \quad (53)$$

Near $T=0$ we expect the largest contribution to the integral from the neighborhood of $x \simeq \omega_0$. Using the expansion for h ,⁵

$$h = (2/3\Delta) \alpha^{-2/3} (1 - \alpha^{2/3})^{-1/2} (x - \omega_0), \quad \alpha = (\Gamma/\Delta) \leq 1, \quad (54)$$

and approximating the denominator in (53) at $x = \omega_0$,

$$D = 2\Gamma\alpha^{-2/3} - \Gamma_{\text{tr}}, \quad (55)$$

we get using (A10)

$$\frac{\sigma}{\sigma_n} = \frac{4}{3} \frac{1 - \alpha^{2/3}}{2\Gamma/\Gamma_{\text{tr}} - \alpha^{2/3}} \frac{\exp(-\beta\omega_0)}{\beta\omega_0} \quad T \gtrsim 0. \quad (56)$$

This result shows the insulating behavior of our system for low impurity concentrations ($\alpha \leq 1$). We should mention that the result conjectured in the work of Jerome, Rice, and Kohn¹ does not agree with our rigorous calculation. The reason for this is that their treatment of the impurity scattering is not adequate to the present problem.

In the gapless region ($\alpha > 1$) we obtain at $T=0$

$$\frac{\sigma}{\sigma_n} = \Gamma_{\text{tr}} \frac{h(x)}{2[\Delta \operatorname{Im}(u^2-1)^{1/2}-\Gamma]+2\Gamma'(1-h)+\Gamma_{\text{tr}}} \Big|_{x=0}. \quad (57)$$

From (A6) we see that the first term in the denominator vanishes at $x=0$, whereas

$$h(x=0) = 1 - \alpha^{-2}. \quad (58)$$

Inserting into (57) we have

$$\frac{\sigma}{\sigma_n} \Big|_{T=0} = \frac{1 - \alpha^{-2}}{1 + (2\Gamma'/\Gamma_{\text{tr}})\alpha^{-2}}, \quad \alpha = \Gamma/\Delta \geq 1. \quad (59)$$

This ratio is obviously smaller than unity, but approaches unity for increasing impurity density ($\alpha \rightarrow \infty$). It is interesting to note that the system, though being in a condensed state of electron-hole pairs, does not have "insulating" properties, if the impurity concentration is high enough ($\alpha > 1$). This situation cannot be explained in simple physical terms, as the description of the gapless region in the quasiparticle picture breaks down. On the other hand, one might say that the qualitative behavior of the conductivity is mainly determined by the existence or absence of a gap in the excitation spectrum and not by the order parameter Δ .

We finally investigate the transition-temperature region, where the system is always in the gapless region ($\alpha > 1$ as $\Delta \rightarrow 0$). Expanding relation (A8) in terms of Δ^2 we get

$$h(x) = 1 - [\Delta^2 \Gamma^2 / (x^2 + \Gamma^2)^2], \quad (60)$$

whereas the denominator leads to

$$D = \Gamma_{\text{tr}} + \frac{2\Delta^2 \Gamma}{x^2 + \Gamma^2} \left(1 - \frac{\Gamma \Gamma_{\text{tr}}}{x^2 + \Gamma^2} \right). \quad (61)$$

Inserting into (53) and expanding in Δ^2 , we obtain finally

$$\sigma/\sigma_n = 1 - A(T_c)\Delta^2, \quad T \lesssim T_c \quad (62)$$

where the coefficient A is

$$A = \frac{1}{2} \beta \int_0^{\infty} dx \operatorname{sech}^2 \frac{1}{2} (\beta x) \left[\frac{2\Gamma}{\Gamma_{\text{tr}}} \frac{1}{x^2 + \Gamma^2} - \frac{\Gamma^2}{(x^2 + \Gamma^2)^2} \right] > 0. \quad (63)$$

The inequality follows from the fact that $2\Gamma \geq \Gamma_{\text{tr}}$. As

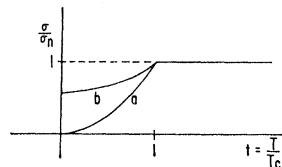


FIG. 1. The dc conductivity as a function of temperature. Curve a: low impurity concentration, $\alpha = (\Gamma/\Delta) < 1$. Curve b: higher impurity concentrations, $\alpha = (\Gamma/\Delta) > 1$, where the gapless region extends to $T=0$.

we have from I [Eq. (60)],

$$\Delta^2 = \text{const}(1-t), \quad t = T/T_c \lesssim 1; \quad (64)$$

we conclude that the ratio σ/σ_n has a finite slope at T_c :

$$\sigma/\sigma_n = 1 - \text{const} \times (1-t). \quad (65)$$

This is in contrast to the infinite slope conjectured in Ref. 1. Figure 1 shows a qualitative plot of the conductivity.

VI. CONCLUSION

We have calculated the dc conductivity of the "excitonic insulator" in the semimetallic limit. This region is especially interesting as the system is supposed to change from a metal to an insulator if it undergoes the transition to the excitonic state. However, we have seen that the simple scattering mechanism conjectured by Jerome, Rice, and Kohn¹ does not hold, as the impurities of the system have a large effect on the description of the excitonic phase itself. We have seen that only for low impurity concentrations the system acquires insulating properties. If the impurity concentration is high enough the normal state is stable down to zero temperature, as discussed in I. For intermediate concentrations the conductivity decreases below the transition temperature, but is still finite at $T=0$. This behavior shows that the conductivity is mainly determined by the presence or absence of a gap in the excitation spectrum and not by the order parameter.

Until now there has been no clear experimental evidence for the existence of the excitonic phase. The question of experimental realizability has been discussed in detail in Ref. 1. It is clear that conductivity measurements are very important. We hope that the results of this paper might stimulate the experimental work.

APPENDIX

Following the discussion of Kadanoff and Falko⁶ we investigate the analytic structure of the Green's function (9) and related functions (10) in the full complex-energy plane. Extending the imaginary discrete frequencies $i\omega_n$ we introduce

$$i\omega_n \rightarrow z, \quad i\tilde{\omega}_n \rightarrow \tilde{z}(z), \quad \tilde{\Delta}_n \rightarrow \tilde{\Delta}(z). \quad (A1)$$

The Green's function (9) may be written as

$$G(z) = - \frac{1}{\epsilon^2 - \tilde{\epsilon}(z)^2} \begin{pmatrix} \tilde{z} + \epsilon & \tilde{\Delta} \\ \tilde{\Delta} & \tilde{z} - \epsilon \end{pmatrix}, \quad (A2)$$

whereas the relations (10) lead to

$$\begin{aligned} \tilde{z} &= z + i\frac{1}{2}\Gamma(\tilde{z}/\tilde{\epsilon}), \\ \tilde{\Delta} &= \Delta - i\frac{1}{2}\Gamma(\tilde{\Delta}/\tilde{\epsilon}), \end{aligned} \quad (A3)$$

with

$$\tilde{\epsilon}(z) = (\tilde{z}^2 - \tilde{\Delta}^2)^{1/2}, \quad \text{Im}\tilde{\epsilon}(z) > 0. \quad (A4)$$

Furthermore, we introduce

$$u(z) = \tilde{z}/\tilde{\Delta}, \quad (A5)$$

which via (A3) satisfies the relation

$$z/\Delta = u - i\alpha[u/(u^2-1)^{1/2}], \quad \alpha = \Gamma/\Delta \quad (A6)$$

such that

$$\begin{aligned} \tilde{z} &= \tilde{\epsilon}[u/(u^2-1)^{1/2}], \\ \tilde{\Delta} &= \tilde{\epsilon}[1/(u^2-1)^{1/2}]. \end{aligned} \quad (A7)$$

The following three statements about the Green's function are derived from spectral representations⁶:

(a) $G(z)$ is analytic except for a cut along the real axis.

(b) $\text{Im}G(z)$ changes sign across the cut whereas $\text{Re}G(z)$ does not change.

(c) The imaginary part of the diagonal Green's functions $G_{b,a}$ is negative-semidefinite in the upper half-plane.

It follows from (a) and (b) that the functions u , $\tilde{\Delta}$, etc., are also analytic, except for the cut. Defining the values of these functions for $z = x + i\delta$ as $u(x)$, $\tilde{\Delta}(x)$, etc., one can derive that just below the cut we have

$$\begin{aligned} \tilde{z}(x-i\delta) &= \tilde{z}(x)^*, \\ \tilde{\Delta}(x-i\delta) &= \tilde{\Delta}(x)^*, \\ u(x-i\delta) &= u(x)^*, \\ \tilde{\epsilon}(x-i\delta) &= -\tilde{\epsilon}(x)^*, \\ [u^2(x-i\delta) - 1]^{1/2} &= -[u^2(x) - 1]^{1/2*}. \end{aligned} \quad (A8)$$

Furthermore, adding the diagonal parts in (A2) and integrating over ϵ , we get from statement (c) the condition

$$\text{Re}(\tilde{z}/\tilde{\epsilon}) \big|_{z=x+i\delta} \geq 0,$$

which via (A6) and (A7) leads to

$$\text{Im}u(x) \geq 0. \quad (A9)$$

As discussed in I, there is a gap in the excitation spectrum as long as $\alpha \leq 1$. The gap ω_0 is given from (A6) as the largest value for which the relation gives a real solution $u = u(x)$ with $|u| < 1$. The result is

$$\begin{aligned} u_0 &= u(\omega_0) = (1 - \alpha^{2/3})^{1/2}, \\ \omega_0 &= \Delta(1 - \alpha^{2/3})^{3/2}, \quad \alpha \leq 1. \end{aligned} \quad (A10)$$

It follows that for $|x| < \omega_0$ there is no discontinuity across the cut, as \tilde{z} , $\tilde{\Delta}$, and u are real and $\tilde{\epsilon}$ purely imaginary. If $\alpha = \Gamma/\Delta > 1$, there is no gap in the excitation spectrum (see I).