A model of a disordered system (A contribution to the theory of "liquid semiconductors")

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A model of the electronic properties of disordered systems of the "liquid-semiconductor" type is proposed. The one-electron Green's function is obtained and leads to a density of states with the characteristic "pseudo-gap" in the energy range corresponding to the forbidden band of the crystal. The dielectric properties, conductivity, and optical absorption are considered. Electron localization of the Bragg type is obtained, together with the analog of interband absorption in an ideal semiconductor. The dielectric properties of the model considered turn out to be intermediate between those of typical metals and insulators. It is noted that the results obtained can be applied to interpret the properties of quasi-one-dimensional systems (of the TTF-TCNQ type) near the Peierls structural transition point.

INTRODUCTION

In recent years interest has grown in both the theory and the experimental studies of the electronic properties of different disordered systems[1]. In particular, great attention has been paid to the experimental study of melts of most of the known semiconductors (see the reviews[2-4]). It has been found that semiconductors can be roughly divided into three groups, according to their kinetic properties in the liquid state.

The first contains substances of the type Ge, InSb and other $A_{III}B_V$, which, on transition to the liquid state, give melts with purely metallic properties. Evidently, this is connected with the fact that, in these substances, not only the long-range order but also the short-range order corresponding to the given crystal is destroyed on melting. The second group is formed by substances of the type PbTe, SnTe, PbSe, In_2Te_3, Ga_2Te_3, etc., which are typical semiconductors in the crystalline state. On melting, their electrical conductivity, in absolute magnitude and in the temperature dependence, has practically the same behavior as in the corresponding crystal. The sign of the thermoelectric power, as a rule, indicates p-type conductivity. In the Hall effect, however, they display typically metallic properties: the Hall constant is almost independent of temperature, its sign corresponds to n-type conductivity, and in absolute magnitude it is slightly greater than the value for a metal with two free electrons per atom. Thus, these substances, which are usually called "liquid semiconductors," form a group intermediate between typical metals and semiconductors. To all appearances, their properties can be considered in the framework of the nearly-free electron approximation, with allowance for strong scattering of the "Bragg" type in the energy range coinciding with the forbidden band of the corresponding crystal. Finally, the third group is formed by substances of the type GeS, SnS, etc., with very low electron mobility, which, evidently, must be treated in the approximation of tight binding of the electrons to the ions.

In this paper we propose a simple model that makes it possible to understand qualitatively the appearance of the distinctive type of "band structure" in the energy spectrum of substances of the second group, which appears in the form of a characteristic "pseudo-gap" (of the type assumed in the work of Mott and other authors[1]) in the density of electron states. Also considered are the dielectric properties, high-frequency conductivity and optical absorption. The "quasi-one-dimensional" character of the model permits us to hope that a considerable proportion of the results obtained below can be applied to describe the properties of one-dimensional systems (of the TTF-TCNQ type) near the Peierls structural transition point.

1. THE ONE-ELECTRON GREEN FUNCTION

We write the Hamiltonian of the interaction of an electron with the ions in the form

$$H_{int}=\frac{1}{N}\sum_{\mathbf{pq}}\langle\mathbf{p}+\mathbf{q}|V|\mathbf{p}\rangle a^{+}_{\mathbf{p}+\mathbf{q}}a_{\mathbf{p}}\rho_{\mathbf{q}}, \qquad (1.1)$$

where

$$\rho_{\mathbf{q}}=\sum_{i}e^{-i\mathbf{q}\mathbf{R}_i}$$

is the Fourier component of the ion density ($\mathbf{R}_i$ are the positions of the ions and N is their total number), $\langle\mathbf{p}+\mathbf{q}|V|\mathbf{p}\rangle$ is a matrix element of the (generally speaking, nonlocal) ionic pseudo-potential[5], and $a^{+}_{\mathbf{p}}$ and $a_{\mathbf{p}}$ are electron operators in second quantization.

We introduce the one-electron Green function in the Matsubara temperature technique:

$$G(\mathbf{p}\tau)=-\langle T_\tau a_{\mathbf{p}}(\tau)a_{\mathbf{p}}^{+}(0)\rangle, \qquad (1.2)$$

and also the Green function of the ion subsystem:

$$F(\mathbf{q}\tau)=-\langle T_\tau \rho_{\mathbf{q}}(\tau)\rho_{\mathbf{q}}^{+}(0)\rangle. \qquad (1.3)$$

For the Fourier transform of (1.3) we have the spectral representation[6]

$$F(\mathbf{q}\omega_m)=\int_{-\infty}^{\infty}d\omega'\frac{A(\mathbf{q}\omega')}{i\omega_m-\omega'}, \qquad (1.4)$$

where $\omega_m = 2\pi m T$ (T is the temperature),

$$A(\mathbf{q}\omega)=Z^{-1}\sum_{mn}\exp\left[-\frac{E_n}{T}\right]|(\rho_{\mathbf{q}})_{mn}|^2\left\{1-\exp\left[-\frac{\omega_{mn}}{T}\right]\right\}\delta(\omega-\omega_{mn}),$$

$$\omega_{mn}=E_m-E_n,\quad (\rho_{\mathbf{q}})_{mn}=\langle m|\rho_{\mathbf{q}}|n\rangle,\quad Z=\sum_m\exp\left[-\frac{E_m}{T}\right], \qquad (1.5)$$

and m and n label the exact level of the ion subsystem.

Next we introduce the dynamical form factor of the liquid[7]

$$S(\mathbf{q}\omega)=Z^{-1}\sum_{mn}|(\rho_{\mathbf{q}})_{mn}|^2\exp\left[-\frac{E_n}{T}\right]\delta(\omega-\omega_{mn}). \qquad (1.6)$$

Comparing (1.5) and (1.6), we see that

$$A(\mathbf{q}\omega)=S(\mathbf{q}\omega)\{1-e^{-\omega/T}\}. \tag{1.7}$$

The simplest contribution to the electron self-energy part has the form

$$\Sigma(\varepsilon_n\mathbf{p})=\frac{T}{N^2}\sum_{\mathbf{q}}|\langle\mathbf{p}+\mathbf{q}|V|\mathbf{p}\rangle|^2\sum_m F(\mathbf{q}\omega_m)\frac{1}{i\varepsilon_n+i\omega_m-\xi_{\mathbf{p}+\mathbf{q}}},$$
$$\varepsilon_n=(2n+1)\pi T, \qquad \xi_p=p^2/2m-\mu. \tag{1.8}$$

We note that the characteristic energies of the ionic excitations (the frequencies at which $S(\mathbf{q}\omega)$ is nonzero) satisfy, in the liquid, the condition $\omega/T \ll 1$, whereas we are interested in the electron spectrum in a substantially wider range of energies $\gtrsim T$. This enables us to neglect the effect of the dynamics of the ion subsystem, i.e., to take into account only the terms with m = n in (1.6):

$$S(\mathbf{q}\omega)\approx S(\mathbf{q})\delta(\omega), \tag{1.9}$$

$$S(\mathbf{q})=\frac{1}{N}\int_{-\infty}^{\infty}d\omega S(\mathbf{q}\omega), \tag{1.10}$$

where $S(\mathbf{q})$ is the static structure factor of the liquid[7]. Using (1.4)—(1.7) and (1.9) in (1.8), we obtain the static approximation

$$\Sigma(\varepsilon_n\mathbf{p})\cong\frac{1}{N}\sum_{\mathbf{q}}|\langle\mathbf{p}+\mathbf{q}|V|\mathbf{p}\rangle|^2S(\mathbf{q})\frac{1}{i\varepsilon_n-\xi_{\mathbf{p}+\mathbf{q}}}. \tag{1.11}$$

This approximation was used by Edwards in his well-known papers[8]. The averaging he used, over all possible ion configurations, is contained implicitly in the definitions (1.5) and (1.6), in which averaging over the canonical ensemble of the liquid is performed.

The static structure factor $S(\mathbf{q})$ is determined experimentally from data on the elastic scattering of x-rays or neutrons. Its typical behavior in a liquid is represented in Fig. 1.

First we shall consider a one-dimensional model of a liquid. We shall model the structure factor by two narrow peaks at q = ±K, this being the natural analog of Fig. 1 in the one-dimensional case. We shall assume that the Fermi level of the free electrons passes through the degeneracy points of their spectrum, at which Bragg gaps are formed in the case of an ideal periodic structure (see Fig. 2). We therefore take $2p_F = K$, where p_F is the Fermi momentum of the free electrons. The latter condition is typical for "liquid semiconductors"[4], K being the analog of the reciprocal-lattice vector of the ideal crystal.

From (1.11) we have (L is the length of the system)

$$\Sigma(\varepsilon_n p)=\frac{L}{N}\int\frac{dq}{2\pi}|\langle p+q|V|p\rangle|^2S(q)\{i\varepsilon_n-\xi_{p+q}\}^{-1}\approx \tag{1.12}$$
$$\approx A^2\{i\varepsilon_n-\xi_{p-K}\}^{-1}+A^2\{i\varepsilon_n-\xi_{p+K}\}^{-1},$$
$$A^2=\frac{L}{N}\int\frac{dq}{2\pi}|\langle p+q|V|p\rangle|^2S(q). \tag{1.13}$$

Here we have made use of the characteristic structure of S(q), with two narrow peaks at q = ±K.

It is not difficult to convince oneself[9] that corrections for the finite width of the peaks are small if the conditions

$$\gamma=\frac{1}{R_c}\ll|p-p_F| \quad \text{or} \quad v_F\gamma\ll 2\pi T, \tag{1.14}$$

are fulfilled, where γ is the width of the peaks, v_F is the Fermi velocity of the free electrons, and the parameter R_c, defined in (1.14), in the one-dimensional case plays the role of the correlation length of the short-range order.

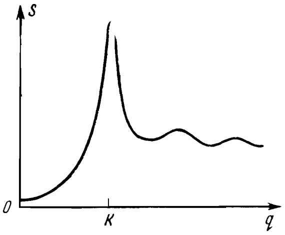

FIG. 1

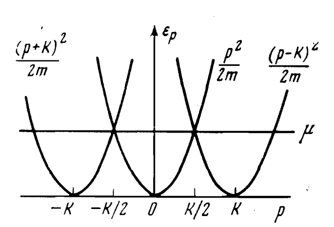

FIG. 2

From Fig. 2 the following symmetry properties of the free-electron spectrum in the one-dimensional case can be seen:

$$\begin{aligned}\xi_{p-K}&=-\xi_p \text{ for } p\sim+K/2\\ \xi_{p+K}&=-\xi_p \text{ for } p\sim-K/2.\end{aligned} \tag{1.15}$$

Then, considering the electron with p ~ +K/2 (the treatment of p ~ −K/2 is analogous), we may take into account only the first term in the right-hand side of (1.12):

$$\Sigma(\varepsilon_n\xi_p)=A^2G_0(\varepsilon_n;\ -\xi_p). \tag{1.16}$$

Thus, the use of the characteristic form of the liquid structure factor makes it possible to replace the real interaction $|\langle p+q|V|p\rangle|^2S(q)$ in the liquid by the model interaction $2\pi NL^{-1}A^2\delta(q-K)$. Then, the remaining perturbation

$$\tilde{A}^2(q)=|\langle p+q|V|p\rangle|^2S(q)-2\pi NL^{-1}A^2\delta(q-K)$$

is unimportant, if the treatment is confined to the region specified by the conditions (1.14). It should be emphasized that the introduction of this model interaction does not imply the introduction of long-range crystalline order. The analysis is performed under the assumption of a microscopically homogeneous liquid, and the conditions (1.14) impose a restriction in the sense that the correlation length of the short-range order should be sufficiently large. The presence of long-range order entails the appearance of "anomalous" Green functions, which describe Umklapp processes[10] and substantially alter the structure of the equations.

With the model interaction introduced above, we can now sum all the important diagrams. It is not difficult to see[9] that, in each order of perturbation theory, diagrams with an alternating sequence of Green functions $\{i\epsilon_n-\xi_p\}^{-1}$ and $\{i\epsilon_n+\xi_p\}^{-1}$ (we are considering p ~ K/2) and an alternating sequence of vertices with incoming or outgoing interaction lines transferring momentum ±K give equal contributions (see Fig. 3). The general term in the expansion for the Green function then has the form

$$g_n(\varepsilon_l p)=\frac{A^{2n}n!}{(i\varepsilon_l-\xi_p)^n(i\varepsilon_l+\xi_p)^n(i\varepsilon_l-\xi_p)}=n!\,z^n(\varepsilon_l\xi_p)G_0(\varepsilon_l\xi_p), \tag{1.17}$$

where A^2 is defined by (1.13), n is the order of perturbation theory in A^2, and $z(\epsilon_l\xi_p)=A^2G_0(\epsilon_l\xi_p)G_0(\epsilon_l;-\xi_p)$. The factor n! arises from simple combinatorial considerations. In fact, there are 2n points to which interaction

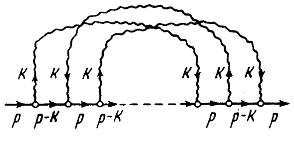

FIG. 3

lines are attached. Of these, n points have an outgoing line, which can enter the remaining n free vertices (corresponding to incoming lines) in any of n! ways. We shall use the identity

$$\sum_{n=0}^{\infty} n!z^n = \sum_{n=0}^{\infty} \int_0^{\infty} d\zeta\, e^{-\zeta}(\zeta z)^n = \int_0^{\infty} d\zeta\, e^{-\zeta}\frac{1}{1-\zeta z}. \qquad (1.18)$$

Then the one-electron Green function is

$$G(\varepsilon_l p) = \sum_{n=0}^{\infty} g_n(\varepsilon_l p) = \int_0^{\infty} d\zeta\, e^{-\zeta}\frac{i\varepsilon_l+\xi_p}{(i\varepsilon_l)^2-\xi_p{}^2-\zeta A^2} \equiv \langle G_{\zeta A^2}(\varepsilon_l pp)\rangle_\zeta, \qquad (1.19)$$

where

$$G_{A^2}(\varepsilon_l pp) = \frac{i\varepsilon_l+\xi_p}{(i\varepsilon_l)^2-\xi_p{}^2-A^2} \qquad (1.20)$$

is the normal Green function of an ideal semiconductor with energy gap 2|A|, and

$$\langle\ldots\rangle_\zeta = \int_0^{\infty} d\zeta\, e^{-\zeta}\ldots$$

is a particular type of averaging over the "fluctuations" of the energy gap. Thus, the model considered for the disordered system is equivalent to an ensemble of ideal semiconductors, in the spectrum of which the energy gap takes random values, with a distribution of a special form.

Performing the analytic continuation to real frequencies in the usual way, we obtain the retarded (or advanced) Green function. The density of electron states can be found from the formula

$$N(\varepsilon) = -\frac{N_0}{\pi}\int_{-\infty}^{\infty} d\xi_p\, \mathrm{Im}\, G^R(\varepsilon\xi_p), \qquad (1.21)$$

where N_0 is the density of free-electron states. From (1.19) we have

$$\mathrm{Im}\, G^{R,A}(\varepsilon,\xi_p) = \mp\pi\int_0^{\infty} d\zeta\, e^{-\zeta}(\varepsilon+\xi_p)\delta(\varepsilon^2-\xi_p{}^2-\zeta A^2)$$

$$= \mp\frac{\pi}{A^2}(\varepsilon+\xi_p)\theta(\varepsilon^2-\xi_p{}^2)e^{-(\varepsilon^2-\xi_p{}^2)/A^2} \qquad (1.22)$$

and the density of states is

$$\frac{N(\varepsilon)}{N_0} = \left|\frac{\varepsilon}{A}\right|\int_0^{\varepsilon^2/A^2} d\zeta\frac{e^{-\zeta}}{(\varepsilon^2/A^2-\zeta)^{1/2}} = 2\left|\frac{\varepsilon}{A}\right|\exp\left[-\frac{\varepsilon^2}{A^2}\right]\mathrm{Erfi}\left(\frac{\varepsilon}{A}\right).$$

$$\mathrm{Erfi}(x) = \int_0^x dx\, e^{x^2} \qquad (1.23)$$

is the error function of imaginary argument. The density of states (1.23) is represented graphically in Fig. 4.

We have thus obtained a "pseudo-gap," of the type proposed in the numerous papers of Mott and other authors in order to interpret the properties of "liquid semiconductors." The width of the pseudo-gap is equal in order of magnitude to the width of the forbidden band of the corresponding crystal. The asymptotic behavior of (1.23) has the form

$$\frac{N(\varepsilon)}{N_0} \to \begin{cases} 1 & \text{if } |\varepsilon|\to\infty \\ 2\varepsilon^2/A^2\to 0 & \text{for } |\varepsilon|\to 0. \end{cases} \qquad (1.24)$$

We emphasize that the Green function (1.19) has no pole singularities in the vicinity of the "Fermi surface" and, in this sense, does not describe the spectrum of the elementary excitations in the region of energies corresponding to the pseudo-gap. The first of the conditions (1.14) indicates that the formulas obtained are inapplicable in the immediate vicinity $\epsilon \sim 0$ of the Fermi level. For $R_c \gtrsim 20a$, where a is the interatomic spacing, this limitation is extended to the region $|\xi_p| \lesssim 0.05\,\epsilon_F$ (ϵ_F is the free-electron Fermi energy), which, for typical $|A| \sim (0.1-0.2)\epsilon_F$ amounts to approximately (1/4)—(1/8) of the width of the pseudo-gap. The situation is improved with increasing R_c, but the vanishing of the density of states in the middle of the pseudo-gap raises doubts. Moreover, for "liquid semiconductors" the estimate $T \sim |A|$ is typical, so that the second condition (1.14) is already fulfilled when $R_c \gtrsim 10a$.

The generalization of the results obtained to the three-dimensional case encounters certain difficulties. In particular, if in (1.11) we make use of the usual local-pseudo-potential approximation, then, on integration over the polar angle between the vectors **p** and **q**, there arises a characteristic logarithmic expression for the self-energy part[8,11-13], which is considerably less singular than (1.12) in the energy region of interest and leads only to weak changes in the density of states as compared with the case of free electrons. It was pointed out by Ziman[13] that, under certain assumptions concerning the higher correlation functions of the ions (in particular, the four-ion correlation function), contributions to the electron self-energy part that have a "one-dimensional" form of the type (1.12) can appear. Without denying this possibility, we should like to remark that these assumptions are too stringent, the more so because, at present, no theoretical or experimental methods exist that permit one to find the higher ionic correlators in the liquid. Incidentally, it turns out to be sufficient to impose only one condition on the ionic pseudo-potential (based essentially on its nonlocal nature) in order to obtain a result of the type (1.16) in the three-dimensional case. The matrix element $\langle\mathbf{p}+\mathbf{q}|V|\mathbf{p}\rangle$ of a nonlocal pseudo-potential depends not only on $|\mathbf{q}|$, but also, in the general case, on $|\mathbf{p}|$ and $|\mathbf{p}+\mathbf{q}|$, i.e., it depends also on the mutual orientation of the vectors **p** and **q**[5]. It then turns out that, in the region $|\mathbf{q}| \sim 2p_F$ of interest, the pseudo-potential corresponding to "almost-backward" scattering is considerably greater than for scattering through small angles[5,12].

A typical dependence of the matrix element $\langle p+q|V|p\rangle$ ($|p| \sim p_F$, $|q| \approx 2p_F$) on the scattering angle is shown in Fig. 5. We shall assume that for the substances in which we are interested there is a sharply pronounced peak in the pseudo-potential in the region of scattering angles $\theta \sim \pi$. Then, from (1.11) we obtain (Ω_0 is the volume per atom)

$$\Sigma(\varepsilon_n\mathbf{p}) = \Omega_0\int_0^{\infty} dq\, q^2\frac{1}{4\pi^2}\int_{-1}^{1}\frac{d\cos\theta|\langle\mathbf{p}+\mathbf{q}|V|\mathbf{p}\rangle|^2 S(\mathbf{q})}{i\varepsilon_n-\xi_{|\mathbf{p}+\mathbf{q}|}} \approx A^2\{i\varepsilon_n-\xi_{|\mathbf{p}|-|\mathbf{K}|}\}^{-1}, \qquad (1.25)$$

and the problem reduces to a one-dimensional one. Here,

$$A^2 = \Omega_0\int_0^{\infty} dq\, q^2\frac{1}{4\pi^2}\int_{-1}^{1} d\cos\theta|\langle\mathbf{p}+\mathbf{q}|V|\mathbf{p}\rangle|^2 S(\mathbf{q}). \qquad (1.26)$$

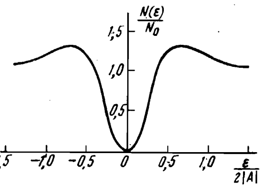

FIG. 4

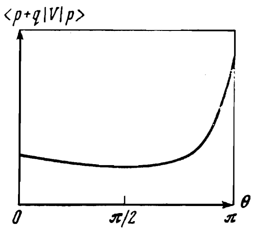

FIG. 5

We assume that the conditions (1.14) are fulfilled and that the integration over cos θ is effectively cut off in the interval

$$|\delta\theta|^2 \ll |p-p_F|/|p_F| \text{ or } |\delta\theta|^2 \ll 2\pi T/\varepsilon_F \tag{1.27}$$

about $\theta \sim \pi$; this singles out a narrow cone, corresponding to the dominant role of the backward scattering. For $|\mathbf{p}-\mathbf{p}_F| \sim 0.05\mathbf{p}_F$ we have $|\delta\theta| \lesssim 0.22$. Therefore, in the three-dimensional variant of our model the real interaction $|\langle\mathbf{p}+\mathbf{q}|V|\mathbf{p}\rangle|^2 S(\mathbf{q})$ is replaced by the model interaction

$$\frac{4\pi^2}{K^2\Omega_0}A^2\delta(q-K)\delta(\cos\theta+1).$$

The remaining perturbation

$$\tilde{A}^2(q,\theta)=|\langle\mathbf{p}+\mathbf{q}|V|\mathbf{p}\rangle|^2 S(\mathbf{q})-\frac{4\pi^2}{K^2\Omega_0}A^2\delta(q-K)\delta(\cos\theta+1)$$

leads to the appearance of the above-mentioned weak renormalizations of the density of states. It is not difficult to see that, in the three-dimensional case, in place of (1.15) we have

$$\xi_{|p|-|K|}=-\xi_{|p|} \quad \text{for } |p|\sim K/2. \tag{1.28}$$

The subsequent treatment coincides with (1.17)—(1.23), and all the formulas remain valid for the three-dimensional system too.

2. THE VERTEX PART, POLARIZATION OPERATOR AND DIELECTRIC FUNCTION

It is of interest to study, in the model under consideration, the properties of the vertex part describing the response of the system to an external electromagnetic perturbation. We have the following expression for the variation of the one-electron Green function on introduction of a weak external field[6]:

$$\frac{\delta G(\varepsilon\mathbf{p})}{\delta A_\mu(\mathbf{q}\omega)}=G(\varepsilon\mathbf{p})J^\mu(\varepsilon\mathbf{p}\varepsilon+\omega\mathbf{p}+\mathbf{q})G(\varepsilon+\omega\mathbf{p}+\mathbf{q}), \tag{2.1}$$

where $\delta A_\mu(\mathbf{q}\omega)=\{\delta\mathbf{A}_{\mathbf{q}\omega};-\delta\varphi_{\mathbf{q}\omega}\}$ is the variation of the external field and $J^\mu(\epsilon\mathbf{p}\epsilon+\omega\mathbf{p}+\mathbf{q})$ is the required vertex part. In this case we have for the free Green function:

$$\frac{\delta G_0(\varepsilon\mathbf{p})}{\delta A_\mu(\mathbf{q}\omega)}=G_0(\varepsilon\mathbf{p})J_0^\mu(\varepsilon\mathbf{p}\varepsilon+\omega\mathbf{p}+\mathbf{q})G_0(\varepsilon+\omega\mathbf{p}+\mathbf{q}), \tag{2.2}$$

where the free vertex

$$J_0^\mu(\varepsilon\mathbf{p}\varepsilon+\omega\mathbf{p}+\mathbf{q})=\begin{cases}-e\mathbf{p}/mc, & \mu=1,2,3\\ e, & \mu=0\end{cases} \tag{2.3}$$

In the model considered, the variational derivative (2.1) can be calculated directly. In fact, from (1.17)—(1.19) we have

$$\frac{\delta G(\varepsilon\mathbf{p})}{\delta A_\mu(\mathbf{q}\omega)}=\frac{\delta}{\delta A_\mu(\mathbf{q}\omega)}\left\{\left\langle\sum_{n=0}^{\infty}[\zeta z(\varepsilon\mathbf{p})]^n\right\rangle_\zeta G_0(\varepsilon\mathbf{p})\right\}$$
$$=\left\langle\sum_{n=1}^{\infty}\sum_{m=1}^{\infty}[\zeta z(\varepsilon\mathbf{p})]^{m-1}\zeta\frac{\delta z(\varepsilon\mathbf{p})}{\delta A_\mu(\mathbf{q}\omega)}[\zeta z(\varepsilon+\omega\mathbf{p}+\mathbf{q})]^{n-m}\right.$$
$$\left.\times G_0(\varepsilon+\omega\mathbf{p}+\mathbf{q})+\sum_{n=0}^{\infty}[\zeta z(\varepsilon p)]^n\frac{\delta G_0(\varepsilon\mathbf{p})}{\delta A_\mu(\mathbf{q}\omega)}\right\rangle_\zeta, \tag{2.4}$$

since $\delta G(\epsilon\mathbf{p})/\delta A_\mu(\mathbf{q}\omega)$ is obtained from the set of diagrams of the type shown in Fig. 3 by inserting external-field lines into any of the electron lines in Fig. 3 (see Fig. 6a). In (2.4), m is the label of that block $z(\epsilon\mathbf{p})$ of Fig. 6a into which the external-field line enters. Using (2.2), it is not difficult to convince oneself that (see Fig. 6b)

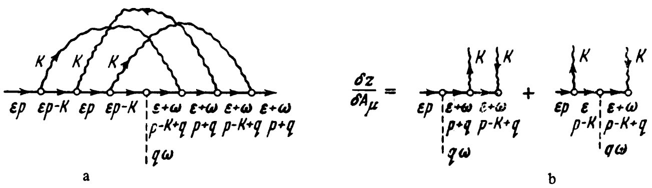

FIG. 6

$$\frac{\delta z(\varepsilon\mathbf{p})}{\delta A_\mu(\mathbf{q}\omega)}=G_0(\varepsilon\mathbf{p})J_0^\mu(\varepsilon\mathbf{p}\varepsilon+\omega\mathbf{p}+\mathbf{q})z(\varepsilon+\omega\mathbf{p}+\mathbf{q})$$
$$+z(\varepsilon\mathbf{p})J_0^\mu(\varepsilon\mathbf{p}-\mathbf{K}\varepsilon+\omega\mathbf{p}-\mathbf{K}+\mathbf{q})G_0(\varepsilon+\omega\mathbf{p}-\mathbf{K}+\mathbf{q}). \tag{2.5}$$

Substituting (2.2) and (2.5) into (2.4), after certain transformations we obtain

$$\frac{\delta G(\varepsilon\mathbf{p})}{\delta A_\mu(\mathbf{q}\omega)}=J_0^\mu(\varepsilon\mathbf{p}\varepsilon+\omega\mathbf{p}+\mathbf{q})G_0(\varepsilon\mathbf{p})G_0(\varepsilon+\omega\mathbf{p}+\mathbf{q})$$
$$\times\left\langle\sum_{n=0}^{\infty}\zeta^n z^n(\varepsilon\mathbf{p})\sum_{m=0}^{\infty}\zeta^m z^m(\varepsilon+\omega\mathbf{p}+\mathbf{q})\right\rangle_\zeta$$
$$+J_0^\mu(\varepsilon\mathbf{p}-\mathbf{K}\varepsilon+\omega\mathbf{p}-\mathbf{K}+\mathbf{q})\left\langle\frac{1}{\zeta A^2}\sum_{n=1}^{\infty}\zeta^n z^n(\varepsilon\mathbf{p})\sum_{m=1}^{\infty}\zeta^m z^m(\varepsilon+\omega\mathbf{p}+\mathbf{q})\right\rangle_\zeta, \tag{2.6}$$

which reduces immediately to

$$\frac{\delta G(\varepsilon\mathbf{p})}{\delta A_\mu(\mathbf{q}\omega)}=J_0^\mu(\varepsilon\mathbf{p}\varepsilon+\omega\mathbf{p}+\mathbf{q})\langle G_{\zeta A^2}(\varepsilon\mathbf{p}\mathbf{p})G_{\zeta A^2}(\varepsilon+\omega\mathbf{p}+\mathbf{q}\mathbf{p}+\mathbf{q})\rangle_\zeta$$
$$+J_0^\mu(\varepsilon\mathbf{p}-\mathbf{K}\varepsilon+\omega\mathbf{p}-\mathbf{K}+\mathbf{q})\langle G_{\zeta A^2}(\varepsilon\mathbf{p}\mathbf{p}-\mathbf{K})G_{\zeta A^2}(\varepsilon+\omega\mathbf{p}-\mathbf{K}+\mathbf{q}\mathbf{p}+\mathbf{q})\rangle_\zeta, \tag{2.7}$$

where $G_{A^2}(\epsilon\mathbf{p}\mathbf{p})$ is defined in (1.20), while

$$G_{A^2}(i\varepsilon_n\mathbf{p}\mathbf{p}-\mathbf{K})=+\frac{A}{(i\varepsilon_n)^2-\xi_p{}^2-A^2} \tag{2.8}$$

is the anomalous Green function of the ideal semiconductor, describing the elementary Umklapp process $\mathbf{p}\to\mathbf{p}-\mathbf{K}$.

We see that, in the model considered, the electromagnetic response is described by the same formulas as in an ideal semiconductor of the excitonic-insulator type, but with a fluctuating energy gap. Finite expressions arise, associated with pair products of anomalous Green functions, while the average (of the type (1.19)) of (2.8) is absent, corresponding to the absence of long-range order in the system. The model interaction introduced above is the direct analog of the Bragg scattering in the ideal crystal and is responsible for the formation of the distinctive kind of band structure (the pseudo-gap) in the electron spectrum. However, like the scattering in the ideal crystal, it is insufficient for a correct description of the kinetics, for which we must take into account the dissipative scattering (the analog of defects and phonons in the crystal) associated with the discarded part of the real interaction.

We now turn to consider the dielectric properties of our system. Since the polarization operator is directly related to the scalar vertex, from (2.7) we have

$$\Pi(\mathbf{q}\omega_m)=-2\int_0^\infty d\zeta\, e^{-\zeta}T\sum_n\int\frac{d^3p}{(2\pi)^3}\{G_{\zeta A^2}(\varepsilon_n\mathbf{p}\mathbf{p})G_{\zeta A^2}(\varepsilon_n+\omega_m\mathbf{p}+\mathbf{q}\mathbf{p}+\mathbf{q})$$
$$+G_{\zeta A^2}(\varepsilon_n\mathbf{p}\mathbf{p}-\mathbf{K})G_{\zeta A^2}(\varepsilon_n+\omega_m\mathbf{p}+\mathbf{q}\mathbf{p}-\mathbf{K}+\mathbf{q})\}\equiv\langle\Pi_{\zeta A^2}(\mathbf{q}\omega_m)\rangle_\zeta. \tag{2.9}$$

Summing over the Matsubara frequencies in the standard manner and performing the analytic continuation $i\omega_m\to\omega+i\delta$, we obtain[14]

$$\Pi_{A^2}(\mathbf{q}\omega)=-\frac{1}{2}\int\frac{d^3p}{(2\pi)^3}\frac{E_\mathbf{p}E_{\mathbf{p}+\mathbf{q}}+\xi_\mathbf{p}\xi_{\mathbf{p}+\mathbf{q}}+A^2}{E_\mathbf{p}E_{\mathbf{p}+\mathbf{q}}}\{f(E_\mathbf{p})-f(E_{\mathbf{p}+\mathbf{q}})\}$$
$$\times\left\{\frac{1}{E_\mathbf{p}-E_{\mathbf{p}+\mathbf{q}}+\omega+i\delta}+\frac{1}{E_\mathbf{p}-E_{\mathbf{p}+\mathbf{q}}-\omega-i\delta}\right\}+\frac{1}{2}\int\frac{d^3p}{(2\pi)^3}\frac{E_\mathbf{p}E_{\mathbf{p}+\mathbf{q}}-\xi_\mathbf{p}\xi_{\mathbf{p}+\mathbf{q}}-A^2}{E_\mathbf{p}E_{\mathbf{p}+\mathbf{q}}}$$
$$\times\{1-f(E_\mathbf{p})-f(E_{\mathbf{p}+\mathbf{q}})\}\left\{\frac{1}{E_\mathbf{p}+E_{\mathbf{p}+\mathbf{q}}+\omega+i\delta}+\frac{1}{E_\mathbf{p}+E_{\mathbf{p}+\mathbf{q}}-\omega-i\delta}\right\} \qquad (2.10)$$

i.e., the polarization operator of an ideal semiconductor. Here $E_p = (\xi_p^2 + A^2)^{1/2}$; $f(E_p) = \{\exp(E_p/T) + 1\}^{-1}$ is the Fermi distribution function.

As $A^2 \to 0$ the second term in (2.10) tends to zero, while the first gives the usual polarization operator of the electron gas. On the other hand, for $T \to 0$ but $A^2 \neq 0$, the first term in (2.10) vanishes, so that

$$\Pi_{A^2}(\mathbf{q}\omega)=\frac{1}{2}\int\frac{d^3p}{(2\pi)^3}\frac{E_\mathbf{p}E_{\mathbf{p}+\mathbf{q}}-\xi_\mathbf{p}\xi_{\mathbf{p}+\mathbf{q}}-A^2}{E_\mathbf{p}E_{\mathbf{p}+\mathbf{q}}} \qquad (2.11)$$
$$\times\left\{\frac{1}{E_\mathbf{p}+E_{\mathbf{p}+\mathbf{q}}+\omega+i\delta}+\frac{1}{E_\mathbf{p}+E_{\mathbf{p}+\mathbf{q}}-\omega-i\delta}\right\}.$$

The dielectric function is

$$\varepsilon(\mathbf{q}\omega)=1+\frac{4\pi e^2}{\mathbf{q}^2}\Pi(\mathbf{q}\omega)=\langle\varepsilon_{\zeta A^2}(\mathbf{q}\omega)\rangle_\zeta, \qquad (2.12)$$

where

$$\varepsilon_{A^2}(\mathbf{q}\omega)=1+\frac{4\pi e^2}{q^2}\Pi_{A^2}(\mathbf{q}\omega) \qquad (2.13)$$

is the dielectric function of the ideal semiconductor.

We shall consider first the case $\omega = 0$. For $v_F q \ll |A|$ we obtain from (2.11)

$$\Pi_{A^2}(\mathbf{q}0)=\frac{v_F^2q^2}{18}\frac{mp_F}{\pi^2A^2}=\frac{q^2}{4\pi e^2}\frac{v_F^2\varkappa^2}{18A^2}, \qquad (2.14)$$

so that

$$\varepsilon_{A^2}(\mathbf{q}0)=1+v_F^2\varkappa^2/18A^2=1+\omega_p^2/6A^2, \qquad (2.15)$$

where $\kappa^2 = 4mp_Fe^2/\pi$ is the square of the inverse Debye screening length and $\omega_p^2 = 4\pi ne^2/m$ is the square of the plasma frequency (n is the total electron density).

On the other hand, for $v_F q \gg |A|$ it follows from (2.10)–(2.11) that

$$\Pi_{A^2}(\mathbf{q}0)=mp_F/\pi^2=\varkappa^2/4\pi e^2, \qquad (2.16)$$

so that

$$\varepsilon_{A^2}(\mathbf{q}0)=1+\varkappa^2/q^2, \qquad (2.17)$$

i.e., we have the usual Debye screening.

We shall use the simplest interpolation from (2.15) to (2.17):

$$\varepsilon_{A^2}(\mathbf{q}0)=1+\frac{\varkappa^2}{q^2+18A^2/v_F^2}. \qquad (2.18)$$

Then for our model of a disordered system we obtain

$$\varepsilon(\mathbf{q}0)=\int_0^\infty d\zeta\, e^{-\zeta}\varepsilon_{\zeta A^2}(\mathbf{q}0)=1-\frac{v_F^2\varkappa^2}{18A^2}\exp\left(\frac{v_F^2q^2}{18A^2}\right)\mathrm{Ei}\left(-\frac{v_F^2q^2}{18A^2}\right), \qquad (2.19)$$

where Ei(−x) is the integral exponential function. For $v_F q \gg |A|$ we use the asymptotic form

$$\mathrm{Ei}(-x)\underset{x\to\infty}{\approx}-e^{-x}/x$$

and obtain (2.17). For $v_F q \ll |A|$ we use

$$\mathrm{Ei}(-x)\underset{x\to 0}{\sim}\ln x,$$

so that

$$\varepsilon(\mathbf{q}0)\approx 1-\frac{v_F^2\varkappa^2}{18A^2}\ln\frac{v_F^2q^2}{18A^2}. \qquad (2.20)$$

Correspondingly, the effective Coulomb interaction takes the form

$$\Gamma(\mathbf{q}0)\approx 4\pi\tilde{e}^2/q^2, \qquad (2.21)$$

$$\tilde{e}^2=e^2\Big/\left(1-\frac{v_F^2\varkappa^2}{18A^2}\ln\frac{v_F^2q^2}{18A^2}\right), \qquad (2.22)$$

which formally resembles the well-known "zero-charge" situation in field theory. Behavior of the type (2.20)–(2.22) has been obtained recently in a treatment of the so-called zero-gap semiconductors[15].

We turn to the analysis of the case $\omega \neq 0$, $v_F q \ll |A|$. From (2.11) we have

$$\mathrm{Re}\,\Pi_{A^2}(\mathbf{q}\omega)=\frac{v_F^2q^2}{12}\frac{mp_F}{2\pi^2}\int_{-\infty}^{\infty}d\xi_p\frac{A^2}{(\xi_p^2+A^2)^{3/2}}\frac{1}{\xi_p^2+A^2-\omega^2/4}, \qquad (2.23)$$

$$\mathrm{Im}\,\Pi_{A^2}(\mathbf{q}\omega)=\frac{v_F^2q^2}{12}\frac{mp_F}{2\pi^2}\frac{\pi}{2}\int_{-\infty}^{\infty}d\xi_p\frac{A^2}{(\xi_p^2+A^2)^2}$$
$$\times\left\{\delta\left[\frac{\omega}{2}-(\xi_p^2+A^2)^{1/2}\right]-\delta\left[\frac{\omega}{2}+(\xi_p^2+A^2)^{1/2}\right]\right\}. \qquad (2.24)$$

We first consider the real part of the dielectric function. From (2.23) we obtain

$$\mathrm{Re}\,\varepsilon_{A^2}(\omega)=1+\frac{\pi}{2}\frac{ne^2}{m}\int_{-\infty}^{\infty}d\xi_p\frac{A^2}{(\xi_p^2+A^2)^{3/2}}\frac{1}{\xi_p^2+A^2-\omega^2/4}. \qquad (2.25)$$

For $\omega \to 0$ ($\omega \ll 2|A|$), (2.15) follows naturally from this. For $\omega \gg 2|A|$ we obtain the plasma limit:

$$\mathrm{Re}\,\varepsilon_{A^2}(\omega)\approx 1-\omega_p^2/\omega^2. \qquad (2.26)$$

We shall use the simplest approximation:

$$\mathrm{Re}\,\varepsilon_{A^2}(\omega)=1+\frac{\omega_p^2}{6A^2}\theta\left(1-\frac{\omega^2}{4A^2}\right)-\frac{\omega_p^2}{\omega^2}\theta\left(\frac{\omega^2}{4A^2}-1\right). \qquad (2.27)$$

Then, from (2.12),

$$\mathrm{Re}\,\varepsilon(\omega)=1-\frac{\omega_p^2}{6A^2}\mathrm{Ei}\left(-\frac{\omega^2}{4A^2}\right)-\frac{\omega_p^2}{\omega^2}\{1-e^{-\omega^2/4A^2}\}. \qquad (2.28)$$

From this, for $\omega \gg 2|A|$, the plasma limit (2.26) follows. For $\omega \ll 2|A|$ we obtain, analogously to (2.21),

$$\mathrm{Re}\,\varepsilon(\omega)\approx 1-\frac{\omega_p^2}{6A^2}\ln\frac{\omega^2}{4A^2}. \qquad (2.29)$$

We emphasize that the qualitative behavior of Re $\epsilon(\omega)$ turns out to be practically independent of the method of interpolation in the formulas of the type (2.19) and (2.27). We can combine (2.20) and (2.29) by writing a single expression, valid with logarithmic accuracy:

$$\mathrm{Re}\,\varepsilon(\mathbf{q}\omega)\approx 1-\frac{\omega_p^2}{6A^2}\ln\frac{\max\{\omega^2;v_F^2q^2\}}{4A^2}. \qquad (2.30)$$

This result is valid only for $\omega \ll 2|A|$, $v_F q \ll |A|$. The interpolation formula (2.28) describes the entire frequency interval. One can easily convince oneself that Re $\epsilon(\omega)$ given by (2.28) has no zeros other than the plasma zero, which arises in the limit $\omega \gg 2|A|$.

The behavior of the imaginary part of the dielectric function is of special interest, since it determines, in particular, the optical absorption in the system. The absorption is determined by the real part of the conductivity, which is related to Im $\epsilon(\omega)$ as follows:

$$\mathrm{Re}\,\sigma(\omega)=\omega\,\mathrm{Im}\,\varepsilon(\omega)/4\pi. \qquad (2.31)$$

From (2.11) and (2.12) we obtain

$$\operatorname{Im}\varepsilon(\omega)=\frac{\pi}{4}\frac{ne^2}{m}\int\limits_0^\infty d\zeta\, e^{-\zeta}\int\limits_{-\infty}^\infty d\xi_p \frac{\zeta A^2}{(\xi_p{}^2+\zeta A^2)^2}$$
$$\times\left\{\delta\left[\frac{\omega}{2}-(\xi_p{}^2+\zeta A^2)^{1/2}\right]-\delta\left[\frac{\omega}{2}+(\xi_p{}^2+\zeta A^2)^{1/2}\right]\right\}$$
$$=2\pi^2\frac{ne^2}{m}\frac{|A|}{\omega^3}\int\limits_0^{\omega^2/4A^2} d\zeta\, e^{-\zeta}\frac{\zeta}{(\omega^2/4A^2-\zeta)^{1/2}}$$
$$=\pi\left(\frac{\omega_p}{\omega}\right)^2\frac{|A|}{\omega}\exp\left\{-\frac{\omega^2}{4A^2}\right\}\left\{\frac{\omega^2}{4A^2}-\frac{d}{d\alpha}\right\}\operatorname{Erfi}\alpha^{1/2}\frac{\omega}{2|A|}\bigg|_{\alpha=1}. \quad (2.32)$$

Correspondingly,

$$\operatorname{Re}\sigma(\omega)=\pi\frac{ne^2}{m\omega}\frac{|A|}{\omega}\exp\left\{-\frac{\omega^2}{4A^2}\right\}\left\{\frac{\omega^2}{4A^2}-\frac{d}{d\alpha}\right\}\operatorname{Erfi}\alpha^{1/2}\frac{\omega}{2|A|}\bigg|_{\alpha=1}. \quad (2.33)$$

We have the following asymptotic behavior for $\omega \gg 2|A|$:

$$\operatorname{Im}\varepsilon(\omega)\approx\pi\left(\frac{\omega_p}{\omega}\right)^2\left(\frac{A}{\omega}\right)^2, \quad (2.34)$$

$$\operatorname{Re}\sigma(\omega)\approx\frac{ne^2}{m\omega}\pi\left(\frac{A}{\omega}\right)^2. \quad (2.35)$$

For $\omega \ll 2|A|$,

$$\operatorname{Im}\varepsilon(\omega)\approx\pi\omega_p{}^2/6A^2, \quad (2.36)$$

$$\operatorname{Re}\sigma(\omega)\approx\frac{ne^2}{m}\pi\frac{\omega}{6A^2}\to 0 \quad \text{for} \quad \omega\to 0. \quad (2.37)$$

The static conductivity in our approximation vanishes, indicating a particular type of Bragg electron-localization. Analogously, the static conductivity of the ideal semiconductor at $T = 0$ equals zero. We have obtained the analog of the usual interband absorption. In addition (2.36) shows that our model describes a substance intermediate between a metal and an insulator: in a metal $\operatorname{Im}\epsilon(\omega) \propto 1/\omega$, and in an insulator $\operatorname{Im}\epsilon(\omega) = 0$ for $\omega = 0$. In our case, $\operatorname{Im}\epsilon(\omega)$ has a finite discontinuity at $\omega = 0$ ($\operatorname{Im}\epsilon(\omega) = -\operatorname{Im}\epsilon(-\omega)$).

It should be noted that, generally speaking, in view of the fact that the entire treatment is invalid (in the sense of the first of the conditions (1.14)) near the center of the pseudo-gap, when $\epsilon \sim \xi_p \sim 0$, our formulas are not valid in the region of low frequencies. Therefore, the calculation performed for the polarization operator is valid, clearly, only in the region of sufficiently high frequencies:

$$\omega\gg v_F\gamma=v_F/R_c, \quad (2.38)$$

where γ and R_c are defined in (1.14). For $R_c \gtrsim 20a$, we are concerned with frequencies greater than or of the order of (1/4)—(1/8) of the width of the pseudo-gap. The condition (2.38) has a clear meaning—in the characteristic time of variation of the external field the electron moves over a distance less than R_c. Naturally, allowance for the finite temperature will also change the asymptotic behavior of $\epsilon(q\omega)$ for small q and ω, because of the appearance of excited carriers in the "upper band".

In conclusion, we note that the model considered and all the results obtained above can be used in the analysis of the properties of one-dimensional systems (of the TTF-TCNQ type) undergoing a Peierls structural transition, since the strong fluctuations of the order parameter in the one-dimensional case make such systems similar in a certain sense to "liquid semiconductors"[16]. Inasmuch as R_c in this case can reach hundreds of interatomic spacings, and the temperatures are sufficiently low, the region of applicability of the theory is substantially broadened.

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177