fusion in terms of microscopic concepts: The difference between $D_\parallel$ and $D_\perp$ is effectively a measure of the gradient of $\nu(\epsilon)$ with respect to energy. For example, when $\nu(\epsilon)$ is an increasing function of energy, collisions occur more frequently as the energy of the carriers is increased, and diffusion parallel to the electric field is reduced in comparison with the perpendicular direction, $D_\parallel \leq D_\perp$ (equality holds at zero field). For the deformation potential, $l=$ const and $\nu \propto \epsilon^{1/2}$, and we find from (17), (18), (23), and (24) that $D_\parallel/D_\perp = 0.5$ (high-field limit) in good agreement with the more exact result of Parker and Lowke.[5]

It is clear that we cannot neglect the dependence of $f^{(0)}$ upon ∇n (as done in Ref. 3), for this implies from (14) and (16) that $\langle\epsilon_1\rangle = 0$, in contradiction to (20). [If $\langle\epsilon_1\rangle$ were set equal to zero, then we would find $D_\parallel = D_\perp$ as given by Eq. (23b).]

The method of moment equations can be extended to the case where optical-phonon scattering is of importance. Here, however, difficulties arise because energy is not equipartitioned and the pressure in (10) becomes a tensor with diagonal entries $n\kappa T_{\parallel,\perp}$. The single equation (11) for energy has to be replaced by two equations, for $T_\parallel$ and $T_\perp$. Because of these increasing complexities, it may not be any more advantageous to pursue this approach than to solve the Boltzmann equation directly. In adopting the latter course, a method recently described by Kumar and Robson[7] appropriate to ions in a neutral gas may be useful in providing a guide to tackling the problem for semiconductors.

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Mobility Gap and Anomalous Dispersion*

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It is shown that anomalous dispersion of quasiparticles leads to nonpropagating states. Therefore regions of anomalous dispersion define a sort of "mobility gap." Using the coherent-potential approximation, we calculate the conditions for obtaining such a mobility gap in a disordered binary alloy. Just outside the mobility edges located at ω_c the mobility vanishes as $|\omega-\omega_c|$.

We consider the question of the existence of a "mobility gap," of whether in a disordered medium there is a range of allowed energy levels which are all nonpropagating states. This concept, first conjectured by Mott,[1] Cohen, Fritzsche, and Ovshinsky,[2] and others, is of great physical interest in the electronic band structure of liquids, amorphous semiconductors, and disordered alloys. It has been shown that in the disordered linear chain *all* states are localized,[3] so that the "mobility gap" could well include all allowed energy levels. In the case of the three-dimensional disordered medium one needs a specific criterion for the existence and location of such a gap. Criteria based on probabilistic concepts have been put forward.[4]

It is the purpose of the present work to present a different sort of criterion, based on the dispersion of quasiparticles. We shall show that if there is a region of *anomalous* dispersion, ordinary wave packets made with states in this region cannot propagate, and we shall therefore identify this region of energy states as constituting a mobility gap. We shall then use the well-known coherent-potential approximation (CPA)[5] to obtain the quasiparticle energies in a special case, as an example to demonstrate conditions under which one finds anomalous dispersion.

Consider a wave packet about an average energy ω_0:

$$F(\vec{r}, t) \equiv \int_{-\infty}^{\infty} d^3k\, e^{i\vec{k}\cdot\vec{r}} \int_{-\infty}^{\infty} d\omega\, f(\omega-\omega_0) e^{-i\omega t}/[\omega - \zeta_k(\omega) - \epsilon_k], \tag{1}$$

where $f(\omega-\omega_0)$ is a given envelope function. With the initial condition that it be centered near the origin at $t=0$, the wave packet propagates out as time goes forward. This causality requirement determines the sign of $\Gamma_k(\omega)$, the imaginary part of the self-energy $\zeta_k(\omega)$:

$$\zeta_k(\omega) \equiv R_k(\omega) - i\Gamma_k(\omega), \quad \Gamma_k(\omega) \geq 0. \tag{2}$$

If Γ is not too large, the above integrand is approximated by a pole located at $\omega_k - i\Gamma_k(\omega_k)$, where ω_k is defined as the solution of

$$\omega_k - R_k(\omega_k) - \epsilon_k = 0. \tag{3}$$

Now assuming $f(\omega-\omega_0)$ to be narrowly peaked about $\omega=\omega_0$, we may expand about ω_0 as follows:

$$\begin{aligned}\omega - \zeta_k(\omega) &= \omega_0 - R_k(\omega_0) + i\Gamma_k(\omega_0) + (\omega-\omega_0)[1 - \partial R_k(\omega_0)/\partial\omega_0 + i\partial\Gamma_k(\omega_0)/\partial\omega_0] + \cdots \\ &= \epsilon_{k_0} + i\Gamma_0 + (\omega-\omega_0)\mu^* + \cdots,\end{aligned} \tag{4}$$

where $\epsilon_{k_0} \equiv \omega_0 - R_k(\omega_0)$, $\mu^* \equiv 1 - \partial R_k(\omega_0)/\partial\omega_0$, and the small correction terms $O(i(\omega-\omega_0)\,\partial\Gamma/\partial\omega)$ (it can be assumed that Γ is slowly varying) and $O((\omega-\omega_0)^2)$ are neglected.

We now average over a large sphere at r:

$$F(r,t) = \exp(-i\omega_0 t)\int d\epsilon_k\, \rho_0(\epsilon_k)\, \frac{\sin kr}{kr} \int d\Omega\, \exp(-i\Omega t)\, \frac{f(\Omega)}{(\epsilon_{k_0} - \epsilon_k) + \Omega\mu^* + i\Gamma_0}, \tag{5}$$

where $\Omega \equiv \omega - \omega_0$. We further expand k about k_0, suitably averaging over angles if necessary,

$$k = k_0 + (\partial\epsilon/\partial k)_0^{-1}(\epsilon_k - \epsilon_{k_0}) = k_0 + z/V_k, \tag{6}$$

which serves to define $V_0 \equiv (\partial\epsilon/\partial k)_0$ and $z \equiv \epsilon_k - \epsilon_{k_0}$. Taking slowly varying factors outside the k integral, we have

$$F(r,t) = \exp(-i\omega_0 t)\rho_0(\epsilon_{k_0})(2ik_0 r)^{-1}\int d\Omega\, f(\Omega)\exp(-\Omega t)[I_1(\Omega) - I_2(\Omega)], \tag{7}$$

where the integrals

$$\begin{aligned} I_1(\Omega) &= \exp(ik_0 r)\int dz\, \exp(izr/V_0)(\Omega\mu^* + i\Gamma_0 - z)^{-1}, \\ I_2(\Omega) &= \exp(-ik_0 r)\int dz\, \exp(-izr/V_0)(\Omega\mu^* + i\Gamma_0 - z)^{-1}\end{aligned} \tag{8}$$

can be evaluated by contour integration. For electronlike particles, $V_0 > 0$ and the contour for I_1 is closed by an infinite semicircle in the upper-half complex z plane and I_2 in the lower half. For holelike particles, $V_0 < 0$ and the respective contours are interchanged. Thus,

$$F(r,t) = -\exp(-i\omega_0 t \mp ik_0 r)[\pi\rho_0(\epsilon_{k_0})/k_0 r]\tilde{f}(t - \mu^* r/|V_0|)\exp(-r\Gamma_0/|V_0|), \tag{9}$$

in which $\tilde{f}(\tau) \equiv \int d\Omega\, f(\Omega)\exp(-i\Omega\tau)$. Except for the $\mp$ sign in the phase factor, this result is independent of the sign of V_0.

The sign of the dispersion parameter μ^* is, however, crucial. For $\mu^* > 0$, $F(r,t)$ is an outgoing spherical wave packet, decaying exponentially as it leaves the origin, because of the incoherent scattering. For $\mu^* < 0$, it becomes an *incoming* spherical wave packet, which *grows* unphysically as it approaches the origin and then ceases to exist at large t. The conclusion that there is a sink at $r=0$, i.e., that the eigenstates are everywhere localized, becomes inescapable. This is in accord with the usual understanding of anomalous dispersion in optics, a familiar phenomenon observed in a narrow range of frequencies near resonant absorption.

It is instructive to consider the example of a retarded Green's function,[6]

$$G_{\rm ret}(\vec{r},t) = -i\theta(t)\langle\{\psi(r,t),\ \psi^\dagger(0,0)\}\rangle = \int_{-\infty}^{\infty} d\omega\, e^{-i\omega t}\, G(\omega + i0^+), \qquad (10)$$

in which $\theta(t)=1$ for $t>0$ and vanishes at $t<0$, and

$$G(\omega) = \int d^3k \int d^3k'\, e^{i\vec{k}\cdot\vec{r}} \langle\langle C_k | C_{k'}{}^\dagger\rangle\rangle_\omega . \qquad (11)$$

We must average over the ensemble of random configurations in the disordered medium, thus restoring translational invariance of a sort:

$$\bar{G}(\omega) = (2\pi)^{-1}\int d^3k\, e^{i\vec{k}\cdot\vec{r}}[\omega - \zeta_k(\omega) - \epsilon_k]^{-1}, \qquad (12)$$

where the self-energy function $\zeta_k(\omega)$ is real for real ω, and is complex, $\zeta(\omega \pm i0^+) = R \mp i\Gamma$, with $\Gamma > 0$, for ω just off the real axis. The branch cut is well approximated by a simple pole, as in Eq. (3). Our previous discussion makes it clear that regions of anomalous dispersion will not contribute significantly to $G_{\rm ret}(\vec{r},t)$. A spectral resolution of $G(\vec{r},t)$ at large r will not show any component belonging to frequencies within this region, corresponding to the notion of a "mobility gap."

It remains to calculate $R_k(\omega)$ and $\Gamma_k(\omega)$, and the CPA now provides a convenient and fairly accurate method for doing so. We take a specific model: the random binary alloy with potential energy $\pm\frac{1}{2}U$ at each site. The CPA equations are

$$\langle\langle C_k | C_{k'}{}^\dagger\rangle\rangle_\omega = (2\pi)^{-1}\delta_{k,k'}[\omega - \zeta(\omega) - \epsilon_k]^{-1}, \qquad (13)$$

where the average T matrix is made to vanish:

$$\bar{T}(\omega) = \frac{\frac{1}{2}U - \zeta(\omega)}{1 - [\frac{1}{2}U - \zeta(\omega)]g(\omega)} + \frac{-\frac{1}{2}U - \zeta(\omega)}{1 - [-\frac{1}{2}U - \zeta(\omega)]g(\omega)} = 0, \qquad (14)$$

where

$$g(\omega) = N^{-1}\sum_k [\omega - \zeta(\omega) - \epsilon_k]^{-1} = \int d\epsilon\, \rho_0(\epsilon)[\omega - \zeta(\omega) - \epsilon]^{-1}. \qquad (15)$$

These yield a self-energy function $\zeta(\omega) = R(\omega) - i\Gamma(\omega)$ (independent of k in the CPA). Supposing the unperturbed bandwidth to be Δ, we introduce dimensionless units such that $U=1$ and $\delta = \Delta/U$, and approximate ρ_0 by the semicircular function,

$$\rho_0(\epsilon) = (4/\pi\delta)[1-(2\epsilon/\delta)^2]^{1/2}, \quad |\epsilon| < \tfrac{1}{2}\delta, \qquad (16)$$

for which a simple algebraic expression can be obtained for $g(\omega)$:

$$g(\omega) = 8\delta^{-2}\{\omega - \zeta - [(\omega-\zeta)^2 - \tfrac{1}{4}\delta^2]^{1/2}\}. \qquad (17)$$

Combining the above with Eq. (14) we obtain a cu-

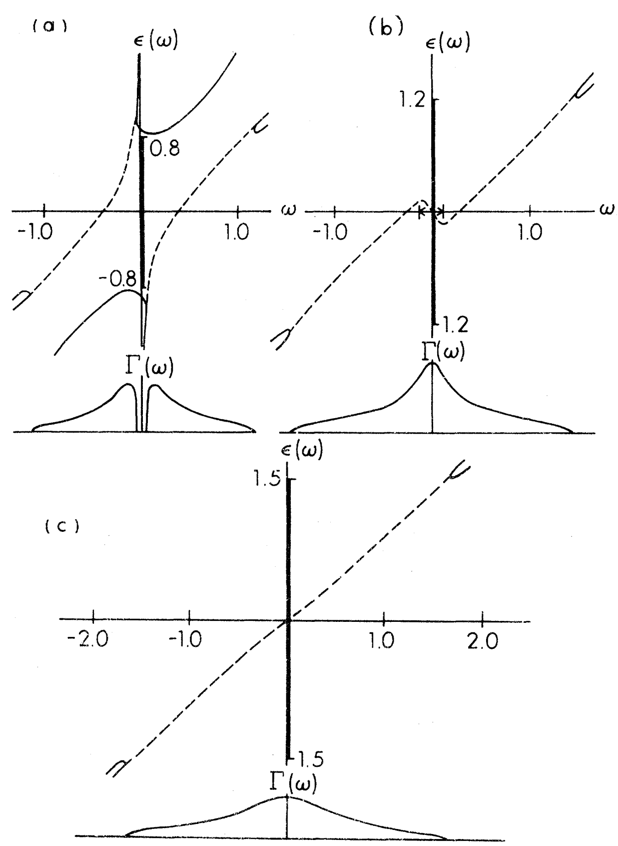

FIG. 1. Dispersion relations, $\epsilon(\omega)$ versus ω, for (a) $\sigma = 1.6$, (b) $\sigma = 2.4$, and (c) $\sigma = 3.0$. Solid lines, real solutions of the cubic equation; dashed lines, real parts of the complex conjugate solutions for ζ; thick line on the $\epsilon(\omega)$ axis, allowed region over which the variable ϵ_k is defined. At the bottom of each figure is shown the imaginary part $\Gamma(\omega)$ of ζ. (a) corresponds to a separated-band case with a finite density-of-states gap, while (b) and (c) are examples with no density-of-states gaps. (b) shows anamalous dispersion, with a mobility gap indicated by an arrow.

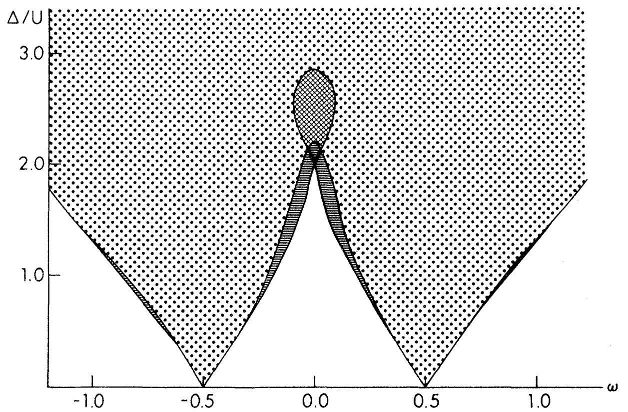

FIG. 2. Dependence of the quasiparticle spectrum and and the mobility gaps upon $\sigma = \Delta/U$ and ω. The density of states is nonvanishing in the dotted regions. Regions of localized states within our mobility gap are cross hatched, and those within the Economou-Cohen gap are single hatched.

bic equation in ζ:

$$\omega\zeta^3 - \tfrac{1}{4}(1 - \tfrac{1}{4}\delta^2)\zeta^2 - \tfrac{1}{4}\omega\zeta + \tfrac{1}{16} = 0. \qquad (18)$$

This is solved numerically to yield $\epsilon(\omega) \equiv \omega - R(\omega)$. When $\epsilon(\omega) = \epsilon_k$, we have located the pole. This is plotted in Fig. 1. For $\delta^2 < 4$, a density-of-states gap opens up about $\omega = 0$ and there is no region of anomalous dispersion. In the range $4 < \delta^2$ one can expand Eq. (17) in powers of ω, and obtain an expression for $\partial\epsilon(\omega)/\partial\omega$ at $\omega = 0$. This quantity turns out negative only in the narrow range $4 < \delta^2 < 8$, and anomalous dispersion again ceases to exist at $\delta^2 > 8$.

It follows from the preceding arguments that the states indicated by an arrowed portion on the ω axis in Fig. 1(b) are localized and that the mobility edges at ω_c are determined by the vanishing of $d\epsilon(\omega)/d\omega$. The mobility gap obtained in this manner is shown in Fig. 2 by cross hatching. In Fig. 2 we contrast our computed regions of anomalous dispersion to the regions of localized states predicted by the probabilistic criterion of Economou and Cohen. The two criteria agree only near $\delta = 2$. This discrepancy appears to be worthy of further study, for it suggests that there may be more than one way to localize waves within a continuum.

Our formulation gives us an insight into the behavior of the mobility edges. Although the mobility is not identically zero for $|\omega| > \omega_c$, it approaches zero when $|\omega| \to |\omega_c|$ because the dispersion parameter $\mu^* = [d\epsilon(\omega)/d\omega]^{-1}$ increases and goes to infinity at the critical energy. As we have $\epsilon(\omega) - \epsilon(\omega_c) \propto (\omega - \omega_c)^2$ near $|\omega_2|$, $1/\mu^* \propto |\omega - \omega_c|$. The mobility μ is defined by $\mu = e^2\tau/\mu^*$. The lifetime τ of a quasiparticle is inversely proportional to $\Gamma(\omega)$, which can now be replaced by $\Gamma(\omega_c)$ since deviation from this value only gives a higher-order correction. As a result, the mobility near the critical point is seen to vanish linearly as $\mu \propto |\omega - \omega_c|$.

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