Dielectric constant and anomalous magnetoresistance of zero-gap semiconductors

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It is shown that for a zero-gap semiconductor the static dielectric constant at infinite wavelength ($\vec{q}=0$) and zero temperature contains a magnetic-field-dependent term of the form of $H^{-1/2}$. Because of this anomalous term, both the longitudinal and the transverse classical magnetoresistance for a p-type sample are expected to have a dependence on the magnetic field other than the usual H^2 behavior in the low-temperature region.

I. INTRODUCTION

There has recently been considerable interest in zero-gap semiconductors, especially in their dielectric properties. In a pure semiconductor with inherent zero energy gap, both the static and the dynamic dielectric functions at zero temperature have been shown to possess singularities. In the static case,[1] the singularity is of the form q^{-1} at small q. The dynamic dielectric function[2] has a $\omega^{-1/2}$ dependence for small ω. These anomalies in the interband polarizability come from the band-edge structure, which is degenerate as required by crystal symmetry. For this reason, the static interband polarizability depends strongly on impurity doping[3] or on temperature.[4] All these effects have been predicted theoretically within the framework of the random-phase approximation (RPA). In view of the subsequent work of Abrikosov and Beneslavskii[5] on the renormalization of the energy spectrum due to electron-electron interactions for zero-gap materials, the form of the RPA anomalous terms may have to be modified within a very small region close to the point where the singularity occurs.

Since the band-edge degeneracy plays a decisive role in these polarizability anomalies, it is expected that any external field which lifts the degeneracy should have a strong effect on the dielectric function. For crystals like α-Sn,[6] HgTe, or HgSe,[7] the degeneracy is required by cubic symmetry, and hence an uniaxial stress should remove it. The dependence of interband polarizability on uniaxial stress is the subject matter of a recent publication by one of us.[8] In this paper we discuss the effect of a uniform magnetic field, which is another means for opening up an energy gap in a zero-gap material. We predict that the interband polarizability should have a $H^{-1/2}$ term from both the spin-flip and the non-spin-flip transitions, where H is the magnetic field strength. With this kind of anomalous screening, the low-temperature classical magnetoresistance of a p-type sample is shown to have a field dependence significantly different from the usual H^2 behavior.

II. CALCULATION OF MATRIX ELEMENT

To calculate the interband polarizability in the presence of a magnetic field, we need to know the matrix element of the perturbing wave field $e^{i\vec{q}\cdot\vec{r}}$ between two Landau level states. Assuming that $\vec{q}$ is along z, which is the direction of the magnetic field, the relevant matrix element is denoted by

$$M \equiv \langle c, n, k_z, \sigma | e^{iqz} | v, n', k_z', \sigma' \rangle , \qquad (2.1)$$

where c and v label the conduction and valence band, respectively; n is the Landau quantum number; k_z is the wave-vector component along the field direction; and σ, which can be either + or −, is the spin index. For α-Sn-type semiconductors, the degenerate band edge is of Γ_8^+ symmetry. Wave functions for the Γ_8^+ edge in a magnetic field have been deduced in the effective-mass approximation by various authors.[9] For our purpose it is more convenient to use the results of Yafet,[10] who had deduced the wave functions by taking only interactions among Γ_8^+ and the two close-by Γ_7^+ and Γ_7^- states into account. The wave functions are given by

$$|c \text{ or } v, n, k_z, \sigma\rangle = \frac{1}{\sqrt{L^3}} e^{ik_y y + ik_z z} \times \sum_{j,k_x} A_{j,n}(k_x, k_z) e^{ik_x(x-\frac{k_y}{s})} u_j , \qquad (2.2)$$

where L^3 is the crystal volume and $s = eH/\hbar c$. If we further confine the expansion of the magnetically perturbed wave function into the four Γ_8^+ band-edge states only, the summation over j in Eq. (2.2) runs over the following four states:

$$u_1 = |(1/\sqrt{2})(X - iY)\downarrow\rangle ,$$
$$u_2 = |(1/\sqrt{6})[(X - iY)\uparrow + 2Z\downarrow]\rangle ,$$
$$u_3 = |(1/\sqrt{6})[(X + iY)\downarrow - 2Z\uparrow]\rangle ,$$

$$u_4 = |(1/\sqrt{2})(X+iY)\uparrow\rangle , \quad (2.3)$$

where X, Y, Z are the Γ'_{25} wave functions which transform as atomic p states and the symbols $\uparrow$ and $\downarrow$ designate the spin-up and spin-down states, respectively. The expansion coefficients $A_{j,n}$ as obtained by Yafet[10] are quoted in Table I. In these coefficients Φ_n is the linear-harmonic-oscillator wave function of the dimensionless variable $k_x/\sqrt{s}$. The energy eigenvalues of the conduction-band Landau levels with + or − spin are given as

$$E^c_{n,\pm} = \tfrac{2}{3}(|P|^2/E_g)[k_z^2 + (2n+1)s] \mp \tfrac{1}{3} s |P|^2/E_g , \quad (2.4)$$

where $E_g = E(\Gamma_8^+) - E(\Gamma_7^-)$ and P is the momentum matrix element, $P = (\hbar/m)\langle iS|p_x|X\rangle$. The wave function S is that for the Γ'_2 state having atomic s symmetry. The valence band has been assumed to be flat and hence the magnetic field splitting of the valence band is to be neglected in this approximation.

With the wave functions given in Eq. (2.2) the matrix element is calculated to be

$$|M|^2 = \delta_{k'_z, k_z+q} \sum_{j,k_x} A^*_{j,n}(k_x, k_z) A_{j,n'}(k_x, k'_z) . \quad (2.5)$$

From Table I it is evident that for non-spin-flip transitions, the selection rule is $\Delta n \equiv n' - n = 0$, and for spin-flip transitions, $\Delta n = \pm 1$. By using the orthonormal properties of linear-harmonic-oscillator wave functions, we can write down in explicit form the matrix element in the small-q limit corresponding to four types of transitions in the following:

(a) $|v, n, -\rangle$ to $|c, n, -\rangle$

$$|M|^2 = \frac{12(n+1)sk_z^2q^2}{[2k_z^2 + (4n+3)s]^2(2k_z^2+ns)} , \quad n \geq 0 . \quad (2.6)$$

(b) $|v, n, +\rangle$ to $|c, n, +\rangle$

$$|M|^2 = \frac{12nsk_z^2q^2}{[2k_z^2 + (4n+1)s]^2[2k_z^2+(n+1)s]} , \quad n \geq +1 . \quad (2.7)$$

(c) $|v, n, -\rangle$ to $|c, n-1, +\rangle$

$$|M|^2 = \frac{6n(n+1)s^2q^2}{(2k_z^2+ns)[2k_z^2 + (4n-3)s][2k_z^2+(4n+3)s]} , \quad n \geq +1 . \quad (2.8)$$

(d) $|v, n, +\rangle$ to $|c, n+1, -\rangle$

$$|M|^2 = \frac{6n(n+1)s^2q^2}{[2k_z^2+(n+1)s][2k_z^2 + (4n+1)s][2k_z^2+(4n+7)s]} , \quad n \geq +1 . \quad (2.9)$$

III. CALCULATION OF DIELECTRIC CONSTANT

We calculate the RPA interband polarizability at zero temperature according to the following expression with a flat-valence-band approximation:

$$4\pi\alpha = \frac{4e^2 s}{Lq^2} \sum_{k_z, n, \sigma} \frac{|M|^2}{E^c_{n,\sigma}} , \quad (3.1)$$

The factor s in Eq. (3.1) is related to the degeneracy of Landau levels (Ls) obtained by restricting k_y/s in the phase factor of Eq. (2.2) to be within a length of L. The summation is over the occupied-valence-band Landau states for a pure sample. Each state is connected with two conduction-band Landau states, one corresponding to spin-flip transitions and one to non-spin-flip transitions.

With the matrix element in Eqs. (2.6)–(2.9) and energy eigenvalues given in Eq. (2.4) the interband polarizability in Eq. (3.1) can be straightforwardly calculated. The result is expressed as

$$4\pi\alpha = \lambda/\sqrt{H} , \quad (3.2)$$

where the constant λ is given by

$$\lambda = \frac{72}{\pi} \frac{E_g}{|P|^2} (e^3\hbar c)^{1/2} \sum_{i=1}^{4} I_i . \quad (3.3)$$

The four numerical constants I_i are contributions from the four types of transitions listed in Eqs. (2.6)–(2.9). They are given explicitly in the following:

$$I_1 = \sum_{n=0} 2(n+1) \int_0^\infty dx \frac{x^2}{(2x^2+4n+3)^3(2x^2+n)} ,$$

$$I_2 = \sum_{n=1} 2n \int_0^\infty dx \frac{x^2}{(2x^2+4n+1)^3(2x^2+n+1)} ,$$

$$I_3 = \sum_{n=1} n(n+1) \int_0^\infty dx [(2x^2+4n-3)^2 \times (2x^2+4n+3)(2x^2+n)]^{-1} , \quad (3.4)$$

$$I_4 = \sum_{n=1} n(n+1) \int_0^\infty dx [(2x^2+4n+7)^2 \times (2x^2+4n+1)(2x^2+n+1)]^{-1} ,$$

TABLE I. Expansion coefficients $A_{j,n}$ for the wave functions in a magnetic field. The harmonic-oscillator wave function Φ_n are functions of $k_x/\sqrt{s}$.

Basis state	$\vert c,n,-\rangle,\ n\geq 0$	$\vert c,n,+\rangle,\ n\geq 0$	$\vert v,n,-\rangle,\ n\geq -1$	$\vert v,n,+\rangle,\ n\geq +1$
u_1	$\left(\frac{3(n+1)s}{2k_z^2+(4n+3)s}\right)^{1/2}\Phi_{n+1}$	0	$\left[\frac{2k_z^2+ns}{2k_z^2+(4n+3)s}\right]^{1/2}\Phi_{n+1}$	0
u_2	$\left(\frac{2k_z^2}{2k_z^2+(4n+3)s}\right)^{1/2}\Phi_n$	$\left(\frac{(n+1)s}{2k_z^2+(4n+1)s}\right)^{1/2}\Phi_{n+1}$	$-\left(\frac{6(n+1)sk_z^2}{(2k_z^2+ns)[2k_z^2+(4n+3)s]}\right)^{1/2}\Phi_n$	$-\left(\frac{3n(n+1)s^2}{[2k_z^2+(n+1)s][2k_z^2+(4n+1)s]}\right)^{1/2}\Phi_{n+1}$
u_3	$\left(\frac{ns}{2k_z^2+(4n+3)s}\right)^{1/2}\Phi_{n-1}$	$-\left(\frac{2k_z^2}{2k_z^2+(4n+1)s}\right)^{1/2}\Phi_n$	$-\left(\frac{3n(n+1)s^2}{(2k_z^2+ns)[2k_z^2+(4n+3)s]}\right)^{1/2}\Phi_{n-1}$	$-\left(\frac{6nsk_z^2}{[2k_z^2+(n+1)s][2k_z^2+(4n+1)s]}\right)^{1/2}\Phi_n$
u_4	0	$\left(\frac{3ns}{2k_z^2+(4n+1)s}\right)^{1/2}\Phi_{n-1}$	0	$\left(\frac{2k_z^2+(n+1)s}{2k_z^2+(4n+1)s}\right)^{1/2}\Phi_{n-1}$

In the integrals above, the upper limit which should be $K/\sqrt{s}$, K being the Brillouin-zone dimension, has been replaced by infinity. The starting n in each of the series summation above is given explicitly for a pure sample. The series do not converge very rapidly. We have estimated the value for each series and obtain $\sum_{i=1}^{4} I_i \sim 0.16$. If we take the values of $E_g = 0.413$ eV and

$$E_p = 2m\,|P\,|^2/\hbar^2 = 24.8 \text{ eV}$$

as calculated by Leung and Liu[11] for α = Sn, we obtain $\lambda_{\alpha\text{-Sn}} = 6\times 10^3\ \text{g}^{1/2}$. This value for λ should only be regarded as an order-of-magnitude estimate.

It is remarked here that for a doped sample of either n or p type, the $H^{-1/2}$ dependence of interband polarizability as given in Eq. (3.2) is not valid when $\sqrt{s} \ll k_F$, k_F being the Fermi momentum for a degenerate sample.

IV. MAGNETORESISTANCE

The anomalous screening discussed in this paper should have an effect on the magnetoresistance at low temperature. For α-Sn, HgTe, or HgSe, the effective mass of the hole is much larger than that of the electron. It is then advantageous to investigate a p-type sample such that suitable temperature and field regions can be chosen to make the conduction-band states quantized, but not the valence-band states. In this way, quantum effects do not set in other than giving rise to a field-dependent impurity screening. Since the impurity scattering dominates at low temperature, the relaxation time τ should show a field dependence through its dependence on the dielectric constant ϵ as given by

$$\tau = \tau_r(\epsilon/\epsilon_r)^2 , \qquad (4.1)$$

where the subscript r refers to an arbitrarily chosen reference point. The dielectric constant ϵ should contain a field-independent part ϵ_0 and an anomalous part given in Eq. (3.2), or

$$\epsilon = \epsilon_0 + \lambda/\sqrt{H} . \qquad (4.2)$$

For a p-type sample, the energy surface is sufficiently warped to give rise even to a longitudinal magnetoresistance.[12] Both the longitudinal and the transverse magnetoresistance ordinarily should have a H^2 dependence on the magnetic field. Now with the field-dependent impurity potential, the quadratic dependence on the magnetic field has to be modified. Since the magnetoresistance $\Delta\rho/\rho_0$ depends on the square of the relaxation time,[12] we expect that

$$\frac{\Delta\rho}{\rho_0} = \left(\frac{\Delta\rho}{\rho_0}\right)_r \left(\frac{H}{H_r}\right)^2 \left(\frac{\epsilon_0+\lambda/\sqrt{H}}{\epsilon_0+\lambda/\sqrt{H_r}}\right)^4 . \qquad (4.3)$$

From the measured value[13] of $\epsilon_0(=24)$ and the calculated value of λ for pure α-Sn, it is expected that the field dependence of the magnetoresistance as given in Eq. (4.3) can be significantly different from the usual H^2 behavior. In the small-field region $\sqrt{s} \ll k_F$, however, the magnetoresistance does not have this anomaly.

An experimental study of the magnetoresistance anomaly is not only of interest for its own sake but also may provide one additional verification of the anomalous screening effect. We suggest certain typical experimental conditions in this paragraph. At 4.2 °K and in a magnetic field below 10 kG, the valence band for all the presently known zero-gap semiconductors should remain unquantized. For a p-type sample containing 10^{15} carriers/cm^3 or less, the magnetoresistance should rise as H^2 at very low field and gradually change to the field dependence given by Eq. (4.3) as the field increases.

A brief account of the present work has appeared elsewhere.[14]

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