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High-frequency conductivity of a two-dimensional electron gas interacting with optical phonons

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We calculate the high-frequency conductivity for a two-dimensional electron gas interacting with optical lattice vibrations. The collision frequency and the optical mass normalization are obtained. The frequency dependence of the (inverse) collision time is presented.

I. INTRODUCTION

When a device of metal-insulator-semiconductor structure is biased, a large accumulation of electrons or inversion layer is produced on the surface of the semiconductor. When the energy bands are bent, as in the case of strong inversion, a potential well appears on the insulator-semiconductor interface which localizes the motion of the electrons normally to the surface. On the other hand, the electrons are free to move in the plane of the surface. Under strong enough bias, the localization of the electrons in the direction normal to the surface, which is characterized by the spread of their wave function, is much smaller than their average distance within the plane. We are thus permitted to use a two-dimensional model for the electron gas in which the electrons are free to move only in the plane of the semiconductor surface.[1]

In treating the response of the electron gas in our system to a dc electric field (transport theory) or an ac electric field (optical properties), collision processes of electrons with ions, impurities, or acoustic phonons have been mainly considered.[2] These can explain results obtained in semiconductors such as Ge and Si. However when compound semiconductors are used, such as InSb, GaAr, etc., which are partially ionic, the interaction of the electrons with longitudinal-optic phonons becomes important and cannot be neglected.[3] A similar situation exists for bulk electrons in compound semiconductors. The effect is particularly notable at low temperature for optical absorption when the photon frequency ω exceeds the longitudinal-optic-phonon frequency Ω_l. Here a new channel of absorption, i.e., a final state with an excited phonon, is operative and influences strongly the optical-absorption coefficient. In Sec. II we present the theory for the high-frequency conductivity of a two-dimensional electron gas with polar optical phonons.

In treating the electron-phonon interaction one should note that the electrons moving on the surface of the semiconductor will interact most strongly with surface rather than bulk phonons.[4] Surface phonons produce a large electrostatic potential in the insulator-semiconductor interface. The potential decreases exponentially to zero away from the interface. The eigenfrequencies of the surface phonons and their interaction with the electrons depend on bulk properties as well as on the dielectric properties of the insulating barrier.

II. CALCULATIONS OF THE CONDUCTIVITY

Our electron-phonon system is described by the Hamiltonian

$$H = H_0 + H_1 \ , \tag{1}$$

where

$$H_0 = \sum_p \epsilon_p a_p^\dagger a_p + \sum_q \omega_q b_q^\dagger b_q \tag{2}$$

and

$$H_1 = \frac{1}{2A} \sum_{p,p',q} v_q a_{p+q}^\dagger a_{p'-q}^\dagger a_{p'} a_p + \frac{1}{A^{1/2}} \sum_{p,q} (C_q a_{p+q}^\dagger a_p b_q + \text{H.c.}) \ . \tag{3}$$

Here ϵ_p is the kinetic energy of an electron having momentum $\vec{p}$, ω_q is the wave-number-dependent longitudinal-optic frequency and a_p, $a_p^\dagger$ (b_q, $b_q^\dagger$) are the destruction and creation operators, respectively, of the electrons (phonons). The coupling term $v_q = 2\pi e^2/q$ is the Fourier transform of the Coulomb interaction for planar electrons and

$$C_q = -i \frac{2\pi e^2}{q} \hbar\omega_l [\epsilon_b(\epsilon_\infty^{-1} + \epsilon_b^{-1})^{3/2} (\epsilon_0^{-1} + \epsilon_b^{-1})^{1/2}]^{-1/2}$$

represents the electron–longitudinal-optic-phonon interaction.

To evaluate the conductivity we start from the Kubo formula which reads

$$\sigma(\omega)=\frac{1}{2A}\int_0^\infty d\tau\, e^{i\omega\tau}\int_0^\beta d\lambda\,\langle\vec{j}(\tau-i\lambda)\cdot\vec{j}(0)\rangle \ , \quad (4)$$

where ω is the frequency of the applied field, $\vec{j}(0)$ is the Fourier transform of the current operator for wave number equal to zero, and

$$\vec{j}(\tau)=e^{iH\tau}\vec{j}(0)e^{-iH\tau} \ . \quad (5)$$

The statistical average of an operator O is given by

$$\langle O\rangle=\mathrm{Tr}(e^{\beta(\Omega+\mu N-H)}O) \ , \quad (6)$$

where H is the total Hamiltonian of the system and Ω is defined by

$$e^{-\beta\Omega}=\mathrm{Tr}(e^{\beta(\mu N-H)}) \ . \quad (7)$$

Here μ and N are the chemical potential and the number operator, respectively, and β is the inverse of the temperature in energy units.

In order to render Eq. (4) in a more convenient form, we integrate by parts and obtain

$$\sigma=\sigma_0+\sigma_1 \ , \quad (8)$$

where

$$\sigma_0=i\frac{e^2n}{m\omega} \quad (9)$$

and

$$\sigma_1=\frac{1}{2\omega A}\int_0^\infty d\tau\, e^{i\omega\tau}\langle[\vec{j}(\tau),\vec{j}(0)]\rangle \ . \quad (10)$$

In Eq. (10) the square brackets denote the commutator.

Calculations of the current-current correlations and the conductivity in the three-dimensional case have been worked out in much detail and are well documented.[5] The calculations for the two-dimensional situation is remarkably similar and we shall present only the final results. We evaluate the conductivity treating electron-phonon collision within the Born approximation (high-frequency conductivity), however treating the self-consistent field of the fluctuating electron gas exactly in the random-phase approximation (RPA). Our expression includes the full dynamic screening of the electrons. We however will consider here a weak electron-phonon interaction and ignore completely the renormalization of the phonon spectrum and line broadening by the electron density fluctuations. Our result for the conductivity reads

$$\sigma=i\frac{ne^2}{m\omega}+\frac{e^2}{2\omega^3m^2(2\pi)^2}\int d\vec{q}\,q^2|C_q|^2\frac{P}{4\pi}\int_{-\infty}^{+\infty}dx\coth\left(\frac{\beta x}{2}\right)\frac{1}{\epsilon_q(x+\omega)}$$
$$\times\left\{\frac{1}{\epsilon_q(x)}[Q_q(x+\omega)-Q_q(x)][D_q(x+\omega)-D_q(x)]-\frac{1}{\epsilon_q{}^*(x)}[Q_q(x+\omega)-Q_q{}^*(x)][D_q(x+\omega)-D_q{}^*(x)]\right\} \ . \quad (11)$$

Here the dielectric function is given by

$$\epsilon_q(x)=1-v_qQ_q(x) \ , \quad (12)$$

where Q, the density fluctuation is defined by

$$Q_q(x)=\frac{1}{(2\pi)^2}\int d\vec{p}\,\frac{f_{p+q/2}-f_{p-q/2}}{\epsilon_{p+q/2}-\epsilon_{p-q/2}-x-i\eta} \ . \quad (13)$$

$D_q(x)$ represents the phonon propagator and is given by

$$D_q(x)=\frac{2\omega_q}{x^2-\omega_q^2} \ . \quad (14)$$

To render our result for the conductivity in a more transparent form we shall identify the effect of the electron-phonon collision with the Drude form of the conductivity. We write for σ,

$$\sigma=i\frac{ne^2}{(m+\delta m)(\omega+i\nu)} \ , \quad (15)$$

where δm, the mass renormalization, and ν, the collision frequency, are small quantities. We therefore identify them as

$$\nu=(8\pi^2\omega mn)^{-1}\,\mathrm{Re}\int d\vec{q}\,q^2|C_q|^2\frac{1}{4\pi}\times P\int_{-\infty}^{+\infty}dx\coth\left(\frac{\beta x}{2}\right)F \ , \quad (16)$$

$$\delta m=-(8\pi^2\omega^2n)^{-1}\,\mathrm{Im}\int d\vec{q}\,q^2|C_q|^2\frac{1}{4\pi}\times P\int_{-\infty}^{+\infty}dx\coth\left(\frac{\beta x}{2}\right)F \ , \quad (17)$$

where

$$F=\frac{1}{\epsilon_q(x+\omega)}\left\{\frac{1}{\epsilon_q(x)}[Q_q(x+\omega)-Q_q(x)][D_q(x+\omega)-D_q(x)] - \frac{1}{\epsilon_q{}^*(x)}[Q_q(x+\omega)-Q_q{}^*(x)][D_q(x+\omega)-D_q{}^*(x)]\right\} . \quad (18)$$

In order to calculate the collision frequency ν we shall use two simplified assumptions which are well justified. First we omit all phonon lifetime effects, thus ignoring the narrow spread of the phonon spectrum for any wave number q. Second, since the momentum transfer q is of the order of the Fermi momentum which in turn is much smaller than lattice momentum, we ignore entirely the dispersion of the phonons and replace ω_q by Ω_l, the longitudinal vibration frequency. After some algebra one obtains

$$\nu=(8\pi\omega mn)^{-1}\int dq\, q^3\left[\frac{|C_q|^2}{v_q}\right] \times\left\{\left[\coth\left(\frac{\beta\Omega_l}{2}\right)+\coth\frac{\beta}{2}(\omega-\Omega_l)\right]\operatorname{Im}\frac{1}{\epsilon_q(\omega-\Omega_l)}+\left[\coth\left(\frac{\beta\Omega_l}{2}\right)+\coth\frac{\beta}{2}(\omega+\Omega_l)\right]\operatorname{Im}\frac{1}{\epsilon_q(\omega+\Omega_l)}\right\} . \quad (19)$$

For most practical situations, the temperature is smaller than the Fermi energy. We therefore are justified in taking the dielectric function at zero temperature. The statistical factor can also be taken at the zero-temperature limit for $k_BT < \hbar\Omega_l$. We thus obtain for the collision frequency at $T=0$,

$$\nu=(4\pi\omega mn)^{-1}\int dq\, q^3\left[\frac{|C_q|^2}{v_q}\right]\operatorname{Im}\left[\frac{1}{\epsilon_q(\omega-\Omega_l)}\right]\Theta(\omega-\Omega_l) . \quad (20)$$

Here, as expected, a threshold for absorption occurs at $\omega=\Omega_l$. The collision frequency rises for $\omega \gtrsim \Omega_l$ and, as we shall see later, behaves as $\omega^{-3/2}$ at high frequencies. The effect of finite temperature when $k_BT < \hbar\Omega_l$ would be mainly to round off the sharp threshold at $\omega=\Omega_l$. Numerical integration of Eq. (20) will be presented later.

The mass renormalization δm can be cast into a simpler form after some algebra and reads

$$\delta m=(8\pi^2\omega^2 n)^{-1}\int dq\, q^3\left[\frac{|C_q|^2}{v_q}\right]\int_0^\infty dx\coth\left(\frac{\beta x}{2}\right) \times\left[\operatorname{Im}\frac{1}{\epsilon_q{}^*(x)}\operatorname{Re}[D_q(x+\omega)+D_q(x-\omega)-2D_q(x)] +\operatorname{Im}D_q(x)\operatorname{Re}\left(\frac{1}{\epsilon_q(x+\omega)}+\frac{1}{\epsilon_q(x-\omega)}-\frac{2}{\epsilon_q(x)}\right)\right] . \quad (21)$$

Numerical calculations of δm as a function of frequency are more difficult than for ν. Here the various terms in the integrand have alternating signs, thus large cancellations do occur. Let us determine the qualitative behavior of δm as a function ω. Here for $\omega\to\infty$, $\epsilon_q(x\pm\omega)$ may be replaced by unity and $D_q(x\pm\omega)$ asymptotically approaches zero as ω^{-2}. We thus conclude that for $\omega\to\infty$ the integral in Eq. (21) approaches a constant and hence $\delta m \sim \omega^{-2}$. On the other hand for $\omega\to 0$ (below the longitudinal phonon frequency) the integrand in Eq. (21) behaves as ω^2, and thus δm becomes a constant when ω approaches zero. A detailed behavior of δm as a function of ω will not be presented here.

We go back now to our Eq. (20) and evaluate the collision frequency ν. Here we consider the situation where the Fermi energy is larger than k_BT and therefore are justified in using for $\epsilon_q(\omega-\Omega_l)$ the zero-temperature dielectric function. Our result reads

$$\frac{\nu}{\omega_l}=\tfrac{1}{2}(\lambda\tilde{c})\frac{1}{\Omega}\int_0^\infty dz\, z\frac{F(z,\Omega-\tilde{\Omega}_l)}{\epsilon(z,\Omega-\tilde{\Omega}_l)}\theta(\Omega-\tilde{\Omega}_l) , \quad (22)$$

where ω_l is the longitudinal-optic-phonon frequency, Ω_l is the surface phonon frequency, $\lambda=[2e^2m/\hbar^2(\pi n)^{1/2}]$ is the plasma parameter of the two-dimensional electron gas and

$$\tilde{c}=\frac{\epsilon_\infty^{-1}-\epsilon_0^{-1}}{\epsilon_b(\epsilon_\infty^{-1}+\epsilon_b^{-1})^{3/2}(\epsilon_0^{-1}+\epsilon_b^{-1})^{1/2}}$$

is the dielectric form factor for the interaction of the electrons with surface phonons. Here $\Omega = \omega/4\epsilon_F$ and $z = q/2k_F$ are, respectively, the frequency and wave numbers normalized with respect to the Fermi energy and momentum. Also $\tilde{\Omega}_l$ is the surface phonon frequency similarly normalized. The integrand in Eq. (22) is given by

$$F(z,x) = D_-\left[1-\left(z-\frac{x}{z}\right)^2\right]^{1/2} - D_+\left[1-\left(z+\frac{x}{z}\right)^2\right]^{1/2} ,$$

$$D\pm = \begin{cases} 0, & \text{if } |z \pm \frac{x}{z}| \geq 1 , \\ 1, & \text{if } |z \pm \frac{x}{z}| < 1 , \end{cases} \tag{23}$$

and

$$\epsilon(z,x) = 1 + \frac{\lambda}{z}\left[G(z,x) + i\frac{1}{2z}F(z,x)\right] , \tag{24}$$

where

$$G(z,x) = \left\{1 - \frac{C_-}{2z}\left[\left(z-\frac{x}{z}\right)^2 - 1\right]^{1/2} - \frac{C_+}{2z}\left[\left(z+\frac{x}{z}\right)^2 - 1\right]^{1/2}\right\} ,$$

$$C\pm = \begin{cases} 0, & \text{if } |z \pm \frac{x}{z}| \leq 1 , \\ \frac{z \pm (x/z)}{|z \pm (x/z)|}, & \text{if } |z \pm \frac{x}{z}| > 1 . \end{cases}$$

Equation (22) can now be integrated using InSb parameters: $\omega_l = 24.4$ meV, $\epsilon_0 = 17.9$, $\epsilon_\infty = 15.7$, and as an example for the oxide layer, $\epsilon_b = 10$ is taken as a reasonable value. The Fermi energy in our calculation is taken to be 100 meV. In this case we obtain for the surface phonon

$$\Omega_l = \omega_l\left(\frac{\epsilon_0^{-1} + \epsilon_b^{-1}}{\epsilon_\infty^{-1} + \epsilon_b^{-1}}\right)^{1/2} = 0.95\omega_l ,$$

which is almost equal to ω_l. Our result for ν as a function of the normalized frequency is presented in Fig. 1. The collision frequency ν is zero for frequencies below the surface phonon frequency. When the light frequency exceeds the surface phonon frequency, ν increases fast up to a constant value and remains so until $\omega = 4\omega_F$. Thereafter ν approaches asymptotically to a constant times $\omega^{-3/2}$, for large ω. This asymptotic form of ν is obtained when screening effects are omitted, i.e., when in Eq. (22) we replace $\epsilon(z, \Omega - \tilde{\Omega}_l)$ by unity.

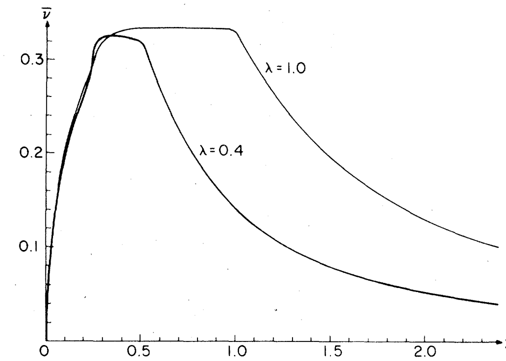

FIG. 1. Normalized collision frequency $\bar{\nu} = 2\nu/\lambda\tilde{C}\omega_l$ as a function of $\bar{x} = (\omega - \Omega_l)/4\omega_F$ for InSb at zero temperature, for $\lambda = 0.4$ and $\lambda = 1$.

In conclusion, we have calculated the collision frequency for a two-dimensional electron gas interacting with optical lattice vibrations. Our result for the collision frequency as a function of the photon energy is plotted in Fig. 1. We find that metal-oxide-semiconductor devices, made up of polar semiconductors, will exhibit a jump in the collision frequency when the photon frequency exceeds the optical-phonon frequency.

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[4]Here we note that the surface longitudinal-optic-phonon frequency is given by $\Omega_l = \omega_l(\epsilon_0^{-1} + \epsilon_b^{-1})^{1/2}(\epsilon_\infty^{-1} + \epsilon_b^{-1})^{-1/2}$ where ω_l is the bulk phonon frequency and ϵ_b is the dielectric constant of the insulator or the oxide.

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