Electron lifetime due to optical-phonon scattering in a graphene sheet

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Abstract. We study scattering between electrons and optical phonons in a graphene sheet. Electron-phonon interaction is derived for zone-center and zone-boundary phonons within the framework of the effective-mass equations. We calculate the electron lifetime due to phonon emission and absorption. The inter-valley scattering induced by the zone-boundary phonons turned out to be dominant in high-field transport.

1. Introduction

Recent experimental realizations [1, 2, 3] of electron transport in a single graphene sheet have induced a large number of studies on unusual properties of massless Dirac electrons in two-dimensional condensed matter systems. There have been many reports on unusual quantum Hall effect [3, 4, 5], suppression of magnetoresistance [6, 7], weak anti-localization [8, 9] and so forth. In these curious transport phenomena, what plays an important role are the two types of pseudo spins: one originates from two sublattices, which we call A and B sites, and the other from distinct two valleys in the band structure which are located around K and K’ points in the Brillouin zone [10]. When an electron goes through a series of scattering events, its pseudo spin with respect to the two sublattices acquires what we call Berry’s phase. The accumulated quantal phase gives rise to interference causing curious transports under the condition that the other pseudo spin is conserved, or there is no inter-valley scattering. However, any disorders randomly changing the directions of both pseudo spins could wipe out such interference effect.

In this paper, we study electron scattering due to the optical phonons in a single graphene sheet [11, 12, 13, 14]. As for the impurity scattering, the inter-valley scattering can be safely neglected unless the potential range of an impurity is smaller than the lattice constant and this seems to be the case in recently prepared graphenes. That is the reason why various interesting phenomena have been found, one after another. With regard to the electron-phonon interaction, zone-center phonons of long wavelength do not cause inter-valley scattering, either. On the other hand, phonons of short wavelength comparable to the lattice constant inevitably generate inter-valley scattering.

Actually, it is the phonon around the K and K’ points that can give an electron the momentum transfer necessary for the transition between the K and K’ points which correspond to the corners in the Brillouin zone. Therefore, zone-boundary phonons are crucial for low-energy inter-valley
electron scattering, while zone-center phonons generate scattering only around each Fermi point, or intra-valley scattering.

2. Electron-phonon interaction
Electrons around the K and K’ points are well described by the effective-mass equations [10]

\[
\begin{pmatrix}
\gamma(\sigma \cdot \hat{k}) & 0 \\
0 & \gamma(\sigma^z \cdot \hat{k})
\end{pmatrix}
\begin{pmatrix}
F^K(r) \\
F^{K'}(r)
\end{pmatrix}
= \epsilon
\begin{pmatrix}
F^K(r) \\
F^{K'}(r)
\end{pmatrix},
\]

where \( k = -i\nabla \) and \( \sigma = (\sigma_x, \sigma_y) \) (Pauli spin matrices). The band parameter \( \gamma \) is equal to \( \hbar v_F \) where \( v_F \) represents the Fermi velocity. Envelope functions \( F^A_K, F^B_K, F^A_{K'}, \) and \( F^B_{K'} \) give the wavefunctions of the electrons at A and B sublattice sites as

\[
\psi_A(R_A) = e^{iK \cdot R_A} F^A_K(R_A) + e^{iK' \cdot R_A} F^A_{K'}(R_A),
\]

\[
\psi_B(R_B) = -\omega e^{iK \cdot R_B} F^B_K(R_B) + e^{iK' \cdot R_B} F^B_{K'}(R_B),
\]

with \( \omega = \exp(2\pi i/3) \). We define the primitive translation vectors as \( a = (1,0)a \) and \( b = (-1/2, \sqrt{3}/2)a \) with the lattice constant \( a \). Then, \( R_A = n_a a + n_b b + \tau \) and \( R_B = n_a a + n_b b \) where \( \tau = (0,1)b \) with the bond length \( b = a/\sqrt{3} \) between adjacent A and B atoms. The wavevectors of the K and K’ points are given by \( K = (2\pi/a)(1/3, 1/\sqrt{3}) \) and \( K' = (2\pi/a)(2/3, 0) \).

In-plane phonon modes are represented by the two lattice displacement vectors \( u_A \) and \( u_B \). First, we focus on the phonon around the \( \Gamma \) point, or the zone-center phonon. The optical modes are characterized by the relative displacement between two sublattice atoms within a unit cell located at \( R \) [15], i.e.,

\[
u^{op}(R) = \frac{1}{\sqrt{2}}(u_A(R) - u_B(R)).
\]

In the second quantized form, this vector is written as

\[
u^{op}(r) = \sum_{q,\sigma} \sqrt{\frac{\hbar}{2NM\omega_F}} (b_{q\sigma} + b^\dagger_{-q\sigma}) e_{q \sigma}(r)e^{iq \cdot r},
\]

where \( N \) is the number of unit cells and \( M \) is the mass of a carbon atom. The index \( \sigma \) denotes the longitudinal or transverse mode and \( e_{q \sigma}(q) \) represents the eigenvector of the mode \( \sigma \). Now, we neglect the dispersion of phonons and assume that both modes have the same frequency \( \omega_F \).

Within the effective mass approximation for electrons, the interaction Hamiltonian is given by

\[
\mathcal{H}_\text{int}^\Gamma = -\sqrt{2} \beta_\Gamma \gamma \begin{pmatrix}
\sigma_x u^{op}_y(r) - \sigma_y u^{op}_x(r) & 0 \\
0 & -\sigma_x u^{op}_y(r) - \sigma_y u^{op}_x(r)
\end{pmatrix},
\]

where \( \beta_\Gamma \) is an appropriate dimensionless parameter [16]. Note that we can derive it from the nearest-neighbor tight-binding model as \( \beta_\Gamma = -d \ln \gamma_0/d \ln b \) with the transfer energy \( \gamma_0 \) and the bond length \( b \). Then, the band parameter \( \gamma \) is equal to \( 3\gamma_0 b/2 \).

Next, we consider the phonon around the K and K’ point, or the zone-boundary phonon. In a manner similar to the extraction of the envelope functions for electrons, the lattice displacement vector is written as

\[
u_A(R_A) = u_A^K(R_A)e^{iK \cdot R_A} + u_A^{K'}(R_A)e^{iK' \cdot R_A},
\]

\[
u_B(R_B) = u_B^K(R_B)e^{iK \cdot R_B} + u_B^{K'}(R_B)e^{iK' \cdot R_B}.
\]

We neglect the dispersion also for the zone-boundary phonon. In general, there exist four independent eigenmodes for each wavevector. However, after straightforward calculations, we
can see that only one mode with the highest frequency contributes to the electron-phonon interaction. This mode is known as a Kekulé type distortion generating only bond-length changes. The interaction Hamiltonian is given by

$$\mathcal{H}^{K,K'}_{\text{int}} = 2\frac{\beta_K}{b^2} \left( \begin{array}{cc} 0 & \omega^{-1} \Delta^{K'}(r) \sigma_y \\ \omega \Delta_K(r) \sigma_y & 0 \end{array} \right),$$

(7)

where $\beta_K$ is another appropriate parameter, which is equal to $\beta_T$ for the tight-binding model, and $\Delta_K(R)$ and $\Delta_{K'}(R)$ are defined by the projection of the displacement to the Kekulé mode,

$$\Delta_K(r) = \omega f^\dagger u_A^K(r) + (f^*)^\dagger u_B^K(r),$$
$$\Delta_{K'}(r) = (f^*)^\dagger u_A^{K'}(r) + f^\dagger u_B^{K'}(r),$$

(8)

and they are complex conjugate to each other, $\Delta_K(r) = \Delta_{K'}(r)^*$. In the second quantized form,

$$\Delta_K(r) = \sum_q \sqrt{\frac{\hbar}{2NM\omega_K}} (b_{Kq} + b_{K'-q}^\dagger) e^{iqr},$$
$$\Delta_{K'}(r) = \sum_q \sqrt{\frac{\hbar}{2NM\omega_K}} (b_{K'q}^\dagger + b_{K-q}^\dagger) e^{iqr},$$

(9)

where $\omega_K$ is the frequency of the Kekulé mode. It is worth noting that $\Delta_K$ cannot be given by a simple summation over the K and K' modes while $\Delta_K$ is written by the summation over the longitudinal and transverse modes. We should take a proper linear combination of the K and K' modes in order to make the lattice displacement a real variable. We can easily understand the operator form of $\Delta_K$ and $\Delta_{K'}$ in the interaction Hamiltonian by considering the momentum conservation with the fact that $2K - K'$ and $K - 2K'$ are reciprocal lattice vectors.

### 3. Electron lifetime

We calculate the electron lifetime $\tau$ due to emission and absorption of an optical phonon. The lifetime of an electron with energy $\varepsilon$ is given by the scattering probability from the initial state to possible final states via emission and absorption of one phonon.

For the zone-center phonon, the interaction Hamiltonian $\mathcal{H}^{K}_{\text{int}}$ (Eq. (5)) has only diagonal components and this is consistent with the fact that inter-valley scattering is prohibited. Then, the final states are limited to the same valley to which the initial electron state belongs. Further, we should evenly evaluate contributions from the longitudinal and transverse modes.

In contrast, only off-diagonal components exist in the interaction Hamiltonian $\mathcal{H}^{K}_{\text{int}}$ (Eq. (7)) for the zone-boundary phonon. Any scattering processes are classified into two types: One is the transition between “one K-electron with one K-phonon” and “one K’-electron”, and the other is between “one K-electron” and “one K’-electron with one K’-phonon”. For example, an electron around the K point can be scattered to the K’ point accompanied by absorption of one phonon around the K point, and this belongs to the former process. The electron scattering from the K to K’ point can also be induced by the emission of one phonon around the K’ point, while this is classified into the latter one.

It appears that there is no remarkable similarity between zone-center and zone-boundary phonons, but calculated scattering probabilities for both phonons are given by the same formula,

$$\frac{\hbar}{\tau} = \pi \lambda_\alpha |n_\alpha \varepsilon + \hbar \omega_\alpha| + (n_\alpha + 1)|\varepsilon - \hbar \omega_\alpha|,$$

(10)
where $\alpha$ represents $\Gamma$ or $K$, $n_\alpha$ is the Planck distribution function for phonon of the frequency $\omega_\alpha$, and $\lambda_\alpha$ denotes the dimensionless coupling constant,

$$\lambda_\alpha = \frac{36\sqrt{3}}{\pi} \frac{\hbar^2}{2Ma^2} \frac{1}{\hbar\omega_\alpha} \left( \frac{\beta_\alpha}{2} \right)^2. \tag{11}$$

On the assumption that $\beta_\alpha$ is independent of $\alpha$ as that in the nearest-neighbor tight-binding model, the phonon frequency is the unique parameter which determines the electron lifetime. For zone-center phonons, $\hbar\omega_\Gamma = 196$ meV and $\lambda_\Gamma = 2.9 \times 10^{-3}(\beta_\Gamma/2)^2$, while $\hbar\omega_K = 161.2$ meV and $\lambda_K = 3.5 \times 10^{-3}(\beta_K/2)^2$ for zone-boundary phonons. As a consequence, the contributions from zone-boundary phonons are larger than those from zone-center phonons.

Moreover, it is reasonable to assume $n_\alpha = 0$ since optical phonons are hardly excited even at room temperature. Namely, the phonon emission process becomes dominant and we have

$$\frac{\hbar}{\tau} = \pi\lambda_\alpha |\varepsilon - \hbar\omega_\alpha|. \tag{12}$$

This simply shows that the electron lifetime is inversely proportional to the coupling parameter $\lambda_\alpha$ and to the density of states at the energy of the final state. What should be stressed here is that the phonon emission is possible only when the energy of the initial electron is larger than that of the phonon to be emitted. Otherwise, the final states are fully occupied at zero temperature and the phonon emission never takes place. In this sense, the zone-boundary phonon has another advantage over the zone-center phonon. Therefore, the zone-boundary phonon gives dominant scattering for high-field transport in graphenes owing to its smaller frequency and larger coupling constant.

**Acknowledgments**

This work was supported in part by Grants-in-Aid for Scientific Research and for Scientific Research on Priority Area “Carbon Nanotube Nano-Electronics” from Ministry of Education, Culture, Sports, Science and Technology Japan.

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