Temperature relaxation and energy loss of hot carriers in graphene

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The temperature relaxation and energy loss of hot Dirac fermions are investigated theoretically in graphene with carrier–optical phonon scattering. The time evolutions of temperature and energy loss for hot Dirac fermions in graphene are calculated self-consistently. It shows that the carrier–optical phonon coupling results in the energy relaxation of hot carriers excited by an electric field, and the relaxation time for temperature is about 0.5–1 ps and the corresponding energy loss is about 10–25 nW per carrier for typically doped graphene samples with a carrier density range of 1–5 × 10^{12} cm^{-2}. Moreover, we analyze the dependence of temperature and energy relaxation on initial hot carrier temperature, lattice temperature and carrier density in detail.

1. Introduction

Owing to its massless Dirac quasi-particles, unique gapless and linear electronic band structure at low energy, graphene has become one of the most important research topics in condensed matter physics, nano-material science and nano-electronics [1,2]. Moreover, graphene-based nano-devices, whose carrier density can be controlled effectively through a gate voltage, exhibit high carrier mobility and quasi ballistic transport over sub-micron scales even at room temperature [3]. Thus, graphene has been proposed as novel high speed and ultrafast electronic devices, such as field-effect transistors [4], p–n junctions [5], and high-frequency devices [6].

On the other hand, the hot carrier phenomenon has become important for the understanding of all modern semiconductor devices. The relaxation of the temperature and energy of hot carriers is one of the central issues to the behavior of semiconductor electronic and optoelectronic devices [7]. However, there have been only a few reports concerning the relaxation process of hot Dirac fermions in graphene using ultra-fast optical techniques [8,9], and very limited investigations in a high electric field. Lei’s group found theoretically that the conductivity exhibits strongly nonlinear behavior and the effect of hot electrons becomes remarkable for an applied high electric field strength E_c > 0.1 kV/cm in graphene [10]. Moreover, it has been found that the electron–optical-phonon scattering plays an important role in energy dissipation, limiting the increase of electron temperature [10].

When a high electric field is applied to a graphene sample, carriers are accelerated and heated because they gain more energy from the electric fields than that lost to the lattice or phonons. Thus, the non-equilibrium distribution of carriers is formed and the carrier temperature (e.g. electron temperature T_e) is higher than the temperature of the surrounding medium (e.g. phonon temperature T_p). Very recent experimental results have indicated that at room-temperature a gated graphene device holds a very high carrier density and source–drain (sd) current along with unusual current–voltage characteristics [11] in a high electric field. The sd current saturation is incomplete and sensitive to the carrier density (or the applied gate voltages) in graphene samples [4,11]. These interesting experimental findings strongly suggest that graphene can also be applied as novel high-field nano-electronic devices. Thus, it is vital to study and understand the relaxation process of hot carriers in order to comprehend the transport properties and performance of graphene high-field devices. In this letter, we present a simple theoretical approach to study the temperature and energy relaxation of hot Dirac fermions in graphene in detail.

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2. Theoretical approach

In this work, we consider a monolayer of graphene with the wavefunction \( \psi_n(r) = 2^{-1/2} (1, \lambda e^{ikr}) \) and energy spectrum \( E_i(k) = \lambda g k \). Here, \( r = (x, y) \), \( k = (k_x, k_y) \) is the wavevector for a carrier (an electron or a hole) along the graphene sheet, \( \gamma = \hbar v_F \) with \( v_F = 10^8 \) cm/s being the Fermi-velocity, \( \phi \) is the angle between \( k \) and the \( x \) direction, and \( \lambda = + \) for an electron and \( \lambda = - \) for a hole [12].

The carriers are accelerated and heated up by the high dc electric fields. Then, the temperature and energy relaxation events occur with carrier–phonon scattering in the absence of the strong electric field. Therefore, the change rate of energy or energy loss rate for hot carriers in graphene is [13]

\[
\frac{dU}{dt} = C_1 \frac{dT_x}{dt} = s \sum_k \frac{\partial E_i(k)}{\partial T_x},
\]

where \( U_t \) and \( T_x \) are respectively the internal energy and temperature of hot carriers in the graphene system, \( t \) is time, \( s = g_g \), \( g_e = 2 \) and \( g_h = 2 \) are respectively the spin and valley degeneracy in graphene, and

\[
C_1 = \frac{dU}{dT_x} = s \sum_k E_i(k) \frac{\partial f_i(\lambda E)}{\partial T_x} = \frac{2}{\pi \gamma \Delta_k} 
\times \int_0^{\infty} d\omega (\lambda E - \mu_\lambda) E^2 f_i(\lambda E)[1 - f_i(\lambda E)],
\]

is the heat capacity of carriers in graphene, where \( f_i(\lambda E) = [\exp(\lambda E/\Delta_k) - 1]^{-1} \) and \( \mu_\lambda \) are respectively the Fermi distribution function and the chemical potential for carriers in graphene.

The carrier–phonon interaction allows energy exchange between the carrier and the lattice system when scattering from a state \( \{ k, \lambda, t \} \) to a state \( \{ k', \lambda, t \} \) with momentum conservation \( k' = k + q \) and energy conservation \( E_i(k') - E_i(k) = \pm \hbar \omega_q \). With Fermi’s golden rule, the change rate of energy for the hot carrier system in graphene due to carrier–phonon scattering is

\[
P_{ep} = -s \frac{2\pi}{\hbar} \sum_{k, k', \lambda} \left[ |U_{\lambda k'}^{ep}|^2 \omega_q \delta[E_i(k) - E_i(k')] \hbar \omega_q \right] 
\times \left[ f_i(k') (1 - f_i(k')) (N_q + 1) - f_i(k) (1 - f_i(k')) N_q \right] 
- |U_{\lambda k'}^{ep}|^2 \hbar \omega_q \delta[E_i(k) - E_i(k')] \hbar \omega_q \]
\times \left[ f_i(k) (1 - f_i(k')) N_q - f_i(k') (1 - f_i(k)) N_q + 1 \right],
\]

where \( N_q \) is the phonon distribution function, and \( |U_{\lambda k'}^{ep}|^2 \) is the square of the carrier–phonon scattering matrix elements. We note that the effect of non-equilibrium phonons is neglected when the transport properties of graphene are investigated in high electric fields [4,10,11,15]. Thus, in this work we neglect the effect of non-equilibrium phonons to study the interaction of carriers with a bath of optical phonons. Moreover, our derived theory is based on the Fermi distribution function and a steady-state Boltzmann equation, which has been verified for a doped graphene sample by Das Sarma et al. [16].

We note that the transport experiments in a high electric field were employed at room temperature [4,11]. Moreover, in doped graphene at relatively high temperatures \( T_R > 200 \) K), the carrier interacts much more strongly with optical phonons than with acoustic phonons due to the larger energy transfer for carrier–optical phonon coupling. As a result, we have [14]

\[
|U_{\lambda k'}^{ep}|^2 = g^2 \gamma^2
\]

for carrier interaction with longitudinal and transverse optical-phonon modes in graphene, where \( g = (\hbar B B')^2/2\hbar \omega_0 \rho = 6.5 \times 10^{-5} \) g/cm² is the area density of the graphene sheet, \( \hbar \omega_0 = 196 \) meV is the optical-phonon energy at the \( \Gamma \)-point at the zone-center, \( B \sim 2 \hbar k_B T \) is a dimensionless parameter, and \( B = a/\sqrt{3} \) is the equilibrium bond length with \( a = 1.42 \) Å [17]. The zone-center phonons of long wavelength mainly cause intra-valley scattering, whereas the zone-boundary phonons at the K-points give dominant inter-valley scattering [18]. The inter-valley scattering takes place in graphene only if the electric field strength is strong enough and the temperature of the carriers is unusually high; however, this can result in breaking down of graphene samples [10]. Thus, here inter-valley scattering can be safely neglected when the electric field strength \( E_c \) is not so strong (e.g. 0.1 kV/cm - \( E_c < 1 \) kV/cm).

In this study, we consider gate-controlled graphene with hot electrons placed on a dielectric SiO₂ wafer. For the case where the conduction carriers are hot electrons \( n_e \sim 10^{12} \) cm⁻², \( n_h = 0 \) for holes (e.g. \( \lambda = \lambda' = + \)) because the valence band is fully occupied by electrons and only the electron–optical phonon interaction in the conduction band is present in the graphene sample. With charge number conservation, we have

\[
n_e = \frac{2}{\pi \gamma^2} \int_0^{\infty} \frac{dx}{x^2} \left[ \lambda(x - \omega_0) f(x) \right] \times \left[ 1 - f(x - \omega_0) \right] \left[ N_0 + 1 - f(x - \omega_0) \right] \left[ 1 - f(x) N_0 \right],
\]

is the energy change via emission of phonons for electrons in graphene, and

\[
n_e = \frac{8\omega_0 g^2}{\pi \gamma^2} \int_0^{\infty} \frac{dx}{x^2} \left[ \lambda(x + \omega_0) f(x) \right] \times \left[ 1 - f(x + \omega_0) \right] \left[ N_0 + 1 - f(x + \omega_0) \right] \left[ 1 - f(x) N_0 + 1 \right],
\]

is the energy change via absorption phonon for electrons in graphene with \( N_0 = \left( e^{\omega_0 \Delta g T}/h \right) - 1 \). Considering energy conservation, the change rate of energy for the electron system is equal to the energy loss rate due to electron–phonon scattering in graphene. Thus, we obtain

\[
C_n dT_n/dt = P_{ep}.
\]

Together with Eqs. (5) and (7), we can evaluate self-consistently the temperature \( T_n \) and energy loss \( P_{ep} \) for hot electrons as a function of time \( t \) in graphene in the presence of electron–optical phonon scattering. We note that this approach can also be applied to the p-type graphene samples, where a negative gate voltage is applied so that the conducting carriers are hot holes in the presence of hole–optical phonon scattering.

3. Results and discussions

In Fig. 1, we show the electron temperature \( T_n \) and energy loss (inset) as a function of time \( t \) at a fixed phonon temperature \( T_R \) and electron density \( n_e \) for the different initial electron temperatures \( T_{e0} \). It is found that the relaxation times for temperature are identical 0.5–1 ps with different initial temperatures \( T_{e0} \) because the higher the temperature of hot electrons, the faster the energy relaxation of hot electrons to the lattice in graphene (see the inset figure in Fig. 1). It means that the emission of phonons becomes
stronger with higher temperature of hot electrons. It shows that
the relaxation process occurs mainly in time $t < 1$ ps and the
energy transfer from electrons to lattice completes mostly within
1 ps. Moreover, we find that the hot electrons with different
temperatures would relax to the same phonon temperature $T_p$
finally. We note that our theoretical results are very similar to those
obtained experimentally [8], though the hot Dirac fermions were
excited by ultrafast laser light in their experiment. It shows that
the relaxation mechanism and process of hot electrons, excited by
electric and optical field, are identical in graphene.

In order to make further clear the time evolution of hot carriers
in graphene, we show the temporal evolution of the population
of hot electrons, which is occupation times the density of state of
graphene, as a function of electron energy $E$ at a fixed initial
electron temperature $T^0_e$, phonon temperature $T_p$ and electron density $n_e$ in Fig. 2. The density of states (DOS) g(E) $|E|/2\pi \gamma^2 \sim E$ is linear in graphene, which is very different from that of a conventional two-dimensional electron gas. It is found that the population of electrons in the conduction band becomes large with time $t$ delay at the low energy regime, while it becomes small with $t$ delay at the high energy regime in graphene. The demarcation energy of electrons is the Fermi energy between low and high energy. This indicates that the effect of electron–phonon scattering and emission of phonons become weak with time delay in graphene system.

In Fig. 3, it shows the electron temperature $T_e$ (upper panel)
and energy loss (lower panel) as a function of time $t$ at a
fixed initial electron temperature $T^0_e$ and electron density $n_e$
for the different phonon temperatures $T_p$. It is found that the
temperature and energy relaxation of hot electrons with the same
initial temperature become fast with environmental temperature
(phonon temperature $T_p$) increasing. The reason is that the
electron–optical phonon interaction becomes strong with phonon
temperature increasing and the relaxation of energy for hot
electrons enhances via emission of phonons in graphene. However,
we must note that the influence of the phonon temperature in
graphene is not so obvious at a high temperature range $T_p =
200–400$ K. The reason behind this is that the energy of the optical-
phonon ($\hbar\omega_{OP} = 196$ meV $\sim 2261$ K) is much larger than that in
usual semiconductor systems or room temperature and it results in
$N_0$ of almost zero. Moreover, the carrier–optical phonon coupling
is very different from that in usual polar semiconductor systems.
It also shows that the effect of non-thermal phonons can be
neglected when the relaxation process of hot carriers excited by
electric fields occurs only intra-band in graphene.

Finally, we plot the electron temperature $T_e$ and energy loss
(insert) as a function of time $t$ at a fixed initial electron temperature $T^0_e$ and phonon temperature $T_p$, for the different
electron densities $n_e$ in Fig. 4. For larger electron density of graphene sample, the relaxation process of hot electrons becomes faster because there are more electrons that can lose energy to the lattice through emission of phonons. It shows that the relaxation of hot carrier is sensitive to the carrier density in graphene, similar to the behavior of the current density [4,11]. The typical relaxation time for temperature and energy is about 0.5–1 ps for graphene samples. The carrier density of graphene devices can be modulated effectively via applying a gate voltage [2,4], so that the relaxation.
process and time of hot Dirac fermions in graphene devices can be modulated successfully by applying gate voltages.

4. Conclusions

In summary, we developed a simple theory to study the temperature relaxation and energy loss of hot Dirac fermions in graphene. We have shown that the temperature and energy relaxation of hot carriers is about 0.5–1 ps and energy loss is about 10–25 nW per carrier for a typically doped graphene due to electron–optical phonon scattering. Most of the energy of hot carriers excited by an electric field is lost after 1 ps in graphene. The relaxation process of hot electrons is very sensitive to carrier density (gate voltage) and the effect of non-equilibrium phonons can be safely neglected in graphene. We hope these theoretical findings are beneficial to understand the graphene system more deeply and to explore its further applications in practical nano-devices.

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